Mitigation of Heavy Ion-Stimulated Gas Desorption from Accelerator Components





TECHNISCHE UNIVERSITÄT DARMSTADT

Verminderung der Schwerionen-induzierten Gasdesorption von Beschleunigerkomponenten

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Mitigation of Heavy Ion-Stimulated Gas Desorption from Accelerator Components Verminderung der Schwerionen-induzierten Gasdesorption von Beschleunigerkomponenten

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Darmstadt, den 27. April 2023

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Abstract

Ion-stimulated desorption is a serious problem regarding intensity limitation for heavy ion circular accelerators. Lost beam ions colliding with the wall of the beam tube trigger the release of huge amounts of gas. This leads to local pressure increases up to three orders of magnitude, which in turn enhances further beam losses. Future accelerators, such as the Facility for Antiproton and Ion Research (FAIR), are designed to deliver ion beams of highest intensities. For stable beam conditions, this requires low desorbing surfaces for beam exposed accelerator components and excellent vacuum conditions with pressures in the range of 10^{-12} mbar.

The objective of this thesis was to develop surfaces with minimal ion-stimulated desorption by testing a large variety of pretreatment methods for copper, tungsten and aluminum samples including extended ex-situ thermal annealing and different combinations of lapping, polishing, etching and milling as well as sputter cleaning with keV argon ions. In addition, coatings with TiZrV, titanium nitride and carbon were tested.

Ion-stimulated desorption was determined by irradiation experiments with calcium or gold ions with 4.8 MeV/u specific energy at the UNILAC beamline M1 at the GSI Helmholtz Center for Heavy Ion Research. In addition, ion-stimulated desorption measurements with highly charged ions (Au⁷⁸⁺) of different specific energies (2, 3 and 4.8 MeV/u) were conducted at CRYRING. For all experiments, desorption was quantified by recording the pressure increase with a total pressure gauge and a quadrupole mass spectrometer. For ion-stimulated desorption, the pressure increase during irradiation is converted into a number of desorbed molecules per impacting ion, the so-called desorption yield, while in complementary thermal desorption experiments outgassing is quantified by the amount of desorbed gas per surface area (mbar·l/cm²).

As surface treatments, diamond milling and polishing turned out to be appropriate solutions. Sputter cleaning with keV argon ions also result in a clear reduction of the desorption yield. Ex-situ annealing at 400 °C for about 4 h under ultra-high vacuum conditions was identified as excellent pretreatment method to reduce ion-stimulated desorption. The low desorption is preserved even after storage in atmosphere for at least 11 months. Storage in argon is recommendable, because these samples show lower desorption compared to atmosphere storage. The fact that the low desorption persists under storage in atmosphere is a strong indication that ion-stimulated desorption is not limited to the surface, but that the bulk also plays a significant role. To prepare accelerator components with minimal outgassing, both surface and bulk properties have to be optimized.

Zusammenfassung

lonen-induzierte Desorption beeinträchtigt das Vakuum und die Strahlqualität in Schwerionen-Ringbeschleunigern. Verlorene Strahlionen setzen bei Kollision mit der Strahlrohrwand große Gasmengen frei. Dies führt zu lokalen Druckanstiegen von bis zu drei Größenordnungen, die weitere Strahlverluste verursachen. Zukünftige Beschleuniger wie die Facility for Antiproton and Ion Research (FAIR) sollen Ionenstrahlen höchster Intensität liefern. Dazu sind hervorragende Vakuumbedingungen mit Drücken im Bereich von 10⁻¹² mbar notwendig. Außerdem müssen strahlexponierte Beschleunigerkomponenten mit niedrig-desorbierenden Oberflächen ausgestattet werden.

Ziel dieser Arbeit war es, Oberflächen mit minimaler Ionen-induzierter Desorption zu entwickeln. Dazu wurde eine Vielzahl von Vorbehandlungsmethoden für Kupfer-, Wolfram- und Aluminiumproben getestet. Die Proben wurden mittels ex-situ Wärmebehandlung und verschiedener Kombinationen von Läppen, Polieren, Ätzen und Fräsen behandelt. Zusätzlich wurden die Reinigung der Oberflächen durch Sputtern mit keV-Argonionen und die Beschichtung mit TiZrV, Titannitrid und Kohlenstoff getestet.

Die Ionen-induzierte Desorption wurde durch Bestrahlungsexperimente mit Calcium- oder Goldionen mit 4,8 MeV/u spezifischer Energie an der UNILAC-Beamline M1 am GSI Helmholtzzentrum für Schwerionenforschung bestimmt. Zusätzlich wurden am CRYRING Desorptionsmessungen mit hochgeladenen Ionen (Au⁷⁸⁺) unterschiedlicher spezifischer Energien (2, 3 und 4,8 MeV/u) durchgeführt. Um die Desorption zu quantifizieren, wurde für alle Experimente der Druckanstieg mit einem Totaldruckvakuummeter und einem Quadrupol-Massenspektrometer gemessen. Anschließend wurde der Druckanstieg während der Bestrahlung in die Anzahl desorbierter Moleküle pro auftreffendem Ion, der sogenannten Desorptionsausbeute, umgerechnet. In ergänzenden Experimenten zur thermischen Desorption wurde die Desorption anhand der Menge von desorbiertem Gas pro Fläche (mbar·l/cm²) quantifiziert.

Als Oberflächenbehandlungen erwiesen sich Diamantfräsen und Polieren als geeignete Lösungen. Auch die Sputter-Reinigung mit keV-Argonionen führt zu einer deutlichen Reduzierung der Desorptionsausbeute. Die vielversprechendste Vorbehandlungsmethode zur Verringerung der Ionen-induzierten Desorption ist eine exsitu Wärmebehandlung bei 400 °C für ca. 4 h unter Ultrahochvakuum-Bedingungen. Die verringerte Desorption bleibt auch nach Lagerung der Proben an Atmosphäre über mindestens 11 Monaten erhalten. Lagerung in Argon ist jedoch empfehlenswert, da diese Proben im Vergleich zur Lagerung an Atmosphäre eine geringere Desorption aufweisen. Die Tatsache, dass die geringe Desorption bei Lagerung an Atmosphäre bestehen bleibt, ist ein starker Hinweis darauf, dass Ionen-induzierte Desorption kein reiner Oberflächeneffekt ist, sondern dass auch tieferliegende Schichten eine bedeutende Rolle spielen. Um Beschleunigerkomponenten mit minimaler Desorption herzustellen, müssen sowohl die Oberflächen- als auch die Bulkeigenschaften optimiert werden.

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1 Introduction

Many fields in today's research rely on high-energy and high-intensity particle accelerators. This concerns in particular basic research in nuclear and particle physics, but also interdisciplinary areas such as materials research, radiotherapy and industry applications. To gain insights in atomic and nuclear processes, which are not accessible with the current technology, higher beam energies are required. Furthermore, higher beam intensities are favorable to reduce the required beam time, improve statistics and open access to new physics.

For stable operation of heavy ion circular accelerators, excellent vacuum conditions in the range of 10⁻¹² mbar are required [Kol06]. However, even at this low pressure, beam ions collide with residual gas particles resulting in losing or picking up of electrons. Ions of altered mass-to-charge ratio leave the set trajectory when passing the next dipole magnet, hit the wall of the beam tube under grazing incidence and stimulate gas desorption. A higher pressure, in turn, increases the probability of collisions with residual gas molecules and thus of charge-exchange processes. This is a self-amplifying process. The pressure rise in the beam tube during the acceleration process of the ions, denoted as "dynamic vacuum", leads to reduced beam lifetime, limited intensity and increased emittance.

For the new Facility for Antiproton and Ion Research (FAIR) currently under construction at the GSI Helmholtz Center for Heavy Ion Research in Darmstadt (Germany), beam energies higher by a factor of about 20 (2.7 GeV/u for U²⁸⁺ and 29 GeV for protons [Gut06]) and intensities increased by a factor of 100 (5E11 particles per pulse [EIH13]) compared to the status at GSI in 2001 are planned. These high intensities require acceleration of ions with rather low charge states to minimize space charge effects and reduce particle losses in the stripping process. Stripping denotes the process where electrons are removed from the ions. It occurs for those electrons whose orbital velocity is slower than the ion velocity. Highest charge states usually require relativistic ion velocities. To increase the charge state of the ions, the beam is passed through a thin foil or gas jet. This creates a charge state distribution from which the ions with the desired charge state are selected by magnetic deflection. All ions having other charge states get lost (stripping losses). The space charge of an ion bunch depends on the charge state of the ions. If the space charge is very high, this results in beam loss, because the ions repel each other (space charge losses). Therefore, ions with low charge state are necessary to produce ion beams with high intensities. However, high-energy ions with low charge states have high cross sections for charge exchange in the collisions with residual gas molecules [Boz17].

Several approaches exist to improve the static and dynamic vacuum such as vacuum bake-out, beam scrubbing, cryogenic pumping, coating of the vacuum chambers with non-evaporable getters or implementation of so-called ion catcher systems. Bake-out is a very common procedure to achieve pressures in the ultra-high vacuum (UHV, $p < 10^{-7} mbar$) regime. The vacuum vessel is heated under vacuum to usually 150–300 °C depending on the used materials to reduce the coverage of adsorbed water molecules on the surfaces. For the depletion of absorbed hydrogen from the bulk, vacuum components could be heated to 800–1000 °C in a high vacuum furnace. This process is called vacuum firing, but so far it is only applied for stainless steel or titanium [Mal20c]. Beam scrubbing denotes the cleaning of surfaces in the accelerator by the ion beam itself.

Cryogenic surfaces and surfaces coated with a getter material enable pumping distributed over a large area. Getter coatings can be applied even inside the magnets where local pumps cannot be mounted. Cryogenic surfaces bind residual gas molecules by van der Waals attraction (physisorption) [Mal20a]. A non-evaporable getter (NEG) is a reactive material that pumps gases by sorption. Reactive gases such as CO, CO₂, O₂, H₂O or N₂ are pumped by chemical reactions while H₂ is dissolved in the NEG layer [Mal20b]. Nobel gases, methane and other hydrocarbons are not pumped. During air venting, a thin layer of carbides, oxides and nitrides is formed, which protect deeper layers of the NEG film. After evacuation to UHV, the film has to be activated by a bake-out process. Typical parameters for NEG activation are 180 °C for 24 h [Mal20b]. Under these conditions, the carbides, oxides and nitrides diffuse into the bulk while H₂ is desorbed and pumped away. The NEG film also

acts as a barrier against diffusion of gas from the bulk into the vacuum. Other advantages are low particlestimulated desorption yields as well as low photo and secondary electron yields [Sue06].

Ion catchers are installed behind the dipole magnets to collect the lost beam ions in a controlled manner. For optimal performance of the ion catchers, the ions have to hit a low desorbing surface under perpendicular incidence, because desorption is lower for perpendicular incident ions compared to gracing incidence. Additionally, vacuum pumps with high pumping speed are installed next to the ion catchers. For optimal vacuum conditions, the ion catchers need surfaces with minimal desorption.

To date, neither the surface nor bulk properties affecting ion-stimulated desorption are fully understood. The yield of desorption stimulated by swift ions depends on many parameters e.g. on the amount of energy deposited in the material by the ion. The deposited energy is characterized by the so-called energy loss dE/dx of the ion. The energy loss depends on energy and charge state of the ion and on the target density. For desorption, the characteristics of the surface (cleanliness, roughness) and the adsorbates are of importance. This work studied different surface and bulk pretreatment procedures to create surfaces with lowest desorption. The treatment methods comprised different combinations of standard surface processes applied for many years, such as lapping, polishing, etching, milling or coating. In addition, methods like sputter cleaning and thermal annealing under ultra-high vacuum conditions were intensively investigated. Ion-stimulated desorption was measured for metals typically used for accelerator components such as tungsten, aluminum and stainless steel with special focus on copper.

The results of these investigations are not only important for FAIR and its heavy ion synchrotron SIS100, but also for other accelerators, which are currently under construction or commissioning such as SPIRAL2 (Système de Production d'Ions Radioactifs en Ligne de 2e génération) in France [Dol19], the High Intensity Heavy-ion Accelerator Facility (HIAF) in China [Ma17] or the Future Circular Collider (FCC) at CERN [Aba19]. To scale the experimental data to the energy range needed for the design of a specific accelerator, additional measurements with different ion energies at the new GSI accelerator CRYRING@ESR were conducted. The objective of this experiment was first the commissioning of the setup, second to investigate the dependence of the desorption yield on the energy loss of the ion, whereupon the energy loss is related to the ion energy and third to conduct desorption experiments with almost fully stripped ions, which results in very high energy losses in the surface of the material.

2 Theoretical Framework

2.1 Desorption Processes in Heavy Ion Accelerators

Processes which influence the vacuum pressure in heavy ion accelerators are manifold: (1) thermal desorption, (2) electron clouds and electron-stimulated desorption, (3) photon-stimulated desorption, (4+5) desorption stimulated by ionized or scattered residual gas molecules and (6+7) desorption stimulated by lost beam ions. The increase of the vacuum pressure in the accelerator due to interacting ions is called "dynamic vacuum". Figure 1 illustrates the typical processes in an ion accelerator.



Figure 1: Overview of processes, which contribute to the dynamic vacuum in heavy ion accelerators. Source: Bender 2020 [Ben20], Fig. 10.1. Reprinted with permission of John Wiley and Sons.

Thermal desorption (Figure 1, process 1) is a phenomenon always present in vacuum even at room temperature. Additional heat, which increases thermal desorption, can be induced in the vessel walls e.g. by hot filaments of pressure gauges.

In every accelerator for positive particles (protons, positrons or positively charged ions) also free electrons exist. Sources for free electrons are secondary electrons produced by energetic primary electron or ion irradiation or photoelectrons produced by synchrotron radiation [Bag20]. They are also created by residual gas ionization or at gas or foil strippers. The free electrons are accelerated in the Coulomb potential of the positive charged particle bunch perpendicular to the beam. The energy gain of the electron is in the order of some 10 eV up to a few keV depending on bunch population and distance to the bunch [Mal08]. The electrons hit the opposite wall of the beam tube and trigger electron-stimulated desorption and the release of secondary electrons. The secondary electrons are then accelerated within the electric field of the next particle bunch and generate again secondary electrons. This resonant effect is called beam-induced electron multipacting [Cim14]. Electron clouds (process 2) are formed by the bunched structure of the ion beam. The electrons from the clouds induce electron-stimulated desorption, resulting in local pressure rises.

Photon-stimulated desorption caused by synchrotron radiation (process 3) also increases the dynamic vacuum. Synchrotron radiation is produced in the magnetic structures of the accelerator when the particles are accelerated perpendicular to their velocity. For heavy ion accelerators, the contribution of this process to the dynamic vacuum is negligible [Ben20].

With increasing pressure, the probability of collisions of beam ions with residual gas molecules grows. If the residual gas molecule is ionized in the collision, it will be accelerated in the beam potential towards the wall of

the beam tube. The kinetic energy of the residual gas ions depend primarily on the beam current and the β -function¹ and can reach up to a few keV [Mal00]. Accelerated residuals gas ions (process 4) or elastically scattered residual gas molecules (process 5) induce low-energy particle-stimulated desorption.

In the collision with a residual gas molecule, the beam ion can also gain or lose one or more electrons. This leads to a change in the mass-to-charge ratio and within the next dipole magnet, the ion leaves its specified trajectory and hits the beam tube with its full energy under grazing incidence (process 6). Grazing incidence results in higher desorption compared to perpendicular incidence. Under these conditions one ion can trigger the desorption of 10^2-10^5 gas molecules [Mah08], causing further beam interactions with the residual gas. This self-amplifying process limits the maximum beam intensity and can lead to vacuum break down and complete loss of the ion beam.

Loss of beam particles also occurs at aperture-limiting devices, stripper foils, targets and beam dumps (process 7). This is high-energy ion-stimulated desorption but under perpendicular incidence, which is less severe. Generally, in heavy ion accelerators the dominate process, which impairs the dynamic vacuum, is desorption by lost beam ions (process 6 and 7).

2.2 Energy Loss of Ions in Solids

2.2.1 General Considerations

If ions penetrate a target, they experience energy loss. The stopping power or more precisely the stopping force S is defined as an energy loss per path length

$$S(E) = -\frac{dE}{dx} \tag{1}$$

The energy loss is a stochastic process involving two main mechanisms: (i) elastic collisions of the projectile ion with target nuclei resulting in a change of the ion direction (nuclear stopping) and (ii) interactions of the projectile with target electrons resulting in ionization and excitation of the target atoms (electronic stopping). Usually the two effects are treated separately, because they are relevant in different energy regimes [Möl17]. The total stopping power is the sum of both contributions

$$S(E) = S_{nucl}(E) + S_{elec}(E)$$
⁽²⁾

Figure 2 shows the contribution of the nuclear and the electronic stopping as a function of specific energy. At low specific energies up to some 10 keV/u the nuclear energy loss dominates, while at higher ion velocities, the electronic energy loss prevails. The electronic energy loss has a maximum at a few MeV/u, the so-called Bragg peak. At relativistic ion velocities, the stopping power increases slightly due to the emission of Cherenkov radiation and other relativistic effects [Lan20]. With low probability, also nuclear reactions take place. In the energy range of a few MeV/u treated in this work, the electronic energy loss dominates, only ≤ 1 % of the total energy loss is due to elastic collisions (nuclear stopping) [Ass07].

Comparing both sides of the Bragg peak, points exist with equal stopping power but different kinetic energies of the ion. The maximum energy transfer to the target electrons and therefore the range of the electron cascade depends directly on the projectile kinetic energy. As a result, at higher ion velocities but equal energy loss the same amount of energy is spread into a larger volume, which leads to a smaller energy density. This is called velocity effect.

During the interaction of the ion with the target electrons, the projectile ion loses or gains electrons. According to Bohr's stripping criterion, all electrons with orbital velocities smaller than the projectile velocity are stripped off. After several tens of nm [Ass17] the ion reaches an effective charge state which depends on its velocity.

 $^{^{1}}$ The β -function is the envelope of all particle trajectories and corresponds to the transvers beam size [Hol16].

For the calculation of the effective charge state Z_{eff} , several approaches exist. In this work, the equation from Schiwietz et al. [Sch01] was used. The authors fitted about 850 experimental data points to deduce the following formula for solid-state targets

$$Z_{eff} = \frac{12\chi + \chi^4}{0.07\chi^{-1} + 6 + 0.3\chi^{0.5} + 10.37\chi - \chi^4}$$
(3)

with

$$\chi = \left(\frac{v}{v_0} \frac{Z_p^{-0.52}}{1.68} Z_t^{-0.019 \cdot Z_p \cdot \frac{v}{v_0}}\right)^{1+1.8/Z_p} \tag{4}$$

where v is the ion velocity, v_0 the electron velocity in the first atomic orbit also called Bohr velocity $(v_0 = 2.19 \cdot 10^6 m/s)$. Z_p and Z_t are the atomic numbers of the projectile and the target, respectively. The uncertainty of equation (3) is $\Delta Z_{eff} = 0.54$, which corresponds to a relative uncertainty of $\Delta Z_{eff}/Z_p = 2.3 \%$.



Figure 2: Nuclear and electronic energy loss as a function of the specific energy for gold and calcium ions in a copper target. Data were calculated with "SRIM Ion Stopping and Range Tables" (Version SRIM-2013, [Zie13]) for ions with equilibrium charge state. The vertical line indicates the specific energy (4.8 MeV/u) at which the experiments at the beamline M1 were conducted.

Several algorithms were developed to calculate stopping powers. In this work, SRIM and CasP were used. SRIM (The stopping and range of ions in matter) [Zie17] is based on the binary collision approximation. The movement of the atoms in a target is described as a sequence of trajectories called "free-flight-path" between two elastic binary collisions [Möl17]. To calculate the nuclear energy loss and the scattering in the collision, an analytical equation called "magic formula" is used [Zie08]. Along the ion's free-flight-path, the ions lose energy by interactions with the target electrons. For heavy ions the electronic stopping power S_{elec} is determined with a semi-empirical approach by scaling the electronic energy loss of a proton $S_{elec,H}$ at the given velocity using the Brand-Kitagawa theory [Möl17; Zie08]

$$\frac{S_{elec}}{S_{elec,H}} = \frac{\left(Z_{eff}\right)^2}{\left(Z_{eff,H}\right)^2} \tag{5}$$

with Z_{eff} as the effective charge state of the ion at the given velocity. The SRIM code calculates the trajectory of every projectile and recoil atom until its energy becomes smaller than the predefined "cutoff energy" or it

reaches the surface [Möl17]. The model can be applied for an energy range from 0.1 keV/u to several MeV/u. The accuracy is about 10 % [Zie08]. SRIM also includes a subprogram called "Stopping and range tables". There only the stopping power is calculated with equation (5) and additionally ion ranges are determined using the "Projected Range Algorithm" [Zie08].

The program CasP (Convolution approximation for swift Particles) [Sch21] calculates the electronic stopping power from the impact-parameter dependent mean electronic energy transfer. This is done using unitary or perturbative convolution approximation [Gra02; Sch11]. Input parameters for the calculation are the projectile velocity, the projectile-screening potential, the target-electron density distribution and the oscillator strengths for the target electrons. The program can be used for ion energies up to a few 100 MeV/u. In contrast to SRIM, CasP is also able to treat non-equilibrium charge states.

2.2.2 Nuclear Energy Loss and Sputtering

Nuclear energy loss occurs due to binary elastic collisions between the projectile ion and the target nuclei. Nuclear stopping plays a role particularly at low energies at the end of the ion path. When the ion interacts with a screened target nucleus, energy is transferred to the target atom and it is displaced from its position. The projectile ion no longer follows a straight path, as it is the case for electronic energy loss. The recoil atoms collide with other target atoms and a collision cascade is induced. The process stops if the kinetic energy of the recoil atom becomes smaller than the displacement energy. The displacement energy is in the order of 10–100 eV depending on the material. The collision cascade creates defects in the solid.

During the collision cascade caused by irradiation with low-energy ions (~keV) in a target, some atoms gain a momentum towards the surface. If the kinetic energy of the atom is larger than the surface binding energy, the atom can leave the surface. This process is called sputtering. About 2/3 of the sputtered particles come out of the topmost atomic layer. For 5 keV argon ions under perpendicular incidence the sputtered atoms originate at maximum from a depth of about 20 Å [Bur88]. The sputter yield (number of sputtered particles per incoming ion) depends on the nuclear energy loss and therefore on the ion energy, and on the incidence angle of the ion [Beh07]. The dependencies are shown in Figure 3 for argon ions impinging on a copper substrate. The sputter yield first increases with increasing incidence angle with respect to the surface normal, because the collision cascade occurs closer to the surface. At angles lager than 70° the sputter yield decreases again, because the number of reflected ions increases [Fau19].



Figure 3: Sputter yields for argon ions on copper as a function of energy at perpendicular incidence (left) and as a function of incidence angle with respect to the surface normal at 1.05 keV ion energy (right). Source: Eckstein 2007 [Eck07], Figs. 27 and 73. Reprinted with permission of Springer Nature.

Sputtering of polycrystalline material usually results in an increased surface roughness, excavation of micro crystals and the creation of steps, pits and elevations [Beh64]. At rough surfaces, changes of the local inclination angle, geometrical shadowing, redeposition and secondary sputtering by reflected ions occur. Surface roughness reduces the sputter yield. The mean inclination angle of a surface is a convenient parameter to describe the sputter yields of rough surfaces [Cup21].

2.2.3 Electronic Energy Loss

If the specific energy of the projectile ion is larger than some 100 keV/u, the ion mainly excites the electronic subsystem of the target. Via ionization δ -electrons are generated and spread around the ion trajectory (time scale 10^{-17} – 10^{-16} s). In the next 10^{-15} – 10^{-14} s the electrons ionize further atoms and an electron cascade arises. After 10^{-13} s the energy is transferred to the atomic lattice via electron-phonon-coupling. Within this model, the ultrafast heating of the atomic system via electron-phonon-coupling is described by the so-called inelastic thermal spike. The heating of the atomic subsystem results in atomic collisions, defects and if the temperature is high enough in local melting. Afterwards the lattice cools down and electrons and holes recombine. The thermal spike ends within about 10^{-12} s for metals and 10^{-10} s for insulators [Ben15].

The temperature in the electronic T_e and atomic system T_a can be calculated by a set of two coupled differential equations ("Two-temperature model") [Ben20]. The equations are classical heat flux equations in radial geometry. For the electronic subsystem, the equation reads as follows

$$C_e(T_e)\frac{\partial T_e(r,t)}{\partial t} = -\frac{1}{r}\frac{\partial}{\partial r}\left(rK_e(T_e)\frac{\partial T_e(r,t)}{\partial r}\right) - g(T_e - T_a) + A(r,t)$$
(6)

The corresponding equation for the atomic subsystem is

$$C_a(T_a)\frac{\partial T_a(r,t)}{\partial t} = -\frac{1}{r}\frac{\partial}{\partial r}\left(rK_a(T_a)\frac{\partial T_a(r,t)}{\partial r}\right) + g(T_e - T_a) + B(r,t)$$
(7)

 $C_{e/a}$ is the specific heat and $K_{e/a}$ is the thermal conductivity of the respective electronic and atomic subsystem. A(r,t) and B(r,t) are source terms linked to the electronic or nuclear energy loss, respectively. $g(T_e - T_a)$ is the coupling term, which ensures the energy transfer from one subsystem to the other. By solving the two equations, one can determine the radial temperature profile around the ion impact as a function of time. There is some criticism about the model, because it assumes equilibrium conditions even for this very short time scales and macroscopic material parameters such as specific heat or thermal conductivity are applied for the short length scales. For insulators, there is also the problem that free electron diffusion is assumed and that holes are not included.

Figure 4 presents the temperature in the electronic and the atomic subsystem as a function of time and radius for a copper and an aluminum target as calculated with the thermal spike program written by Zimmermann [Zim19]. The projectile is a gold ion with 4.8 MeV/u specific energy. The input parameters and their values are listed in chapter 11.1 in the appendix. Due to the higher energy loss, for copper the temperature increase of the electronic subsystem is much higher than for aluminum. For copper, the maximum temperature is 412,500 K, while for aluminum it is only 294,820 K. After electron-phonon-coupling, also the temperature of the atomic lattice is higher for copper with a maximum temperature of 679 K, while the maximum lattice temperature of aluminum is 579 K. The time evolution of the temperature is comparable for both materials.

In several materials, the fast heating and quenching along the ion trajectory result in a cylinder of damaged material, the so-called ion track. In the inelastic thermal spike model, an ion track is formed if the temperature around the ion path exceeds the melting temperature of the target material. The diameter of the ion track depends on the energy loss of the ion and is typically in the range of 5–20 nm [Ass07]. A threshold value for the track formation exists, below a critical dE/dx value which depends on the material no tracks are produced [Lan20]. Metals are less sensitive to track formation, because the energy deposited by the ion is spread very

efficiently in the electronic subsystem due to the high electron mobility. Moreover, the high thermal conductivity results in a fast energy distribution in the atomic system, which leads to a smaller temperature increase compared to e.g. insulators. Consequently, so far no tracks were observed in gold, copper or silver, but for example in iron, titanium or amorphous metallic alloys. In contrast, insulators such as oxides, ceramics or polymers are very sensitive to track formation, while semiconductors have a medium sensitivity [Lan20].



Figure 4: Temperature in the electronic and atomic subsystem for copper and aluminum as a function of time and radius around the ion track after impact of a gold ion with 4.8 MeV/u specific energy as determined with the inelastic thermal spike model.

In the energy regime of electronic energy loss, sputter yields were observed which could not be explained by the collisional sputtering described in the previous chapter. This so-called electronic sputtering is caused by evaporation due to the pressure and/or thermal spike in the atomic lattice [Ass07]. For electronic sputtering, the sputter yields strongly depend on the energy loss and therefore on the target material (if it is a metal or an insulator and crystalline or amorphous) and on the charge state of the ion. Similar to track formation, electronic sputtering only occurs above a material dependent energy loss threshold [Ass07].

At low ion velocities ($v \ll v_0 Z^{2/3}$), the electronic stopping power can be calculated with the Lindhard-Scharff formula [Möl17]

$$S_{elec}(v) = \frac{8\pi e^2 a_0}{4\pi\epsilon_0} \cdot \frac{Z_p^{7/6} Z_t}{\left(Z_p^{2/3} + Z_t^{2/3}\right)^{3/2}} \cdot \frac{v}{v_0}$$
(8)

v denotes the ion velocity and v_0 the Bohr velocity. Z_p and Z_t are the atomic numbers of the projectile and the target, respectively. e is the elementary charge, a_0 the radius of the first atomic orbit and ϵ_0 the vacuum

electric permittivity. The Bethe formula describes the stopping power at energies higher than the Bragg peak $(v \gg v_0 Z^{2/3})$ [Bet53; Möl17]

$$S_{elec}(v) = \frac{4\pi e^4 (Z_{eff})^2}{m_e v^2} NB$$
(9)

 Z_{eff} denotes the effective charge state of the ion, m_e the electron mass and N the atomic density of the target. B is called stopping number. For non-relativistic velocities B is given by

$$B = Z_t \ln\left(\frac{2m_e v^2}{l}\right) \tag{10}$$

and for relativistic velocities by

$$B = Z_t \left[\ln\left(\frac{2m_e v^2}{l}\right) - \ln(1 - \beta^2) - \beta^2 \right]$$
(11)

with $\beta = v/c$ (c: speed of light) and I as mean ionization potential.

2.3 Desorption

2.3.1 Thermal Desorption and Thermal Desorption Spectroscopy

Thermal desorption occurs if the thermal energy of the adsorbed particle is larger than the desorption energy E_{des} . For Physisorption, the desorption energy is just the binding energy, for chemisorption, it is the sum of binding and activation energy. The number of particles per surface area $\Delta\sigma$ with sufficient energy as a function of the substrate temperature T is described by Boltzmann statistics [Jou18b]

$$\Delta \sigma = \sigma \cdot \exp\left(-\frac{E_{des}}{RT}\right) \tag{12}$$

where σ is the number of adparticles per surface area und R the universal gas constant. From this formula the Polanyi-Wigner equation [Red62] for determining the desorption rate j_{des} is derived as

$$j_{des} = -\frac{d\sigma}{dt} = v_i \cdot \sigma^i \cdot \exp\left(-\frac{E_{des}}{RT}\right)$$
(13)

i is the order of the desorption reaction and v_i the so-called pre-exponential factor. The number of particles on the surface can be also expressed as surface coverage θ , which is defined as

$$\theta = \frac{\sigma}{\sigma_{mono}} \tag{14}$$

 $\sigma_{mono} \approx 10^{15} cm^{-2}$ [Jou18b] is the number of adparticles per surface area in one monolayer. The preexponential factor v_i can be interpreted in first-order desorption as the oscillation frequency of the adparticles. v_1 can be estimated by equating the energy of a harmonic oscillator hv and the thermal energy kT[Jou18b]

$$\nu_1 = \frac{kT}{h} \tag{15}$$

h is the Planck constant. At room temperature v_1 is in the order of 10^{13} s⁻¹. But experimental values are in the range from $10^4 - 10^{15}$ s⁻¹ [Jou18b]. For second-order desorption the following equation applies [Red93]

$$\nu_2 = \sqrt{2} \cdot d_{col} \sqrt{\frac{\pi RT}{2M}} \tag{16}$$

where d_{col} is the collision diameter of an adsorbed atom. $\sqrt{\pi RT/2M}$ is the average velocity of the adatoms migrating on the surface and M the molar mass of the adatom. If the adatoms are bound to dedicated adsoption sites and are only able to jump from one site to another, v_2 is calculated as [Kle78]

$$v_2 = \frac{v_{dif}}{\sigma_s} \tag{17}$$

where v_{dif} is the average jump frequency of the adatoms on the surface and σ_s is the number of adsorption sites per surface area. For second-order desorption, the desorption energy is $E_{des} = 2E_B - E_{dis}$ with E_B as binding energy of the adatom and E_{dis} as dissociation energy of the molecule.

The order of desorption is related to the desorption mechanism. First-order desorption occurs with desorption of atoms or non-dissociated molecules. The desorption rate is proportional to the coverage. If the recombination of two particles is the rate-limiting step, this is indicated as second-order desorption. With zero-order desorption the desorption rate is independent from the coverage. It occurs with desorption from multilayers or if the particles desorb from a few dedicated sides with the remaining particles forming a reservoir. Fractional orders of desorption characterize desorption from clusters, which requires to break bonds between the adparticles [Kre86].

The parameters of the Polanyi-Wigner equation such as desorption energy, pre-exponential factor or order of desorption can be determined by thermal desorption spectroscopy (TDS). In this method, the sample is heated with a defined temperature ramp and the amount of desorbed gas is quantified as a function of temperature. The TDS curve shows peaks at specific temperatures, which correspond to the desorption energies. A simple method for the evaluation of thermal desorption spectra was proposed by Redhead [Red62]. The desorption energy depends not only on the adsorbate-substrate system but also on the coverage and the location of the adsorption side [Kre86].

2.3.2 Ion-Stimulated Desorption

Ion-stimulated desorption (ISD) is described as the release of gas molecules adsorbed at the surface or absorbed in near surface layers. Depending on the type of binding, two types of adsorption are distinguished: For physisorption, the adparticles are bound by van der Waals forces with desorption energies below 40 kJ/mol, while chemisorbed particles are bound by covalent or ionic bonds usually with higher desorption energies between 80 and 800 kJ/mol [Jou18b]. Sputtering is the emission of atoms or clusters of the target material. During ion irradiation, both processes, desorption and sputtering, can occur. However, sputtered particles are non-volatile, they are readily chemisorbed at the wall of the vacuum chamber and do not contribute to the dynamic vacuum to a significant extent [Ben20].

The energy required for ion-stimulated desorption can be deposited via two mechanisms whose contribution depends on the ion velocity. For ions in the keV energy range (nuclear energy loss), adparticles are released by the atomic collision cascade (sputtering, cf. chapter 2.2.2). At high ion energies (~MeV/u), the energy is initially deposited in the electronic subsystem, heating the atomic system after electron-phonon-coupling. Desorption may be due to electronic excitation processes or due to the local temperature increase around the ion impact as described by the inelastic thermal spike model (cf. chapter 2.2.3). In the latter case, it is expected that the local temperature increase leads to thermal desorption of the adparticles [Ben09]. Assuming the two-temperature model and the Polanyi-Wigner equation (equation (13)) combined with the assumption of first-order desorption, the desorption yield η can be predicted by

$$\eta = 2\pi \int_0^{t_{max}} \int_0^{r_{max}} \nu_1 (T(r,t)) \cdot \sigma(r,t) \cdot \exp\left(-\frac{E_{des}}{RT(r,t)}\right) r \, dr \, dt \tag{18}$$

The desorption yield η is defined as the number of desorbed particles per impacting ion. At high ion energies desorption yields for metals are typically in the order of 10^2-10^5 molecules/ion, in contrast at low energies the yields are usually below 10 molecules/ion [Mal20c]. For high-energy ions of several MeV/u, the contribution of desorption induced by secondary particles (electrons, sputtered ions) to the total desorption yield is very small

in the order of 5–10 % [Hed09] because of the low production rates of the secondary particles and their small desorption yields.

The ISD yield depends on the one hand on energy and charge state of the ion and the energy loss and on the other hand on the target properties (strength of the electron-phonon-coupling, electrical and thermal properties) and the adsorbate (binding energy, coverage). Existing data suggest that the desorption yield scales with the electronic energy loss as

$$\eta \sim \left(\frac{dE}{dx}\right)_{elec}^{n} \tag{19}$$

The expected exponent is between n = 1 - 3 [Car03; Kol09; Mol07] and is related to the desorption mechanism. Thermodynamic models such as the thermal spike model predict n = 1.5 - 2, but larger values are also reported.

Grazing incidence of the ions results in higher desorption yields than perpendicular incidence as observed for various materials, but the dependence on the incidence angle φ with respect to the surface normal is less pronounced than the $1/cos(\varphi)$ -dependence known from sputtering or secondary electron yields. Experimental ISD yields scale with

$$\eta \sim (1/\cos\varphi)^m \tag{20}$$

with m = 0.12 - 0.31 [Mol07]. Table 1 shows the scaling factor for different incidence angles. Large deviations of the desorption yield are only observed for grazing incidence. For an incidence angle of 45°, which was used in this work, a deviation of only about 7 % compared to perpendicular incidence is expected.

Table 1: Scaling factor of the ion-stimulated desorption yield for different incidence angles calculated with m = 0.2

φ	0°	45°	70°	80°	85°	89°
$(1/\cos\varphi)^m$	1	1.07	1.24	1.42	1.63	2.25



Figure 5: Correlation of the desorption yields (4.2 MeV/u Pb⁵⁴⁺ ions, grazing incidence) for various beam tube materials and the carbon and oxygen surface concentration as determined by X-ray photoemission spectroscopy after 300 °C bakeout in UHV. The dashed line indicates the possible correlation. Source: Mahner et al. 2011 [Mah11], Fig. 5. Licensed under CC BY 3.0.

Several studies (e.g. [Hed09; Loz02; Mah03]) observe that the ISD yield decreases with increasing ion fluence Φ due to surface cleaning by the ion beam (denoted as beam scrubbing). Surface concentration of carbon and oxygen influence the ISD yield as shown in Figure 5 [Mah11]. The yield decrease can be fitted with the following equation

$$\eta(\Phi) = \eta(\Phi^*) \left(\frac{\Phi^*}{\Phi}\right)^{\alpha}$$
(21)

The ISD yield $\eta(\Phi^*)$ at the corresponding fluence Φ^* can be taken at any point of the observed yield-fluence curve. α lies between 0 and 0.5 [Mal20c].

2.3.3 Electron- and Photon-Stimulated Desorption

As described in chapter 2.1, in particle accelerators also photons from synchrotron radiation and electrons contribute to the dynamic vacuum. Electron-stimulated desorption (ESD) and photon-stimulated desorption (PSD) are caused by electrical excitation of the binding of the adsorbate. This process is referred to as "desorption induced by electronic transitions". The desorption mechanism strongly depends on the adsorbate-substrate system.



Figure 6: Potential curves and transitions according to the MGR model, x: reaction coordinate, I: ionization energy of the adsorbate, ϕ : work function of the substrate, H_a : adsorption energy, E_{ex} : transition energy to the antibonding state, E': electronic excitation after transition to the bonding curve. Source: Menzel et al. 1964 [Men64b], Fig. 15. Reprinted with permission of AIP Publishing.

An early model to describe ESD with low-energy electrons from metal surfaces was developed by Menzel and Gomer [Men64a; Men64b] and independently by Redhead [Red64]. The model can also be applied for PSD from substrates with low-energy antibonding states, which can be excited by UV-photons [Chu83]. According to the MGR (Menzel-Gomer-Redhead) model (Figure 6), the incident electron or photon excites the system of adsorbate (A) and metal substrate (M) from the ground state (M+A) to an antibonding state (M+A)[‡] or ionic state (M^-+A^+). In the excited state, the particle experiences a repulsive potential. The particle is accelerated

away from the surface and gains kinetic energy. If the lifetime of the excited state is long enough, the particle can desorb directly along the antibonding or ionic potential curve. Alternatively, the transition in an excited bonding state (M*+A or M**+A) or the ground state (M+A) is possible. The particle desorbs if the particle gained enough kinetic energy before the transition to overcome the barrier for recapture. Many more models exist for the description of desorption induced by electronic transitions. Examples can be found e.g. in [Ram91] for ESD and in [Chu83] for PSD.

High-energy electrons also interact with the substrate. Some of the electrons are reflected and additionally, secondary electrons are generated, which both interact with the adsorbate. At electron energies above 1 keV these processes dominate [Dri78]. Photons generate photoelectrons if the energy is higher than the work function. Photoelectrons cause ESD, too. Irradiation with high electron or photon intensities may result in substrate heating and consequently thermal desorption.

2.4 Diffusion

Gas molecules are not only adsorbed at the surface, they also penetrate into the bulk (absorption). In the solid, they occupy vacancies or interstitial sites. Following a concentration gradient $\nabla c(\vec{r})$, absorbed particles diffuse through the bulk. The diffusion process is characterized by Fick's laws [Jou18b]. Fick's first law describes the particle flux rate j_{dif}

$$j_{dif}(\vec{r}) = -D \cdot \nabla c(\vec{r}) \tag{22}$$

The temporal dependence of the particle concentration c is described by Fick's second law

$$\frac{\partial c}{\partial t} = D \cdot \Delta c \tag{23}$$

with *D* being the diffusion coefficient. Generally, the diffusion coefficient is a second-order tensor, but for metals with cubic structure, it simplifies to a scalar [Peg70]. *D* depends on the jump frequency ν and the characteristic jump distance a_{jump} , which is related to the lattice structure

$$D = a_{jump} \cdot \nu^2 \tag{24}$$

Various theories exist for the determination of the jump frequency. All of them result in an exponential dependence of D on the temperature

$$D = D_0 \cdot \exp\left(-\frac{E_{dif}}{RT}\right) \tag{25}$$

but they differ in interpretation and calculation of the pre-exponential factor D_0 , which can be temperature and mass dependent [Peg70]. The activation energy for diffusion E_{dif} is the difference between the energy of the atom in its equilibrium position and the potential barrier, which the atom has to overcome to move to the next vacancy or interstitial site [Köt70].

The different diffusion mechanisms can be divided into two groups: volume diffusion and interface diffusion. Grain boundary diffusion, pipe diffusion (along dislocations) and surface diffusion are typical examples for interface diffusion. Usually for interface diffusion the diffusion coefficients *D* are some orders of magnitude larger than for volume diffusion [Häs70]. For volume diffusion, in particular two mechanisms are of importance: (i) vacancy diffusion, where atoms jump to a neighboring vacancy creating a new vacancy and (ii) interstitial diffusion for foreign atoms with small atomic radii, which occupy interstitial sites. Vacancy diffusion results in a flux of diffusing atoms in one direction and a vacancy flux in the opposite direction. It occurs in most metals and is the dominant mechanism in face-centered cubic metals [Peg70]. Interstitial diffusion occurs particularly for gas atoms (hydrogen, oxygen, nitrogen) or carbon atoms in metals. The atoms jump from one interstitial site to another. In the cubic lattice the foreign atoms occupy octahedron or tetrahedron sites [Köt70].

Among all interstitial diffusion atoms, hydrogen has the highest mobility and the lowest activation energy. As a result, the outgassing is strongly affected by surface processes, which occur in this case with lower rates. This impedes the experimental determination of bulk diffusion parameters and measured values for the activation energy differ by orders of magnitude in the literature [Köt70]. Metals which absorb hydrogen in an endothermic reaction like iron, tungsten or copper, contain only small fractions of hydrogen. Because of the low concentration, the diffusion is significantly influenced by lattice defects. Vacancies, dislocations, voids or impurity phases can trap hydrogen atoms and hinder the diffusion [Bor88]. The effect depends on defect type and concentration and decreases with increasing temperature, because the hydrogen atoms are released from the traps with increasing temperature [Köt70].

3 Experimental Setups and Accelerator Facility

3.1 Setup for Offline Desorption Measurements

Measurements on thermal desorption were done at an offline desorption measurement setup (denoted as "TDS-setup"). The setup was also used for sample annealing and offers the possibility for experiments on electron-stimulated desorption. The setup consists of two vacuum chambers, which are separated by an aperture (Figure 7 and Figure 8). The aperture is made out of a stainless steel outer part with cooling channels for water-cooling and an inner gold-coated ceramic aperture with low thermal conductivity. The arrangement limits the heating of the aperture to less than 45 °C during the measurements. This minimizes thermal desorption from the aperture.



Figure 7: Schematic view of the offline desorption measurement setup with the two vacuum chambers, the load lock at the top and the pumping system at the bottom, Source: Velthaus et al. 2021 [Vel21].

The left chamber, denoted as "sample chamber", contains a movable sample holder, the connection to a load lock and a Faraday cup. The sample holder is made out of copper (Cu-ETP) and can be heated up to 500 °C using a PBN/PG ceramic heater (Momentive HTR1001) with temperature controller (JUMO DICON touch). The temperature is monitored by two type K thermocouples (uncertainty ≤ 0.25 %), one is attached to the sample holder close to the sample and the other one is fixed to the ceramic aperture. The temperature can be adjusted with an accuracy of ± 0.5 K. The vacuum in this chamber is maintained by a turbo molecular pump (Pfeiffer HiPace 700, nominal pumping speed 685 l/s for N₂) and controlled by a wide-range gauge (WRG, Leybold ITR 90).

The second chamber ("analysis chamber") contains the vacuum diagnostic and an electron source for ESD measurements. The pressure is measured by an extractor vacuum gauge (Pfeiffer IMR 430 with controller Leybold IM 540) and a quadrupole mass spectrometer (QMS, MKS Microvision 2). For calibration measurements, a gas inlet line with a liquid nitrogen cold trap and a connection to the prevacuum is attached to the analysis chamber via a dosing valve. A bypass line with an angle valve connects the analysis chamber to

the turbo molecular pump of the sample chamber. After bake-out, the valve in the bypass line in closed and the chamber is pumped by a sputter ion pump (SIP, Varian Starcell, nominal pumping speed 50 l/s for N₂) and a titanium sublimation pump (TSP). A final pressure of about 3E-11 mbar is achieved in the analysis chamber and of <5E-10 mbar in the sample chamber.

For the desorption measurements, the sample holder is placed in front of the aperture in such a way that the aperture is completely covered by the sample. Hence, the pumping speed through the closed aperture is reduced to approximately 1 % of the pumping speed of the analysis chamber. Therefore, only gas desorbed from the sample is measured in the analysis chamber. Gas from the heating system is pumped by the turbo molecular pump and its contribution can be neglected. When heating up the sample holder without sample to 400 °C, the total pressure in the analysis chamber increases only by $\leq 1E-11$ mbar. For sample exchange, a load lock containing a transfer rod with a sample carrier for 18 samples, a turbo molecular pump (Pfeiffer HiPace 300, nominal pumping speed 260 l/s for N₂), a WRG (MKS QuadMag 974B) and a quick access door is available. More details about the offline desorption measurement setup can be found in [Vel17] and [Vel21].



Figure 8: Photograph of the offline desorption measurement setup from top, (1) load lock, (2) sample chamber, (3) aperture, (4) analysis chamber, (5) extractor gauge, (6) quadrupole mass spectrometer, (7) WRG, (8) bypass and (9) gas dosing valve.

The effective pumping speed of the analysis chamber is not constant in time, because it depends on the condition of the titanium layer in the titanium sublimation pump. A fresh-deposited titanium layer has the highest pumping speed, which decreases while the layer becomes saturated. If the titanium layer is fully saturated, the pumping speed of the TSP is zero and the chamber is only pumped by the sputter ion pump. The

effective pumping speed of the analysis chamber was measured for different gases as a function of the amount of pumped gas since the last evaporation process. For the measurements, nitrogen, carbon monoxide, carbon dioxide, hydrogen or argon were injected into the analysis chamber up to a pressure of 9E-9 mbar. Then the aperture was closed by the sample holder and the pressure increase was measured. For the effective pumping speed S_{eff} , the following equation is valid

$$p = \frac{q}{S_{eff}} \tag{26}$$

where p is the pressure in the analysis chamber and q the gas flow into the chamber. Here the gas flow originates from the gas injected via the dosing valve. Using equation (26), two conditions can be defined. For the closed aperture holds

$$p_{closed} = \frac{q}{S_{eff}} \tag{27}$$

while if the aperture is open

$$p_{open} = \frac{q}{S_{eff} + S_{aperture}} \tag{28}$$

is valid. By measuring the pressure difference in the sample chamber when opening and closing the aperture, the conductance of the aperture was determined to be $C_{aperture} = 6.5 \pm 0.2 l/s$. This is in good agreement with a simulation with the program "MC-Leitwert" [Lux03], which yields $C_{aperture} = 6.66 l/s$. The effective pumping speed through an aperture $S_{aperture}$ with conductance $C_{aperture}$ is calculated as follows

$$S_{aperture} = \frac{S_{turbo}}{1 + \frac{S_{turbo}}{C_{aperture}}}$$
(29)

The turbo molecular pump has a pumping speed of $S_{turbo} = 685 l/s$. This results in an effective pumping speed through the aperture of $S_{aperture} = 6.28 \pm 0.2 l/s$. By equating equation (27) and (28), the following expression for the effective pumping speed of the analysis chamber is obtained

$$S_{eff} = \frac{p_{open} \cdot S_{aperture}}{p_{closed} - p_{open}}$$
(30)

The results of the measurements are shown in Figure 9. The amount of pumped gas Q is determined by integrating the pressure over time for each measurement and summarizing all measurements. The measured data points are fitted with an exponential function

$$S_{eff} = S_0 \cdot \exp\left(-\frac{Q}{\tau}\right) + S_1 \tag{31}$$

The fit results are shown in Table 2. Measurements with water vapor are very difficult to realize, therefore for H₂O the pumping speed of N₂ was used and multiplied with $\sqrt{28}/\sqrt{18}$, because the pumping speed scales with the molecular mass *M* as $1/\sqrt{M}$ [Jou18a]. All measurements were performed at room temperature (22 ± 2 °C)

Table 2: Fit parameters for the effective pumping speed of the analysis chamber for different gases

Gas	S ₀ [l/s]	S ₀ error [l/s]	au [mbar·l]	au error [mbar·l]	<i>S</i> ₁ [l/s]	S ₁ error [l/s]
H ₂	113.3	3.8	0.0380	0.0034	159.3	4.2
N ₂	34.7	1.2	0.0173	0.0026	41.0	1.0
со	6.1	1.4	0.0034	0.0021	80.8	0.3
Ar	2.9	0.2	0.0079	0.0009	19.8	0.2
CO ₂	6.7	1.0	0.0080	0.0036	66.5	0.7



Figure 9: Effective pumping speed of the analysis chamber as a function of the amount of pumped gas.

3.2 Accelerator Facility at GSI

Most of the measurements on ion-stimulated desorption were conducted at the beamline M1 at the M-branch of GSI. The M-branch is located directly behind the linear accelerator UNILAC (Figure 10). The gold ions are provided from a Penning Ionization Gauge (PIG) source in the south terminal. The beam is preaccelerated to 1.4 MeV/u and stripped to a charge state of $q_{ion} = 25$ or 26. The calcium ions (Ca¹⁰⁺) come from an Electron Cyclotron Resonance (ECR) ion source and are directly transported to the UNILAC without stripping. In the UNILAC, the beam is accelerated to a specific energy of 4.8 MeV/u for the desorption experiments. An additional stripper foil can be inserted in front of the M-branch beamline. This offers the possibility to further increase the charge state of the ions by electron stripping. The dipole magnets in the arc of the beamline are used to select a charge state from the charge state distribution created by the stripper foil. For the desorption measurements Ca¹⁹⁺ or Au⁵²⁺ ions were selected, because these charge states are close to the equilibrium charge states of 18+ (Ca) and 53+ (Au) at 4.8 MeV/u when using a carbon foil [Sch01] and therefore offers the highest beam intensities. However, when using the stripper foil at the M-branch, the intensity is 0.5–1 order of magnitude lower compared to the unstripped beam.

Four beam times were conducted at M1 from 2019 to 2022. All ions had a specific energy of 4.8 MeV/u, which is for gold ions in copper close to the Bragg peak, where the ions exhibit their maximum energy loss. The beam conditions such as repetition rate and pulse length varied slightly between the different beam times but were constant during one beam time block. The variations did not have significant influence on the desorption experiments, because the pressure changes always occur at much longer time scales than the beam pulse length. The beam pulses had a length of 1–5 ms and a repetition rate of 2.4–15 Hz depending on the number of experiments running in parallel. The beam intensity varied from beam time to beam time, but the results of the desorption measurements are normalized by the beam intensity. The only major difference between the different beam times were the used charge states, because the charge state influences the energy loss of the

ions in the sample. Figure 11 shows the energy loss of gold ions in copper for the different charge states. The used charge states for the calcium and gold ions and the corresponding intensities are listed in Table 3.

Been time	Intensity [ions/s]					
beam time	Ca ¹⁰⁺	Ca ¹⁹⁺	Au ²⁵⁺	Au ²⁶⁺	Au ⁵²⁺	
2019	5E7	3E8	-	2E7	-	
2020	5E9	1E9	-	7E8	7E7	
2021	1E10	-	9E8	-	-	
2022	2E10	-	-	4E9	-	

Table 3: Used charge states and average intensities during the different beam times



Figure 10: Scheme of the accelerator facility at GSI with the M-branch behind the UNILAC and the CRYRING at the end of the accelerator chain. Source: GSI Helmholtzzentrum für Schwerionenforschung GmbH, 2021 [GSI21], modified.

CRYRING@ESR [Les15] is the newest accelerator at GSI located at the end of the accelerator chain (Figure 10). It is designed as a storage ring with an acceleration/deceleration section for tuning the energy of highly or fully stripped ions injected from the Experimental Storage Ring (ESR). It is possible to adjust independently the kinetic energy and the potential energy (charge state) of the beam. For the desorption experiment, hydrogen-like ions were selected. At high charge states, the energy loss of the ions is much larger than of the ions used at the UNILAC (Figure 11), because the energy loss scales with the square of the charge state. The large energy loss is relevant to the desorption problem and may have implications for the UHV conditions required for the operation of CRYRING.

For the desorption experiment at CRYRING, the gold ions coming from the PIG ion source were accelerated in the UNILAC to 11.4 MeV/u. After stripping to Au⁶⁵⁺, the ions are accelerated in the heavy ion synchrotron SIS18 to 147.2 MeV/u. Then the beam is extracted using fast extraction, stripped again to the final charge state (Au⁷⁸⁺) and transferred to the Experimental Storage Ring. In the ESR, the beam is cooled and decelerated to 10 MeV/u. Beam cooling reduces the longitudinal and transversal momentum spread of the beam and therefore decreases the beam diameter and its emittance [Pot90]. In ESR and CRYRING, electron cooling of the

beam is used. The cooled ions are finally transported to CRYRING. In the CRYRING, the beam is further cooled, decelerated to the desired energy, cooled again and then fast extracted to the irradiation chamber. For the desorption experiment, ion energies between 2–4.8 MeV/u were used. Due to the use of several accelerators and the multiple stripping processes, the achievable repetitions rates and beam intensities at CRYRING are rather low. In the gold beam time for the desorption experiment, the pulses had a repetition rate of only 0.026 Hz and a pulse length of approximately 0.23 μ s. At extraction, each pulse contained about 4.4E5 ions at 2 MeV/u, 7.7E5 ions at 3 MeV/u and 9.2E5 ions at 4.8 MeV/u, which is much less than at the M-branch.



Figure 11: Electronic energy loss of gold ions in copper for the used charge states as calculated by CasP (version 5.2, model: UCA, screening function: general, [Sch13]).

3.3 Setup at M-branch

Figure 12 presents a schematic view of the experimental setup installed at the M1 beamline, which was used for the ISD measurements. The core is the spherical irradiation chamber (diameter 350 mm). It contains the sample holder, a total pressure gauge and a quadrupole mass spectrometer. The sample holder has a resistive heater for sample annealing and to bake the sample holder after chamber venting. For the pressure measurement during ion irradiation, an extractor gauge (Leybold IE 514 with controller Prevac MG 14) and a quadrupole mass spectrometer (MKS Microvision 2) is used. For the QMS calibration, the chamber has a gas inlet line with a liquid nitrogen cold trap and a prevacuum connection. The irradiation chamber is connected to the pumping vessel via a 295 mm long DN100 tube. The setup is evacuated by a turbo molecular pump (Pfeiffer HiPace 700 M, nominal pumping speed 685 I/s for N₂) and by a combination pump. Another small turbo molecular pump (Pfeiffer HiPace 80, nominal pumping speed 67 I/s for N₂) is connected to the irradiation chamber to evacuate an argon ion source, which was not used in this work. For pressure control, a second extractor gauge (Leybold IE 514 with controller Prevac MG 14) is mounted to the pumping vessel. The base pressure in the irradiation chamber is usually $\leq 1E-9$ mbar.



Figure 12: Schematic view of the setup at the M1 beamline with the load lock on the left, the irradiation chamber in the middle and the pumping vessel on the right. Beam direction is from right to left. Source: Velthaus et al. 2023 [Vel23].



Figure 13: Photograph of the end of the M1 beamline and the irradiation chamber, (1) irradiation chamber, (2) quadrupole mass spectrometer, (3) load lock with beam diagnostic, (4) gas inlet line, (5) pumping vessel, (6) slit pairs and (7) Faraday cup. Beam direction is from right to left.

The load lock system is used to bring the samples into the vacuum without venting the irradiation chamber. A gate valve connects the load lock to the irradiation chamber. The load lock contains a self-designed transfer rod with a carrier for 14 samples, a turbo molecular pump (Pfeiffer HiPace 80), a wide-range gauge (MKS QuadMag 974B) and a quick access door. Additionally, for beam diagnostic a Faraday cup and a beam screen (YAG:Ce with ITO coating at one side) moved by a stepper motor is placed in the load lock. Another beam screen (chrome-doped Al_2O_3) can be place in the sample holder. A second Faraday cup is located in front of the whole setup (Figure 13). Two pairs of adjustable slits between the first Faraday cup and the pumping vessel are used to cut the beam to the desired size.

To quantify the amount of desorbed gas, it is necessary to know the effective pumping speed of the setup. The effective pumping speed was determined by simulating the pressure distribution in the setup with the program "Molflow+" [Ker19; Ker20]. Molflow+ calculates pressure distributions under molecular flow conditions by using a test-particle Monte-Carlo method. Because of a change in the experimental setup in 2022, two simulations with different geometries were done, one for the beam times in 2019–2021 and a second one for the beam time in 2022. The geometry of the first design is shown in Figure 14. The resulting pressure distribution is presented in Figure 15. To calculate the effective pumping speed S_{eff} , equation (26) is applied. In this calculation p is the pressure in the center of the chamber and q the desorbed gas flow, which is set to 1 mbar·l/s for easy calculation, because S_{eff} does not depend on q. This results in $S_{eff} = 181 l/s$ for the beam times 2019–2021. Before the beam time 2022 the electrostatic bender (cf. Figure 14) was removed, this results in a higher effective pumping speed of $S_{eff} = 190 l/s$.



Figure 14: Model for the Molflow+ simulation for the beam times in 2019–2021.



Figure 15: Result of the Molflow+ simulation for the beam times in 2019–2021. The pressure distribution is shown as color-code.

The effective pumping speed of the small turbo molecular pump at the argon ion source could not be included in the simulation, because the geometry inside the argon ion source is not known. The effective pumping speed was determined by measuring the pressure rise, which occurs when the valve in front of the small turbo molecular pump is closed. When the valve is closed, the following condition is valid

$$p_{closed} = \frac{q}{S_{eff,main\,pumps}} \tag{32}$$

When the valve is open, the condition changes to

$$p_{open} = \frac{q}{S_{eff,main\,pumps} + S_{eff,ion\,source}}$$
(33)

The gas flow q is equal under both conditions. Therefore, the equations can be equated. The effective pumping speed of the turbo molecular pump at the argon ion source is calculated as

$$S_{eff,ion\ source} = S_{eff,main\ pumps} \cdot \frac{p_{closed} - p_{open}}{p_{open}}$$
(34)

Using $S_{eff,main\,pumps} = 181 \, l/s$ from the Molflow+ simulation, the effective pumping speed of the small turbo molecular pump is $S_{eff,ion\,source} = 13 \, l/s$. The same measurement was done opening and closing the valve to the beamline. This results in a pressure difference of only 3E-13 mbar, which correspond to 0.2 l/s effective pumping speed and is therefore neglected. For the evaluation of the desorption measurements, the sum of the effective pumping speed of the main pumps from the Molflow+ simulation and the measured pumping speed of the turbo molecular pump at the argon ion source was used, which is $S_{eff,total} = 194 \, l/s$ for the beam times in 2019–2021 and $S_{eff,total} = 203 \, l/s$ for the beam time in 2022. These values are valid for nitrogen. Based on the nitrogen data, the effective pumping speeds for all relevant gases were calculated and are shown in Table 4.

Table 4: Effective pumping speed of the setup at M1 for different gases based on the Molflow+ simulation for nitrogen and scaled by $1/\sqrt{M}$ to the other gases

Gas	Molecular mass M	S_{eff} [l/s] beam times 2019–2021	S_{eff} [l/s] beam time 2022
N ₂	28	194	203
H₂	2	726	760
H₂O	18	242	253
СО	28	194	203
Ar	40	162	170
CO2	44	155	162

3.4 Setup at CRYRING

An overview of the experimental setup at the CRYRING extraction beamline is presented in Figure 16 and Figure 17. The sample handling system in the CRYRING chamber contains a sample holder and a load lock. The sample holder is a customized 5-axis manipulator with space for two samples or for one sample and a beam screen (chrome-doped Al_2O_3). The load lock includes a transfer rod with a sample carrier, a WRG (Pfeiffer PKR 361), a turbo molecular pump (Pfeiffer HiPace 300, nominal pumping speed 260 l/s for N_2) and a quick access door.

At the main chamber, several vacuum pumps are installed. A turbo molecular pump (Pfeiffer HiPace 300) is used for pumping down. After the vacuum bake-out, the valve in front of the turbo pump is closed and the chamber vacuum is maintained by a sputter ion pump (Gamma Vacuum 500T DI TiTan Ion Pump, nominal pumping speed 400 l/s for N₂), a titanium sublimation pump (Gamma Vacuum) and a NEG pump (SAES CapaciTorr). The vacuum diagnostic consist of an extractor gauge (Leybold IE 514 with controller Leybold IM 540), a quadrupole mass spectrometer (Pfeiffer PrismaPlus QMG 220) and a WRG (Pfeiffer PBR 260). The base pressure is about 2E-9 mbar. In the beam tube connecting the irradiation chamber with the extraction beamline, a combination of SIP (Gamma Vacuum 75S DI TiTan Ion Pump, nominal pumping speed 60 l/s for N₂) and NEG pump (Gamma Vacuum N300, nominal pumping speed 43 l/s for N₂) is mounted together with a second WRG (Pfeiffer PBR 260) for vacuum monitoring.



Figure 16: Schematic view of the irradiation chamber at the CRYRING extraction beamline.



Figure 17: Photograph of the CRYRING setup, (1) quadrupole mass spectrometer, (2) extractor gauge, (3) load lock and (4) sputter ion pump. Beam direction is from right to left.

4 Methods

4.1 Thermal Desorption

4.1.1 Measurement Process and Data Analysis

Sample annealing and measurement of thermal desorption can be done in one procedure. The sample is transported from the load lock into the sample holder and the samples holder is placed in front of the aperture. The sample is heated with a linear temperature ramp of 6 K/min from room temperature to the desired annealing temperature, which is usually 400 °C. Then the temperature is kept constant. During the whole process, the temperature and the total and partial pressures are recorded. An example is shown in Figure 18. The quadrupole mass spectrometer (QMS) is used in the so-called "bar chart mode", where the center of each mass up to m/q 50 is scanned. During the heating up, the pressure evolution first shows a steep increase, starting when the adparticles have enough thermal energy to desorb. After a small local maximum, the pressure rises slower and reaches a global maximum before or at the end of the temperature ramp. After the global maximum, the pressure decreases exponentially and finally saturates. The pressure evolution determines the duration of the annealing process. The heater is switched of, when the total pressure falls below a value of approximately 1E-10 mbar. For the OFCu samples, this value is usually reached 4 h after the start of the temperature ramp.



Figure 18: Temperature (top) and pressure (bottom) evolution during the annealing process of a milled OFCu sample. The fluctuations in the total pressure are caused by small deviations (\pm 1 °C) in the ambient temperature due to the switching hysteresis of the air conditioning. Source: Velthaus et al. 2023 [Vel23].

The intensities measured by the QMS are displayed in mbar in the software, but these values do not correspond to the real partial pressures, because they are calculated based on a general sensitivity, which is equal for all masses. To determine true partial pressures, calibration measurements for individual gases were conducted. Gases, which are known to be important for desorption measurements, were injected into the vacuum chamber up to different pressures and the pressure was measured with the extractor gauge and the QMS. The extractor gauge is calibrated for nitrogen. To correct the pressure readings for the different electron

impact ionization probabilities of the gases, correction factors were applied. Except for argon, the correction factors were calculated from the quotient of the ionization cross section of the considered gas and the ionization cross section of nitrogen at 120 eV, as described in [Jou23]. 120 eV corresponds to the kinetic energy, which the electrons acquire by passing through the potential difference in the extractor gauge. The gas correction factors are listed in Table 5. For each gas the corrected pressure of the extractor gauge as a function of the pressure of the corresponding mass in the mass spectrum was fitted by the following power function

$$p(gas) = a \cdot p(QMS)^b \tag{35}$$

In theory, the relationship between the intensity measured by the QMS and partial pressure should be linear. However, there are always some non-linearities, which are better described by a power function.

Gas	Gas correction factor	Reference
H ₂	2.81	[Kim04]
H ₂ O	1.12	[Kim04]
СО	1.00	[Kim04]
CO2	0.69	[Kim04]
Ar	0.65	[Elk19]

Table 5: Gas correction factors for the extractor gauge

The sensitivity of the microchannel plate, which is used in the QMS as detector, is not constant over a longer time period. For this reason, a normalization factor was introduced. The normalization factor is determined for each individual calibration and desorption measurement. The normalization factor is chosen in such a way, that the curve of the sum of all scanned masses of the QMS multiplied with the normalization factor fits to the total pressure-time curve (cf. Figure 18) measured by the extractor gauge for the measurement under consideration. Each individual measurement has its own normalization factor.

Figure 19 and Table 6 and Table 7 show the results from the fits of the calibration measurements. These equations are used to calculate the real partial pressures. Conducting a calibration measurement with water vapor is very difficult. Therefore, for H_2O the calibration for N_2 was used corrected by the corresponding gas correction factor. For the calculation of the partial pressure of CO one extra step has to be done, because part of the molecules fragment in the QMS. For example, CO_2 breaks into CO and O. As a result, the signal at mass 28 contains a contribution from "real" CO and CO, which originates from fractured CO_2 . For calculating the partial pressure of CO₂ is determined using the following calibration equation for CO_2 and mass 44

$$p(CO_2) = a \cdot p(mass \, 44)^b \tag{36}$$

The contribution of CO_2 to mass 28 can be calculated using the inverse of the calibration equation of CO_2 and mass 28

$$p(mass \ 28 \ from \ CO_2) = \left[\frac{p(CO_2)}{a}\right]^{1/b}$$
(37)

The fraction of CO at mass 28 is the difference between the intensity at mass 28 and the fraction of CO₂

$$p(mass \ 28 \ from \ CO_2) = p(mass \ 28) - p(mass \ 28 \ from \ CO_2)$$
 (38)

With this value the partial pressure of CO is calculated using the calibration equation for CO

$$p(CO) = a \cdot p(mass \ 28 \ from \ CO)^b \tag{39}$$

For H₂ and Ar, equation (35) with the parameters for the corresponding gas is applied.



Figure 19: Calibration measurements for different gases and corresponding fit curves for 2019–2021. Note the double-logarithmic scale.

Gas	Recorded m/q	a	<i>a</i> error	b	b error
N ₂	28	0.1138	0.0031	0.8607	0.0016
СО	28	0.1513	0.0081	0.8753	0.0032
CO ₂	28	0.0673	0.1371	0.7672	0.1074
CO ₂	44	0.0366	0.0339	0.7802	0.0520
H ₂	2	0.4848	0.0609	0.9565	0.0072
Ar	40	0.2216	0.0050	0.8980	0.0013

Table 6: Parameters for the calculation of the real partial pressures for the TDS-setup for 2019-2021

Table 7: Parameters for the calculation of the real partial pressures for the TDS-setup for 2022

Gas	Recorded m/q	a	<i>a</i> error	b	b error
N ₂	28	2.3948	0.4798	1.0072	0.0114
СО	28	1.0585	0.2348	0.9565	0.0126
CO2	28	45.0553	8.4778	1.0929	0.0098
CO2	44	0.2766	0.0367	0.8767	0.0073
H ₂	2	4.5090	2.4851	1.0513	0.0305
Ar	40	1.0707	0.0539	0.9650	0.0028

To compare the results of the thermal desorption measurements quantitatively, first the pressure increase Δp is determined by baseline subtraction. Then the calibration equations are applied and the pressure curves of selected masses (2, 18, 28, 40 and 44) and the total pressure are integrated. The integration interval starts at 40 °C sample temperature and has a duration of 6000 s. Afterwards the results are converted into the amount of desorbed gas Q per surface area A

$$\frac{Q}{A} = \frac{\int \Delta p(t) \cdot S_{eff} dt}{A}$$
(40)
A corresponds to the area of the aperture, which is $A = 0.785 \ cm^2$. S_{eff} is the effective pumping speed. Its determination is described in chapter 3.1. During a measurement, S_{eff} is assumed to be constant. Therefore, the equation simplifies to

$$\frac{Q}{A} = \frac{S_{eff}}{A} \int \Delta p(t) dt \tag{41}$$

For the calculation of the experimental errors, Gaussian error propagation was used. This was done in two steps. First, the errors of the partial pressures were calculated as follows

$$\Delta(p(gas)) = \sqrt{[p(QMS)^b \cdot \Delta a]^2 + [a \cdot \ln(b) \cdot p(QMS)^b \cdot \Delta b]^2 + [a \cdot b \cdot p(QMS)^{b-1} \cdot \Delta p(QMS)]^2}$$
(42)

 Δa and Δb result from the fits and are listed in Table 6 and Table 7. $\Delta p(QMS)$ is assumed to be ±20 %. This is a conservative estimation of the typical standard deviation of a mean value calculated for a constant pressure. In the second step the errors for the amount of desorbed gas are calculated

$$\Delta(Q/A) = \sqrt{\left[\frac{p_{int}}{A} \cdot \Delta S_{eff}\right]^2 + \left[\frac{S_{eff}}{A} \cdot \Delta p_{int}\right]^2 + \left[-\frac{S_{eff} \cdot p_{int}}{A^2} \cdot \Delta A\right]^2}$$
(43)

 p_{int} is the value of the integral $\int \Delta p(t) dt$. The relative error of p_{int} is the same as the relative error of $\Delta p(t)$, which results from equation (42). ΔS_{eff} is assumed to be ±20 %. ΔA is ±0.015 cm², which corresponds to a diameter uncertainty of ±0.1 mm. The mean relative errors are listed in Table 8. The errors of each individual measurement are shown in Table 26 to Table 30 in the appendix.

Table 8: Mean relative errors of the TDS measurements in percent

	Total pressure	H ₂	H ₂ O	СО	CO ₂	Ar
Mean relative	28.4	35.4	27.9	28.5	85.9	27.2
error [%]						

4.1.2 Simulation of Thermal Desorption

To analyze the influence of different parameters on the thermal desorption measurements, the pressure increase during TDS was simulated. The simulation is based on Fick's second law (cf. equation (23)) in 1D space

$$\frac{\partial c(x,t)}{\partial t} = D(t) \cdot \frac{\partial^2 c(x,t)}{\partial x^2}$$
(44)

with

$$D(T(t)) = D_0 \cdot \exp\left(-\frac{E_{diff}}{R \cdot T(t)}\right)$$
(45)

For the simulation the software MATLAB [Mat21] was used. It offers a solver for parabolic or elliptical partial differential equations of type

$$u\left(x,t,c,\frac{\partial c}{\partial x}\right)\frac{\partial c}{\partial t} = x^{-m_{PDE}}\frac{\partial}{\partial x}\left(x^{m_{PDE}}f\left(x,t,c,\frac{\partial c}{\partial x}\right)\right) + s\left(x,t,c,\frac{\partial c}{\partial x}\right)$$
(46)

where $f\left(x, t, c, \frac{\partial c}{\partial x}\right)$ is a flux term and $s\left(x, t, c, \frac{\partial c}{\partial x}\right)$ a source term. m_{PDE} is 0, 1 or 2 for planar, cylindrical or spherical geometry, respectively. For the problem treated here, planar geometry was used ($m_{PDE} = 0$) and the terms are

$$u = 1, \qquad f = D \frac{\partial c}{\partial x}, \qquad s = 0$$
 (47)

The boundary conditions have to adopt the following form

$$p(x,t,c) + q(x,t)f\left(x,t,c,\frac{\partial c}{\partial x}\right) = 0$$
(48)

where p und q have to be defined in the simulation code. f corresponds to the flux term in the partial differential equation (cf. equation (46) and (47)). The left boundary is the surface facing the vacuum. Here desorption is assumed. Therefore, the boundary condition is

$$p(x = 0, t, c) = j$$

$$q(x = 0, t) = -1$$
(49)

because $f = D \frac{\partial c}{\partial x}$ and according to Fick's first law $j = -D \frac{\partial c}{\partial x}$. At the surface, j is equal to the desorbing particle flux. To calculate the desorbing particle flux, first the volumetric particle concentration c at the surface is converted into an areal particle density σ by integrating the particle concentration in a defined surface layer with thickness $x_{surface}$ over the x-direction

$$\sigma(t) = \int_0^{x_{surface}} c(x, t) dx$$
(50)

 $x_{surface}$ is set to 3 nm, which corresponds to approximately 10 atomic layers. In this small depth interval, the particle concentration can be assumed to be constant. Therefore, the equation (50) simplifies to

$$\sigma(t) = c(x=0,t) \int_0^{x_{surface}} dx = c(x=0,t) \cdot x_{surface}$$
(51)

The desorption rate j is determined by the Polanyi-Wigner equation (cf. equation (13)) for second-order desorption

$$j(t) = \frac{\nu_{dif}}{\sigma_s} \cdot \sigma^2(t) \cdot \exp\left(-\frac{E_{des}}{R \cdot T(t)}\right)$$
(52)

Second-order desorption was chosen, because the simulation focuses on hydrogen and for desorption of hydrogen, two atoms have to recombine to a hydrogen molecule. For v_{dif} , the approach $v_{dif} = kT/h$ [Wis91] was chosen

$$j(t) = \frac{k \cdot T(t)}{h \cdot \sigma_s} \cdot \sigma^2(t) \cdot \exp\left(-\frac{E_{des}}{R \cdot T(t)}\right)$$
(53)

The number of adsorption sites σ_s is assumed to be equal to the number of adparticles in one monolayer $\sigma_s = \sigma_{mono} = 1 \cdot 10^{19} \ particles/m^2$. The values calculated for ν_2 with this approach agree well with the values reported in the literature [Red93]. For the temperature the following condition applies

$$T(t) = \begin{cases} t \cdot a_{ramp} + 273 \, K & \text{for } t < T_{max}/a_{ramp} \\ T_{max} + 273 \, K & \text{for } t \ge T_{max}/a_{ramp} \end{cases}$$
(54)

where a_{ramp} is the slope of the temperature ramp in K/s. T_{max} is the final temperature of the sample in °C. The right boundary at x = d, where d is the samples thickness, is assigned to be the backside of the sample, which is attached to the sample holder. Therefore, no particle flux across this boundary occurs and the boundary condition is

$$p(x = d, t, c) = 0$$

$$q(x = d, t) = 1$$
(55)

The initial condition is the particle concentration in the sample

$$c(x,t=0) = c_0(x)$$
(56)

To run the simulation, first the MATLAB-function "pdepe" is called using equations (47), (49) and (56). This function solves the partial differential equation and returns the particle concentration c for the defined steps

in position and time. Afterwards the function "pdeval" is used to calculate the derivative of the concentration with respect to the position $\partial c/\partial x$. Fick's first law is applied to determine the diffusion rate

$$j_{dif}(x,t) = \left| -D(T(t)) \cdot \frac{\partial c}{\partial x}(x,t) \right|$$
(57)

Equation (54) gives the temperature, which is needed to calculate the diffusion coefficient D(T(t)) by means of equation (45). The particle flux out of the sample $j_{out}(t)$ is determined by the following equation

$$j_{out}(t) = A \cdot j_{dif}(x = 0, t) \tag{58}$$

where A is the sample surface. Finally, the pressure increase can be calculated

$$\Delta p(t) = \frac{j_{out}(t) \cdot k \cdot T_{chamber}}{S_{eff}}$$
(59)

k is the Boltzmann constant, $T_{chamber}$ the temperature of the vacuum vessel and S_{eff} the effective pumping speed. The total number of desorbed particles N_{tot} can be determined by integrating the desorbing particle flux over time

$$N_{tot} = \int_{t=0}^{t_{end}} j_{out}(t) \, dt$$
 (60)

This is realized by a trapezoidal numerical integration. The total number of desorbed particles can then be converted into a total amount of desorbed gas per surface area

$$\frac{Q}{A} = \frac{N_{tot} \cdot k \cdot T_{chamber}}{A}$$
(61)

When applying suitable integration limits, this quantity can be compared to the results of the TDS measurements. The code of the simulation can be found in chapter 11.2 in the appendix.

To examine the different contribution of desorption and diffusion, two more models are tested: (i) a model applying only thermal desorption from a partially covered surface and (ii) a model assuming that every diffusing particle which reaches the surface is released immediately to the vacuum. The simulation of desorption without diffusion is based on the Polanyi-Wigner equation for second-order desorption (equation (53)). The ordinary differential equation is solved using the MATLAB-solver "ode15s". For the initial condition, the surface coverage of the sample has to be known. The coverage θ as a function of the vacuum pressure in the chamber $p_{chamber}$ is defined by adsorption isotherms. For low coverages, the coverage is proportional to the pressure, which is described by the Henry adsorption isotherm [Jou18b]

$$\theta = \frac{s_0 \tau_0 \exp\left(\frac{E_{des}}{RT_{sample}}\right)}{\sigma_{mono}\sqrt{2\pi m_0 k T_{gas}}} \cdot p_{chamber}$$
(62)

where s_0 is the sticking coefficient, σ_{mono} the number of adparticles in one monolayer and m_0 the molecular mass. T_{sample} and T_{gas} are the temperature of the sample or gas, respectively. $\tau_0 = \frac{1}{\nu_1} = \frac{h}{kT}$ is the period of the lattice oscillations. The resulting initial condition is

$$\sigma(x,t=0) = \theta \cdot \sigma_{mono} \tag{63}$$

To model the second case, where all particles reaching the surface are immediately desorbed, the boundary condition for the surface facing the vacuum is changed to

$$p(x = 0, t, c) = c(x = 0, t) - n_0$$

$$q(x = 0, t) = 0$$
(64)

This means that at the surface a constant particle concentration n_0 is applied, which is determined from the base pressure in the vacuum chamber $p_{chamber}$ as

$$n_0 = \frac{p_{chamber}}{kT} \tag{65}$$

This is a simplification, because in reality the pressure in the vacuum chamber changes during the experiment. It will be shown in the results that in the important range from 1E-11 to approximately 3E-8 mbar the chamber pressure has no influence.

4.2 Ion-Stimulated Desorption

4.2.1 Continuous Bombardment Method (M-branch)

For the ISD measurements at the M1 beamline of the M-branch, the samples were irradiated with 4.8 MeV/u calcium and gold ions of various charge states (Ca¹⁰⁺, Ca¹⁹⁺, Au²⁵⁺, Au²⁶⁺ or Au⁵²⁺). To avoid cleaning of the samples by the ion beam (beam scrubbing), the irradiation duration was limited to 2 min. The samples were irradiated under 45° beam incidence, because the sample holder has to be compatible with another experiment.

The beam current was measured using the two Faraday cups available in the setup. The front cup is located in front of the beam slits and has a fast pneumatic drive. The rear cup is placed behind the sample in the load lock and moved by a stepper motor. For a desorption measurement, first the beam current was measured using the front cup. Then the cup was moved out, the beam hit the sample and desorption was measured. After 2 min the front cup was moved back into the beam to stop the irradiation of the sample and to measure again the beam current. The current value used for data analysis is the mean value of the current reading before and after sample irradiation. The stability of the beam intensity during irradiation was monitored by recording the current of the beam halo on an aperture in front of the setup (not shown in Figure 12). Because of limited space at the beamline, the slits are located behind the front Faraday cup. Thus, the current reading does not correspond to the current at the sample if the beam is cut by the slits. In this case, the rear cup was used to determine the transmission of the slits. The ion current on the sample was calculated by multiplying the current reading from the front cup with the transmission factor.



Figure 20: Representative evolution of the pressure as a function of time during the irradiation of a plasma electrolytic polished OFCu sample for the total pressure and selected masses.

At the M-branch, desorption was measured under continuous bombardment. The ion pulses arrive with a repetition rate of several Hz. This is much faster than the time, which the pressure needs to recover after an individual ion pulse. Therefore, an equilibrium state is reached, where the flow of desorbed gas and the flow of gas pumped from the chamber result in a constant pressure. The pressure increase is measured with the extractor gauge and the QMS. For the ISD measurements, the QMS is set to the so-called "peak jump mode", where only selected masses are recorded to speed up the acquisition of one scan cycle. The recorded masses were 1, 2, 12, 14, 16, 17, 18, 28, 29, 32, 40 and 44, which correspond to the relevant gases H₂, H₂O, CO, CO₂ and Ar and their fragments. An example for the pressure evolution during an ISD measurement is shown in Figure 20. The calibration of the QMS and the calculation of the partial pressures were done as described for the thermal desorption measurements in chapter 4.1.1. The only difference is that no normalization factor was needed here, because for each beam time a new calibration measurement was conducted. The results of the fits of the calibration measurements are presented in Table 9.

Gas	Recorded m/q	Beam time	a	<i>a</i> error	b	b error
N ₂	28	2019	4.86E+01	1.72E+01	1.039	0.0183
N ₂	28	2020	1.29E+03	1.23E+02	1.343	0.0254
N ₂	28	2021	2.51E+05	1.57E+05	1.694	0.0366
N ₂	28	2022	4.94E+04	3.50E+04	1.567	0.0408
СО	28	2019	4.74E+01	1.02E+01	1.043	0.0112
СО	28	2020	1.13E+03	1.05E+02	1.343	0.0254
СО	28	2021	2.01E+03	1.10E+03	1.430	0.0318
СО	28	2022	2.73E+04	1.88E+04	1.534	0.0396
CO2	28	2019	7.21E+01	1.74E+00	1.003	0.0012
CO2	28	2020	2.89E+03	1.81E+02	1.343	0.0254
CO ₂	28	2021	2.45E+01	3.01E+00	1.073	0.0064
CO2	28	2022	5.34E+02	3.15E+02	1.215	0.0311
CO2	44	2019	3.21E+01	8.88E+00	0.998	0.0139
CO2	44	2020	1.62E+03	1.36E+02	1.343	0.0254
CO2	44	2021	4.07E+02	1.96E+02	1.308	0.0270
CO2	44	2022	2.50E+04	2.16E+04	1.515	0.0489
H ₂	2	2019	1.88E+02	5.22E+01	1.094	0.0136
H ₂	2	2020	1.62E+03	1.36E+02	1.343	0.0254
H ₂	2	2021	1.45E+05	1.01E+05	1.571	0.0394
H ₂	2	2022	1.45E+05	1.01E+05	1.571	0.0394
Ar	40	2021	1.91E+01	2.01E+00	1.096	0.0058

Table 9: Parameters for the calculation of the real partial pressures at M1 for various gases and beam times

To determine the desorption yield η , the number of desorbed molecules is calculated from the measured pressure increase Δp using the ideal gas law

$$\eta = \frac{\Delta p \cdot V}{N_{ion} \cdot k \cdot T} \tag{66}$$

with V as vessel volume and N_{ion} as number of impacting ions. k is the Boltzmann constant and T the absolute temperature. This equation is only valid for a single ion pulse. To calculate the desorption yield under continuous bombardment, the equation has to be differentiated in time

$$\eta = \frac{\Delta p \cdot \frac{dV}{dt}}{\frac{dN_{ion}}{dt} \cdot k \cdot T}$$
(67)

 $\frac{dV}{dt}$ is the pumped volume, which correspond to the effective pumping speed S_{eff} . $\frac{dN_{ion}}{dt}$ is the number of ions per time interval, which is calculated from the beam current I_{beam} on the sample

$$\frac{dN_{ion}}{dt} = \frac{I_{beam}}{q_{ion} \cdot e} \tag{68}$$

where q_{ion} is the ion charge state and e the elementary charge. When combining equation (67) and (68), the desorption yield during continuous bombardment can be calculated from the measured quantities

$$\eta = \frac{\Delta p \cdot S_{eff} \cdot q_{ion} \cdot e}{I_{beam} \cdot k \cdot T}$$
(69)

To determine the pressure increase Δp , in each pressure curve the baseline is subtracted and afterwards mean value and standard deviation over the constant region of the pressure increase are calculated. If no constant region exists, a small region in the area of the maximum pressure was chosen. Then the calibration equations are applied to calculate the partial pressures. Finally, with the derived values and equation (69) the desorption yields are calculated.

The errors of the partial pressures $\Delta(\Delta p)$ are calculated analogously to the ones of thermal desorption (cf. chapter 4.1.1). As error of the QMS values, the standard deviation of the mean values are used. The errors for the desorption yields are calculated as follows

$$\Delta \eta = \sqrt{\left[\frac{S_{eff} \cdot q_{ion} \cdot e}{I_{beam} \cdot k \cdot T} \cdot \Delta(\Delta p)\right]^{2} + \left[\frac{\Delta p \cdot q_{ion} \cdot e}{I_{beam} \cdot k \cdot T} \cdot \Delta S_{eff}\right]^{2} + \left[-\frac{\Delta p \cdot S_{eff} \cdot q_{ion} \cdot e}{I_{beam}^{2} \cdot k \cdot T} \cdot \Delta I_{beam}\right]^{2}}$$
(70)
$$+ \left[-\frac{\Delta p \cdot S_{eff} \cdot q_{ion} \cdot e}{I_{beam} \cdot k \cdot T^{2}} \cdot \Delta T\right]^{2}$$

 ΔS_{eff} is conservatively assumed to be ±15 % and ΔI_{beam} = ±10 %. The temperature is 296 ± 3 K. Table 10 shows the mean relative errors for each gas for the different beam times. The errors change from beam time to beam time, because they are dominated by the errors of the parameters used in the calibration. The errors for each individual measurement can be found in Table 31 to Table 41 in the appendix.

	Beam time 2019	Beam time 2020	Beam time 2021	Beam time 2022
Total pressure	18.1	18.1	18.1	18.1
H ₂	40.8	40.1	75.6	73.4
H₂O	44.4	28.6	68.1	74.8
CO	28.5	22.6	58.0	71.4
CO ₂	33.9	21.4	51.6	88.6

Table 10: Mean relative errors of the desorption yields in percent for the different gases and beam times

4.2.2 Single Shot Method (CRYRING)

Desorption measurements were performed at CRYRING for the first time. The experiment was part of the commissioning phase of the extraction beamline and had the primary goal to test if desorption measurements are possible under the confined beam conditions (i.e. low beam intensity and low repetition rate). Future scientific objectives will focus on desorption measurements with ions of different kinetic energies and high charge states. Due to the high energy loss of highly charged ions, huge desorption yields may result in a severe degradation of the dynamic vacuum even at low beam intensities.

At CRYRING, the samples were irradiated with hydrogen-like gold ions (Au⁷⁸⁺) at three different energies (2, 3 and 4.8 MeV/u). The beam hit the samples under perpendicular incidence. For the desorption measurements at CRYRING, the so-called single shot method was used, because of the low repetition rate. Thereby the

pressure increase of each individual ion pulse was recorded. The acquisition of the pressure values had to be carried out with a high frequency to capture the maximum of the pressure pulse. Commercial vacuum gauge controllers are not designed for fast measurements. At UHV conditions, the controller IM 540 used at CRYRING can only record one data point every 800 ms. Therefore, a fast triggered pressure measurement was implemented.

The pressure was measured with the extractor gauge. In an extractor gauge, electrons are accelerated between a circular cathode and an anode cage to 120 eV. The electrons ionize gas molecules. The gas ions are extracted by the electric filed in the gauge to an ion catcher and create there an electric current, which is measured by the gauge controller. The pressure p is proportional to the measured ion current I_{ion} and to the reciprocal of the electron emission current I_{emis}

$$p = \frac{I_{ion}}{I_{emis} \cdot C_{EXT}} \tag{71}$$

The proportionality constant is the reciprocal of the calibration factor C_{EXT} , which is unique for each gauge and provided by the manufacturer. For the extractor gauge at CRYRING, the emission current is 1.592 mA and the calibration factor is 5.16 mbar⁻¹. The base pressure of 1.7E-9 mbar corresponds to a current reading of approximately 18 pA, which increased up to 45 pA during irradiation.

For the fast pressure measurements, the ion current produced in the gauge was recorded using a femtoammeter (Keithley 6514 System Electrometer). The controller only served to provide the supply voltages. The data acquisition with the ammeter was started by a trigger pulse from the accelerator. As trigger event, the beginning of the so-called pre-extraction beam process was used. The duration of the pre-extraction was set to 0.4 s. This allowed collecting a few data points before the beam pulse arrived to determine the background pressure. The trigger signal started the acquisition of 100 data points. The integration time of the A/D converter in the femtoammeter was set to 20 ms, which turned out to be a good compromise between speed and signal noise. An acquisition rate of 14.8 Hz was achieved. The range of the ammeter was set to 200 pA. During acquisition, the values were stored in the buffer of the instrument. Afterwards the data points were read out by a PC, stored in a file and the ammeter was initialized for the next measurement. During data analysis, the measured current values were converted into pressure values using equation (71). The pressure increase was determined calculating the difference between the maximum of the pressure pulse and the mean value of the data points before the pressure increase. The pressure increase could only be detected by the extractor gauge. For the QMS, the pressure pulse was below the detection limit due to the low beam intensity.

The extraction beamline at CRYRING houses a Faraday cup, but this cup cannot be used, because the electromagnetic pulse of the kicker magnet, which extracts the beam, disrupts the beam current measurement. Therefore, the number of Au^{78+} ions in the ring was measured by a calibrated beam transformer (YR08DT1ML). Figure 21 shows the typical evolution of the beam intensity during an accelerator cycle. After injection of the ion bunch delivered by the ESR with 10 MeV/u, the beam is cooled while the number of particle stays almost constant. During the deceleration process to 2, 3 or 4.8 MeV/u, the intensity decreases. The amount of lost ions depends on the final energy. Then the beam is cooled again and afterwards extracted to the target. The number of ions per pulse impacting on the sample was determined from the number of ions in the ring before the extraction multiplied with the extraction efficiency. The latter parameter was deduced from an earlier beam time, where track etching technology was used. A polyethylene terephthalate and a polycarbonate foil were irradiated, while each ion creates a track of damaged material in the foil. These tracks were etched selectively in NaOH forming nanopores. The number of pores was counted using SEM images. Comparing the fluence on the sample with the total number of ions, which were in the ring before the extraction, for all pulses hitting the sample, the extraction efficiency was determined to be $54 \pm 10 \%$ [Vom21]. This is a mean value. There is no information available about the pulse-to-pulse deviation.

The desorption yield for each ion pulse is calculated using equation (66). The volume was determined using the physical dimensions of the vacuum vessel. For each sample and beam energy, mean value and standard deviation of the desorption yield over all recorded ion pulses were calculated.



Figure 21: Number of Au⁷⁸⁺ ions in CRYRING during one accelerator cycle measured by the beam transformer. After injection, the beam is cooled while the number of particle stays almost constant. During the deceleration process, the intensity decreases. Finally, the beam is cooled again and extracted to the target.

5 Samples

5.1 Sample Materials

For the samples, materials typically used for the production of accelerator components were selected. Copper was chosen, because it has at high electrical and thermal conductivity. Therefore, the energy deposited by the incoming ions is rapidly spread in the bulk reducing the temperature increase. The high melting temperature of tungsten is of interest for accelerator components exposed to very high beam intensities like beam dumps or the production target for rare isotopes at SPIRAL2 [Ben15]. Aluminum alloys are promising candidates for the manufacturing of vacuum chambers, because of their very low outgassing rates [Mal20c], their high electrical and thermal conductivity and their lightness. Stainless steel is widely used for any vacuum components, because of its mechanical strength, corrosion resistance and the easy processing [Mal20c].

5.2 Sample Preparation

5.2.1 Copper and Tungsten Sheet Samples

Samples denoted as "sheet samples" are cut from 1 mm thin sheets. They have the shape of Omicron sample plates (Figure 22) with $18x15x1 \text{ mm}^3$ size. All copper samples are made out of rolled oxygen-free copper (OFCu, purity 99.95%) sheets. The tungsten has a purity of 99.95%. For each material, a series of six samples with different surface treatments was produced for the beam time in 2019. The first sample was just cleaned in isopropanol in an ultrasonic bath for about 15 min. The applied treatment steps for the other samples are listed in Table 11 in the sequence as they were applied. For the sheet samples, lapping was carried out with alumina and polishing with diamond abrasive. For etching, the samples were inserted in $C_2H_2O_4$ (0.2 mol/l, room temperature) until a shiny surface became visible. After the etching, the samples were rinsed with pure water. All samples were prepared by the GSI target lab. For both materials, two sample series were prepared one without and one with annealing at 400 °C. The annealing was done as described in chapter 4.1.1.

Sample No.	Lapping	Etching	Polishing	Final etching
1				
2	х			
3	х			х
4	х		х	
5	х	х	х	
6	х	х	х	х

Table 11: Overview of the surface treatment procedures, which were applied to the OFCu and tungsten sheet samples

According to DIN 8589-15, lapping is defined as chipping with loose grains distributed in a fluid or paste guided over a usually sharp-transferring counterpart featuring undirected cutting paths of the grains [DIN03]. Lapping produces very planar surfaces. Material removal is caused by rolling grains and by grains, which are temporally fixed in the lapping disk [Klo09]. The overlapping indentations of the lapping grains induce a crater-like microstructure (cf. Figure 25b and Figure 26b).

For polishing, no exact definition exists. Similar to lapping, typically abrasive particles finely dispersed in a liquid medium are moved over the workpiece surface. Polishing particles are much smaller than abrasive particles for lapping. The smoothing mechanisms are different and still not fully understood. According to various theories, smoothening could be caused by abrasive removal of material, by plastic deformation or by chemical reactions [Klo09].



Figure 22: Photograph of the sample series with different surface treatments, top row: tungsten, lower row: oxygen-free copper.

5.2.2 Milled and Polished Copper Samples

All other OFCu samples (denoted as "disk samples") have a size of 15x13x4 mm and were cut from a 6.35 mm thick OFCu disk. To remove impurities in the surface from the manufacturing, the samples were milled to a thickness of 4 mm (Figure 23). During milling, material is removed by a rotating, usually multi-tooth cutting tool [Klo11]. The final milling step was done with a diamond milling tool. The samples were cleaned in an ultrasonic isopropanol bath for at least 15 min.

For the beam time 2020, different surface treatments were applied to these samples. Four samples were prepared again by the GSI target lab by lapping, polishing or lapping and polishing (Figure 23) as described in chapter 5.2.1. In comparison to lapping, polishing is a process, which is not standardized. Therefore, different polishing methods were tested. Seven samples were polished with calcium carbonate ("Wiener Kalk"). The company "Breidert Galvanik GmbH" polished another seven samples using silicon carbide. Additionally, in 2021 four samples were treated by plasma electrolytic polishing by the company "plasotec GmbH". During plasma electrolytic polishing, the samples are inserted in an aqueous ammonium sulfate solution [pla22]. When applying a voltage >200 V, discharges occur at the sample surface, which acts as anode. A vapor skin is formed around the workpiece in which a plasma layer builds up. The material is removed by electrochemical reactions, plasma reactions and hydrothermal reactions [Nes16].



Figure 23: Light microscopy images of OFCu samples as milled (left) and after additional lapping and diamond polishing (right).

5.2.3 Coated Samples

During the beam time in 2021, OFCu samples, which were first milled and afterwards coated with titanium nitride or amorphous carbon, were investigated. TiN was chosen because it exhibits low thermal outgassing rates [Mam14]. Amorphous carbon is used in proton accelerators, because of its low secondary electron yield [Val11]. The coatings were produced by the GSI target lab by sputtering with argon as process gas. Two different layer thicknesses were prepared: 200 and 500 nm. Before coating the OFCu samples were cleaned with oxalic acid and pure water and subsequently in a glow discharge. For each material and layer thickness, three different samples were prepared: (i) without annealing, (ii) with annealing before coating and (iii) with annealing after the coating. This was done to disentangle the contributions to desorption from the substrate and the coating layer.

Four stainless steel samples (304 / 1.4301) were coated with a non-evaporable getter (NEG). For this work, an alloy of titanium, zirconium and vanadium was used as NEG. The samples were coated by DC magnetron sputtering with krypton as process gas. The samples were prepared by the vacuum department at GSI. The layers have a composition of approximately 35 % titanium, 36 % zirconium and 29 % vanadium and a thickness of about 2.5 μ m [Bel07]. To pump gases by sorption, the NEG film has to be activated by a bake-out process typically at 180 °C for 24 h [Mal20b]. Three different heat treatments were applied to the samples. The first sample was measured "as received" without heat treatment. The second sample was annealed for 3.6 h at 400 °C according to the annealing process described in chapter 4.1.1. The third sample was activated only exsitu in the TDS-setup at 180 °C for 24.4 h. The fourth sample was first activated ex-situ in the TDS-setup at 180 °C for 24.4 h. The fourth sample was performed with Au²⁵⁺ ions, followed by a second in-situ activation in the irradiation chamber at 177 °C for 13.8 h and a second ISD measurement with Au²⁵⁺ ions. For the subsequent calcium beam time, the fourth sample was activated again in-situ in the irradiation chamber at 177 °C for 25.2 h one day before the ISD measurement with Ca¹⁰⁺.

5.2.4 Sputter Cleaning

Another desorption study was conducted on samples, which were pre-cleaned by irradiation with keV argon ions. For the preparation of the samples for the beam time 2021, an extractor ion source (SPECS IQE 11/35 with power supply PU-IQE11) was used. Because of a failure of this source, the samples for the beam time 2022 were prepared using a homemade cold cathode ion source. Both ion sources provide Ar^+ ions with energies up to 5 keV. At 5 keV the extractor ion source delivers beam currents about 9 μ A and the cold cathode ion source about 5 μ A. During the preparation of the sputter cleaned samples, different parameters were tested. The following parameters were changed: (i) substrate material, (ii) ion energy, (iii) incidence angle and (iv) irradiation time, which results in different ion fluences. In addition, some of the samples were annealed after sputter cleaning. Table 12 to Table 15 specifies the parameters, which were used for each sample arranged according to the different beam time blocks. The incidence angle is defined with respect to the surface normal, i.e. 0° means perpendicular incidence. For the extractor ion source, the distance between ion source and sample was 310 mm. For the cold cathode ion source, it was 120 mm in the standard configuration. For the preparation of the samples with 60° incidence angle, deflection plates had to be installed in order that the argon beam still hit the sample center. This increased the sample distance to 300 mm.

During the preparation of the samples for the beam time 2021, no online current measurement was available. The beam current was measured with a Faraday cup before and after the sputter process. Due to the different distances between ion source and sample and ion source and Faraday cup, it is not clear if the current in the Faraday cup and on the sample are in good agreement. It was also very difficult to determine the size of the beam spot. Therefore, the data on ion fluence has very large uncertainties for the samples prepared in 2021. For the sample preparation for the beam time 2022, the samples were connected to an ammeter to measure the ion current during the sputter process. An aperture in front of the sample biased at -30 V suppressed the

emission of secondary electrons and therefore improved the accuracy of the current measurement. More details about the sample preparation can be found in [Gre21] for 2021 and [Reh23] for 2022.

Sample No.	Substrate	lon energy [keV]	Ion incidence angle	Ion fluence [ions/cm ²]	Comments
8-16	OFCu milled	5	30°	2.96E18	ISD measurement before and after annealing
5-5	OFCu polished (CaCO ₃)	5	30°	2.94E18	ISD measurement before and after annealing
5-20	OFCu polished (SiC)	5	30°	2.92E18	

Table 12: Sputter cleaned samples for the gold beam time 2021

Table 13: Sputter cleaned samples for the calcium beam time 2021

Sample	Substrate	Ion energy	Ion incidence	Ion fluence	Comments
No.		[keV]	angle	[ions/cm ²]	
8-16	OFCu milled	5	30°	2.96E18	after annealing
5-5	OFCu polished (CaCO ₃)	5	30°	2.94E18	after annealing
5-20	OFCu polished (SiC)	5	30°	2.92e18	
8-17	OFCu milled	5	30°	1.17E18	ISD measurement before and after annealing
8-18	OFCu milled	5	30°	2.21E18	ISD measurement before and after annealing
8-19	OFCu milled	5	30°	3.67E18	ISD measurement before and after annealing
8-20	OFCu milled	5	30°	4.35E18	ISD measurement before and after annealing
8-21	OFCu milled	5	45°	3.29E18	
8-22	OFCu milled	5	45°	3.29E18	
8-23	OFCu milled	5	0°	3.40E18	

Table 14: Sputter cleaned samples for the calcium beam time 2022

Sample No.	Substrate	lon energy [keV]	Ion incidence angle	lon fluence [ions/cm ²]	Comments
8-20	OFCu milled	5	30°	4.35E18	after annealing, sample from 2021
8-23	OFCu milled	5	90°	3.40E18	sample from 2021
12-3	OFCu milled	5	0°	1.57E17	
12-2	OFCu milled	5	0°	2.36E17	
12-4	OFCu milled	5	0°	2.95E17	
12-9	OFCu milled	5	0°	2.99E17	
12-6	OFCu milled	5	0°	3.90E17	
12-7	OFCu milled	5	0°	4.68E17	
12-1	OFCu milled	5	0°	1.03E18	
12-11	OFCu milled	3	0°	3.02E17	
12-10	OFCu milled	4	0°	3.02E17	

12-24	Copper single	5	0°	3.02E17	
	crystal				
11-5	Al6061	5	0°	3.02E17	
11-6	Al6061	5	0°	1.03E18	

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Table 15: Sputter	cleaned s	samples	for the	gold beam	time 2022

Sample	Substrate	Ion energy	Ion incidence	Ion fluence	Comments
No.		[keV]	angle	[ions/cm ²]	
8-20	OFCu milled	5	30°	4.35E18	after annealing, sample from
					2021
8-23	OFCu milled	5	90°	3.40E18	sample from 2021
12-14	OFCu milled	5	0°	1.96E16	
12-19	OFCu milled	5	0°	3.90E16	
12-18	OFCu milled	5	0°	7.85E16	
12-17	OFCu milled	5	0°	1.17E17	
12-3	OFCu milled	5	0°	1.57E17	
12-2	OFCu milled	5	0°	2.36E17	
12-4	OFCu milled	5	0°	2.95E17	
12-9	OFCu milled	5	0°	2.99E17	
12-6	OFCu milled	5	0°	3.90E17	
12-7	OFCu milled	5	0°	4.68E17	
12-1	OFCu milled	5	0°	1.03E18	
12-11	OFCu milled	3	0°	3.02E17	
12-10	OFCu milled	4	0°	3.02E17	
12-24	Copper single	5	0°	3.02E17	
	crystal				
11-5	Al6061	5	0°	3.02E17	
11-6	Al6061	5	0°	1.03E18	
12-13	OFCu milled	5	0°	1.96E16	sample distance 300 mm
12-16	OFCu milled	5	0°	3.91E16	sample distance 300 mm
12-15	OFCu milled	5	0°	7.79E16	sample distance 300 mm
12-12	OFCu milled	5	0°	1.17E17	sample distance 300 mm
12-22	OFCu milled	5	60°	3.90E16	sample distance 300 mm
12-21	OFCu milled	5	60°	7.79E16	sample distance 300 mm
12-20	OFCu milled	5	60°	1.17E17	sample distance 300 mm

The here applied sputter cleaning process is similar to glow discharge cleaning, which is used for the conditioning of accelerator vacuum vessels. For the glow discharge cleaning, one or more anodes are inserted into the vacuum chamber, while the vessel wall acts as cathode. When injecting gas into the vessel to a pressure of 5E-4 to 1E-2 mbar, a discharge can be created, which removes surface and near-surface impurities. Gases, which are typically used, are H₂, Ar, Ar/O₂, O₂ or He/O₂. The ion energies are in the order of 200 eV [Dyl88; Mat87], which is much lower that the energy of the ions from the ion source. The fluences are slightly higher in the order of 1E18–1E19 ions/cm² [Dyl88]. The glow discharge also offers higher current densities in the range of 10–100 μ A/cm². Glow discharge cleaning is caused by a combination of sputtering and ion- or neutral-stimulated desorption. This results in lower particle-stimulated desorption, which persists even after air exposure [Dyl88]. A problem of argon glow discharge cleaning is the subsequent desorption of implanted argon atoms [Mat87].

5.2.5 Other Samples

To analyze the influences of grain boundaries on the diffusion processes of the gas particles towards the surface, single crystals of copper were tested. The crystals have (100) orientation, a purity of 99.9999 %, a thickness of 1 mm and a diameter of 15 mm. They were polished to Rz<0.01 μ m surface roughness by the manufacturer "MaTeck Material Technologie & Kristalle GmbH". Two single crystals were measured in the beam time 2020, one without and one with annealing at 400 °C for 4.4 h.

Three other materials were investigated in 2020. The compound material tungsten-copper (WCu) was chosen because it combines typical properties of tungsten and copper such as high tensile strength and high thermal conductivity. WCu has a heterogeneous structure. By sintering of tungsten powder, first a porous blank is produced. Afterwards the pores are filled with liquid copper. Another production method is liquid-phase sintering [WHS14]. For this work, WCu with 25 ± 2 % copper was used (class D). The WCu samples were milled but without the surface finishing by the diamond tool, because of the great hardness of WCu.

Furthermore, samples from two different types of aluminum were measured. Al1050 is aluminum with 99.5 % purity. Al6061 (AlMg1SiCu) is an alloy, which is commonly used for the manufacturing of vacuum chambers. The surfaces of all aluminum samples were milled with the diamond tool. For the annealing of the aluminum samples, attention has to be paid to the vapor pressures of the alloying elements. For Al6061 the annealing temperature was thus limited to 100 °C, because of the high vapor pressure of magnesium. For one of the Al1050 samples the temperature was set to 280 °C, while for a second sample in 2021 400 °C was applied.

If not otherwise stated, all samples are stored in atmosphere. For the beam time 2022, eight samples were stored under argon atmosphere in an argon glovebox. The samples were shortly exposed to air for the transport from the TDS-setup to the glovebox and from the glovebox to the irradiation chamber at the M-branch. Further eight samples were stored in vacuum at approximately 10⁻⁸ mbar in a dedicated vacuum chamber. This setup does not have at load lock. Therefore, all stored samples were exposed to atmosphere for about 15 min, when new samples were put into the chamber. Three different storage durations were chosen: 3, 6 and 9 months for the calcium beam time. The gold beam time took place two months after the calcium beam time. Therefore, the storage time increased to 5, 7 and 11 months.

5.2.6 Samples for the Measurements at CRYRING

For the CRYRING measurements in 2022, five different samples were used. Because of the low beam intensities at CRYRING, samples with rather high desorption yields were selected. The first sample was a milled OFCu sample and the second one was lapped OFCu, as described in chapter 5.2.1 and 5.2.2, respectively. Furthermore, the lapped and etched OFCu sheet sample from the beam time 2019 (cf. chapter 5.2.1) and a TiN-coated OFCu samples with 500 nm layer thickness without annealing (cf. chapter 5.2.3) were tested. To achieve a very high desorption yield, a polycarbonate foil with 100 μ m thickness mounted on a stainless steel sample carrier was irradiated.

5.3 Sample Characterization

Several selected samples were analyzed by scanning electron microscopy (SEM) and atomic force microscopy (AFM). With AFM, five squares of $3x3 \ \mu m^2$ were scanned for each sample using tapping mode. By measuring a calibration sample with different precise known step heights, the AFM results were converted into height values. To compensate for tilts of the samples, for each square a mean plane was calculated and subtracted. An example of the height profile of the lapped and polished tungsten sample is shown in Figure 24a. For each square three different surface parameters were calculated: (i) arithmetical mean height *Sa*, (ii) mean

inclination angle δ_m and (iii) ration of true surface area to geometrical surface area $A_{relative}$. The arithmetical mean height is defined as

$$Sa = \frac{1}{N_{pixel}} \sum_{n=1}^{N_{pixel}} |h_n|$$
(72)

where h_n is the difference between the height of the n-th pixel and the mean height. N_{pixel} is the number of pixels.

For the calculation of the mean inclination angle and the true surface area, the height profile was divided into small triangles, where the vertices are defined by the measured pixels, as shown in Figure 24b. The triangle is spanned by the two vectors \vec{u} and \vec{v} . The normal vector of the triangle is

$$\overrightarrow{n_{\Delta}} = \overrightarrow{u} \times \overrightarrow{v} \tag{73}$$

The inclination angle δ is calculated as

$$\delta = \arccos\left(\frac{\overrightarrow{n_{\Delta}} \cdot \overrightarrow{n}}{|\overrightarrow{n_{\Delta}}||\overrightarrow{n}|}\right)$$
(74)

 \vec{n} is the normal vector of the measured square, here defined as a normal vector in z-direction. The mean inclination angle is the mean value of the inclination angle of all triangles. To determine the true surface area, the area of each triangle is calculated

$$A_{\Delta} = \frac{1}{2} |\vec{u} \times \vec{v}| \tag{75}$$

Then the area of all triangles is summed up. The true surface area is compared to the geometrical surface area

$$A_{relative} = \frac{A_{true}}{A_{geometrical}} - 1 \tag{76}$$

For each sample, the surface parameters are averaged over the five measured squares. The surface parameters of all samples measured with AFM are summarized in Table 25 in the appendix.



Figure 24: a) Topography of the lapped and polished tungsten sample as determined by AFM. The scale of the z-axis is magnified. b) Definition of the parameters used for the calculation of the inclination angle and the true surface area.



Figure 25: SEM images of various OFCu sheet samples, a) untreated, b) lapped, c) lapped and etched, d) lapped and polished, e) lapped, etched and polished, f) lapped, etched, polished and etched. Note the different magnifications.

The scanning electron microscopy (SEM) images of the analyzed samples show characteristic surface features, as presented in Figure 25 for OFCu sheet samples pretreated by different combinations of lapping, etching and polishing. The untreated sample (Figure 25a) has the least textured surface with a rather small roughness of Sa = 19 nm. The lapping process results in a very rough surface as seen in the SEM image (Figure 25b) and confirmed by an AFM measurement (Sa = 77 nm). Subsequent polishing smoothes the surface again (Figure 25d). The polished surfaces exhibit a grainy structure. Most of the grains were identified by energy-dispersive X-ray spectroscopy (EDX) as grains from the lapping and polishing agent. The etching process does not result in

any visible change, but increases the AFM surface roughness: the lapped and polished sample (Figure 25d) has a roughness of 13 nm, the etching step between lapping and polishing (Figure 25e) increase the roughness to 45 nm and the final etching (Figure 25f) to 80 nm.



Figure 26: SEM images of the tungsten samples, a) untreated, b) lapped, c) lapped and etched, d) lapped and polished, e) lapped, etched and polished, f) lapped, etched, polished and etched. Note the different magnifications.

The SEM images of the tungsten samples are presented in Figure 26. The untreated sample (Figure 26a) has a very rough surface from the manufacturing process (Sa = 53 nm). Lapping results in a microstructure (Figure 26b) of comparable roughness (Sa = 57 nm). Subsequent etching increases the roughness to 122 nm. The

microstructure is removed by polishing (Figure 26d, Sa = 12 nm). But the lapped and polished sample still contains holes and trenches. The trenches are flattened by etching between lapping and polishing (Figure 26e, Sa = 7.2 nm). The final etching process increases the surface roughness again to 13 nm (Figure 26f). On the tungsten samples, also some lapping or polishing grains remain as verified by EDX.



Figure 27: SEM image of a milled OFCu sample.



Figure 28: SEM images of the polished OFCu samples, a) polished with diamond abrasive, b) polished with silicon carbide (image includes a dust grain), c) polished with calcium carbonate, d) plasma electrolytic polished.

Figure 27 shows a SEM image from a milled OFCu sample. Its surface exhibits some grooves, scratches and dark spots. The different polished samples are presented in Figure 28. The samples polished with diamond or SiC abrasive (Figure 28a and b) have quite smooth surfaces, only containing grooves from the polishing grains. Both samples have a comparable surface roughness of 4.8 nm and 5.0 nm for polishing with diamond or SiC, respectively. The sample, which was polished with calcium carbonate (Figure 28c), has a slightly higher roughness of 6.4 nm und looks very different. It has many dark areas along and between the grooves. EDX identified the dark areas as oxides. The plasma electrolytic polished sample shows no grooves, but a higher roughness of approximately 23 nm.



Figure 29: SEM images of the NEG-coated stainless steel samples with different heat treatments, a) untreated, b) 3.6 h at 400 °C, c) 24.4 h at 180 °C, d) in total 60 h at 180 °C.

SEM images of the NEG-coated stainless steel samples are presented in Figure 29. The untreated sample and the sample annealed at 400 °C for 3.6 h (Figure 29a and b) looks rather similar. They exhibit a laminar surface structure with some grains on top. During the activation process of the NEG film (>24 h at 180 °C), recrystallization took place. The NEG film (Figure 29c and d) adopt the grain structure of the stainless steel substrate, which looks very similar (Figure 30). The samples have different roughness of 15 nm for the untreated sample and 29 nm, 45 nm and 32 nm for the samples annealed at the conditions mentioned in the caption of Figure 29, respectively.

The results of the sputter cleaning are shown in Figure 31. Irradiation with 5 keV argon ions leads to an increase in surface roughness (Figure 31a). During sputtering, steps are created and small grains are excavated, because different orientated grains erode at different rates [Beh07]. After annealing (Figure 31b), the surface is smoothed again and a very clean surface with few structures is created. The surface roughness

increases with increasing ion fluence, this can be measured even after annealing (cf. Table 25). Figure 31c shows an image of the polished copper single crystal (Sa = 5.7 nm). Its surface exhibit lots of bright spots and also larger structures. Annealing reduce the roughness to 3.1 nm. After the sputter cleaning, the surface is very smooth and clean, containing only very few holes. One hole is shown in Figure 31d as an example.



Figure 30: SEM image of an uncoated stainless steel sample.



Figure 31: SEM images, a) OFCu after sputter cleaning, b) OFCu after sputter cleaning and annealing, c) copper single crystal (polished), d) copper single crystal after sputter cleaning (3.02E17 ions/cm²).

6 Results and Discussion

6.1 Thermal Desorption

6.1.1 Experimental Results

For thermal desorption, the desorbed gas is mainly composed of hydrogen, water, carbon monoxide and carbon dioxide. For the OFCu disk samples, H_2 is the dominant gas species. Argon makes only a significant contribution for the samples, which were cleaned by sputtering with keV argon ions. Usually also a small increase of the masses 15, 26 and 27 is observed, but typically these pressure increases are about 2 orders of magnitude smaller than the one of the main gases. Mass 15 is a fragment of methane and 26 and 27 correspond to hydrocarbons.

The results of the OFCu and tungsten sheet samples treated with different combinations of lapping, etching and polishing are shown in Figure 32. All OFCu sheet samples desorb huge amounts of gas. The lapped and etched OFCu sample has the highest desorption. The desorption of the other OFCu sheet samples is comparable. In contrast, the tungsten samples show very low desorption, with the highest desorption for the lapped sample and the second highest for the lapped and etched one. The three other tungsten samples are comparable and have the lowest desorption among all samples analyzed by TDS.



Figure 32: Thermal desorption (final temperature 400 °C) of OFCu and tungsten sheet samples treated by different combinations of lapping (lap.), etching (etch.) and polishing (pol.). The y-axis shows the amount of desorbed gas Q per surface area A (cf. equation (41)). Note the different scales for OFCu and tungsten.



Figure 33: a) Thermal desorption of OFCu samples with different surface treatments (left) and of samples sputter cleaned with 5 keV argon ions (incidence angle 30°) of different fluences (in ions/cm²) (right). b) Magnification of chart a) without hydrogen to illustrate the contributions of the other gases.

In Figure 33 the amount of desorbed gas for OFCu samples treated with different surface techniques are presented. The two milled samples show a large deviation in the desorption behavior, although they were prepared in the same manner. The samples are obviously not equal even if they were treated identically. The desorption of the polished OFCu sample is comparable to the milled ones, but the fraction of H₂O, CO and CO₂ is higher than for the milled samples (Figure 33b). The lowest desorption has the polished copper single crystal. Two effects might result in the low desorption of the single crystal: (i) the single crystal has a very high purity of 99.9999 % and (ii) it has almost no grain boundaries. At grain boundaries diffusion occurs much faster than in the crystal lattice [Häs70]. The absence of grain boundaries the transport of gas atoms to the surface and reduces the desorption.

Thermal desorption of the sputter cleaned samples is slightly lower than of the milled or polished samples. In the applied fluence regime, no dependence on the ions fluence during sputter cleaning is observable for the total desorption yield, but a slight decrease with increasing fluence is observed for H_2O , CO and CO_2 . In Figure 33b the amount of desorbed H_2O , CO, CO_2 and Ar is shown. The sputter cleaned samples desorb a significant amount of argon, because argon ions were implanted into the sample during sputtering. The range of 5 keV argon ions in copper is about 3.5 nm [Zie13]. During the annealing process, the argon atoms diffuse to the surface and desorb. For all other samples desorption of argon is at least one order of magnitude smaller than for H_2O , CO and CO_2 if observed at all.

In preparation of the samples for the beam time 2021, thermal desorption was measured for milled OFCu samples at different temperatures (Figure 34). All samples were heated at a rate of 6 K/min, but the final temperature was varied between 300 and 500 °C. The results were quite surprising: the 400 °C sample had the highest desorption followed by the 500 and 300 °C sample. To check the results, the measurements were repeated in 2022 with two samples for each temperature. Here some small deviations between the two samples for each temperature were found, but in general the desorption increase slightly with increasing temperature.



Figure 34: Thermal desorption of milled OFCu samples with different final temperatures during the TDS measurement.



Figure 35: Thermal desorption of OFCu samples with different coatings (left) and of WCu, aluminum and NEG-coated stainless steel (right).

Figure 35 presents thermal desorption results of milled OFCu samples coated with titanium nitride or carbon. The samples coated with TiN and carbon exhibit the same desorption. In both cases, the amount of desorbed gas increases with increasing layer thickness. For the TiN samples, the fraction of H_2O is slightly higher. In Figure 35 also the results of some other materials are shown. Desorption of the tungsten-copper sample is higher than of the tungsten or the milled OFCu samples (not shown in Figure 35). It is in the range of the OFCu

sheet samples. The Al1050 and the NEG-coated stainless steel samples have very low desorption. The desorbed gas contains almost exclusively hydrogen. Numeric values for thermal desorption of all samples can be found in Table 26 to Table 30 in the appendix.



Figure 36: Evolution of the total pressure increase (as nitrogen equivalent) as a function of time for some selected samples. The fluctuations in the falling part of the curves are related to small deviations in the room temperature caused by the switching hysteresis of the air conditioning. For the NEG-coated sample, the heater was switched off after approximately 13000 s, because the pressure reaches again a value below 1E-10 mbar. The black curve shows the temperature evolution.

The materials diverge not only in the amount of desorbed gas, but also in the temporal development of their pressure curves. Some examples are shown in Figure 36. The positions of the local maxima in the rising part of the curves are related to the desorption energies of the corresponding gas and substrate. Also the slopes of the falling part and the final pressures differ. The tungsten sample shows the slowest pressure decrease in the long time behavior, while the NEG-coated sample has the fastest decrease.

6.1.2 Simulation Results for Thermal Desorption

The model for the simulation is based on a combination of diffusion and desorption (cf. chapter 4.1.2). All simulations were carried out for a time interval of 14400 s (4 h) with 500 temporal nodes. The depth interval is set to 4 mm for copper and 1 mm for stainless steel with 101 nodes, which corresponds to the samples thickness of disk or sheet samples, respectively. Except of the thickness of the surface layer $x_{surface} = 3 nm$ and the number of particles in one monolayer $\sigma_{mono} = 1 \cdot 10^{19} particles/m^2$, all parameters are treated as free parameters which are chosen, in the range of the physical reasonable values, in such a way that the simulation reproduce the experimental data as good as possible. For all simulations of copper samples, the following input parameters were used: $E_{des} = 64 kJ/mol$, $E_{dif} = 40 kJ/mol$, $D_0 = 8.5 \cdot 10^{-6} m^2/s$ and $c_0 = 3 \cdot 10^{23} m^{-3}$.

Figure 37 shows the expected pressure increase during the annealing process for the system hydrogen-copper determined with the three different models: (i) the model assuming that every diffusing particle reaching the surface is released immediately to the vacuum, (ii) the model combining diffusion and thermal desorption and (iii) the model applying only thermal desorption from a partially covered surface. For diffusion with thermal

desorption, the outgassing at low temperatures is suppressed compared to the model with immediate particle release. This is in agreement with the fact that the particles need a particular thermal energy for desorption. The implementation of desorption also results in a slower decrease of the pressure curve at constant temperature due to the slower outgassing in the beginning. The particle concentration in the bulk decreases slower resulting in a longer outgassing process in the latter state. For the desorption model without diffusion, the pressure shows only a distinctive peak at low temperatures. After the maximum, the pressure decreases very fast, because only a small number of particles is available at the surface compared to the amount of gas in the bulk. Due to the very small surface coverage of only 1E12 particles/m² at 3E-11 mbar (the sticking coefficient was set to 0.1 in equation (62)), the pressure increase is very small. Experimentally this pressure increase is far below the sensitivity limit of the pressure measurement.



Figure 37: Simulated pressure increase for the system hydrogen-copper for three different scenarios: (i) assuming that every diffusing particle reaching the surface is released immediately to the vacuum, (ii) a combination of diffusion and thermal desorption and (iii) only thermal desorption from a partially covered surface. Note the different scale of the y-axis for the desorption model (orange curve).

The model with immediate particle release at the surface was also used to analyze the influence of the base pressure in the vacuum chamber on the diffusion. Figure 38 presents the pressure increase for two different chamber pressures of 1E-11 and 1E-7 mbar. In this pressure range, which is of interest for the annealing process, no influence is observed.

Figure 39 presents two simulations comparing diffusion with first- and second-order desorption. The second-order process includes the recombination of two hydrogen atoms to a molecule. For both cases a desorption energy of 64 kJ/mol was chosen to facilitate the comparison. In reality, the desorption energy should differ for the different desorption orders, because for second-order desorption the desorption energy also includes the dissociation energy. All other parameters were kept constant for both simulations. For first-order desorption, the pressure starts to increase at slightly lower temperatures and the rising slope is steeper. Then a shoulder appears and the pressure increase flattens. Both pressure curves have a maximum when the final temperature is reached and then decrease. For first-order desorption, the slope of the falling part is steeper and shows an exponential decay, while for second-order desorption, the slope has a slower decline. For the following considerations, second-order desorption is chosen, because hydrogen is usually solved as atoms in the metal [Bor88] and requires molecule formation for desorption.



Figure 38: Pressure increase due to diffusion with two different constant base pressures in the vacuum chamber for the system hydrogen-copper.



Figure 39: Comparison of the pressure increase during annealing simulated for first- and second-order desorption as boundary condition for the system hydrogen-copper.

The left diagram of Figure 40 shows measured pressure increases of three milled OFCu samples (4 mm thickness) heated to 400 °C with a temperature ramp of 6 K/min and the corresponding simulation. The simulation represents well the overall evolution of the pressure as a function of time, but it does not reproduce the local maximum in the rising part of the pressure curve. It is reasonable to assume that the simulation so far does not cover all effects which contribute. The local maximum can be implemented by assuming a surface layer with depleted hydrogen concentration. In practice, this can occur when hydrogen

diffuses out of the first layers during the storage, because in atmosphere the hydrogen concentration is very small (much less than 0.5 ppm [Ish03]). For an improved simulation, the initial condition was transformed to

$$c(x,t=0) = \begin{cases} c_{surface} & \text{for } x \le x_d \\ c_0 & \text{for } x > x_d \end{cases}$$
(77)

To reproduce the measured data as best as possible, $c_{surface}$ is set to 1E22 particles/m³ and x_d to 120 µm. With larger x_d the local maximum in the rising part of the pressure curve moves to larger times. In reality, diffusion of hydrogen out of the sample during storage would not result in a rectangular concentration profile. However, another e.g. exponential or Gaussian profile is not applicable, because this surface layer contains only four spatial nodes. In the right diagram of Figure 40, the simulation under this modified initial condition is shown. The corresponding particle concentration as function of depth and time is presented in Figure 41. The upper blue curve in Figure 41 presents the initial concentration with the depleted surface layer. With increasing time, first the depletion zone is filled with hydrogen atoms and then the concentration in the whole samples decreases.



Figure 40: Simulation results and comparison with experimental TDS data of OFCu samples. For the simulation in the left diagram, a constant initial particle concentration was chosen. For the second simulation (right), a lower concentration in the surface layer was applied to reproduce the local maximum in the rising part of the curve (marked with the red circle).

The activation energy for diffusion E_{dif} and the pre-exponential factor D_0 define the diffusion coefficient. They influence the slope of the falling part of the pressure curve and also the height and position of the global pressure maximum. The desorption energy E_{des} determines the slope of the rising and falling part of the curve. The initial particle concentration c_0 influences the overall height of the pressure curve. In Table 16 literature values for the discussed parameters are listed. For all parameters, the values vary among the literature, for D_0 by more than one order of magnitude, because they are difficult to measure and depend on the sample history. For the desorption energy, the value used for the simulation is within the range of the literature values. The literature values for the activation energy of diffusion agree rather well among each other and with the value selected for the simulation. To reproduce the measurement data, for D_0 a higher value is chosen than the literature values. The determined initial concentration is much smaller than stated in the references, but literature values were only found for oxygen-free, phosphorus-doped copper. Maybe the undoped OFCu has a lower hydrogen content.



Figure 41: Particle concentration for the system hydrogen-copper as a function of depth and time for the simulation with 400 °C final temperature and a depleted surface concentration. The curves correspond to different time steps. The corresponding time values are shown in the legend.

Parameter	Simulation value	Literature values	Reference	Comments
E _{dif}	40	38.9 ± 0.27	[Kat71]	Cu single crystal
[kJ/mol]		42.0	[Mag17]	Oxygen-free, phosphorus-
				doped copper (Cu-OFP),
				Fit for several measurements
				from different authors
		44.53	[Ish85]	Cu foil
D_0	8.5E-6	(1.131 ± 0.40)E-7	[Kat71]	Cu single crystal
[m²/s]		1.74E-6	[Mag17]	Cu-OFP,
				Fit for several measurements
				from different authors
		2.11E-6	[Ish85]	Cu foil
E _{des}	64	66.071.3	[Fic14]	Polycrystalline Cu, <i>E</i> _{des}
[kJ/mol]				depends on surface coverage
		68.6 ± 8.0	[Koj80]	Polycrystalline Cu foil
		50.296.3	[Ang89]	Cu single crystal, <i>E</i> _{des} depends
				on surface coverage
<i>c</i> ₀	$3E23 1/m^3 =$	0.58 ± 0.03 wt ppm	[Mar12]	Cu-OFP
	0.055 wt ppm	0.66 wt ppm	[For21]	Cu-OFP

Table 16: Input parameters of the simulation compared to literature values for hydrogen in copper

To test the reliability of the simulation, TDS measurements and simulations for milled OFCu samples (thickness 4 mm) with different final temperatures and temperature ramps were compared. The results are presented in Figure 42 and Figure 43. The chosen input parameters reproduce the different measurements well. Small deviations are observed for the rising part of the pressure curve between the local and the global maximum. The experimental data with 3 and 12 K/min temperature ramp show a faster pressure decrease in the constant temperature part compared to the simulation.



Figure 42: Simulation results for a final temperature of 300 °C (left) and 500 °C (right) together with experimental TDS data of OFCu samples.



Figure 43: Simulation results for a temperature ramp of 3 K/min (left) and 12 K/min (right) together with experimental TDS data of OFCu samples.



Figure 44: Measured and simulated pressure increase during TDS of a stainless steel sheet sample. The input parameters for the simulation are given in the text.

Figure 44 shows simulation and experimental results for a 1 mm thick stainless steel 304 sample. For this measurement, the simulation reproduces the rising part of the pressure curve not very well. For stainless steel, an activation energy for diffusion of 51 kJ/mol and a desorption energy of 98 kJ/mol was selected. For D_0 a value of 7E-7 m²/s was deduced. The initial particle concentration was set to 3E24 1/m³, the surface concentration to 2E24 1/m³ and x_d to 40 µm. The values for E_{dif} , D_0 and c_0 agree very well with values reported in the literature (Table 17). For E_{des} , the value in the simulation is slightly higher than the literature values, but the values differ very much among the references. This might be related to different surface treatments of the samples.

Parameter	Simulation value	Literature values	Reference	Comments
E _{dif}	51	48.0	[Out83]	347 stainless steel
[kJ/mol]		48.8 ± 0.9	[Qui79]	310 stainless steel
		52.3	[Phi68]	321 stainless steel
$D_0 [{ m m}^2/{ m s}]$	7E-7	7.01E-7	[Out83]	347 stainless steel
		(5.15 ± 3.17)E-7	[Qui79]	310 stainless steel
		7.33E-7	[Phi68]	321 stainless steel
E _{des}	98	59 ± 9	[Rez94]	347 stainless steel
[kJ/mol]		97	[Tag83]	304LN stainless steel
		7090	[Gro95]	
<i>c</i> ₀	3E24 1/m ³ =	2.1E24 1/m ³ =	[Out83]	347 stainless steel
	0.63 wt ppm	0.44 wt ppm		

Table 17: Input parameters of the simulation compared to literature values for hydrogen in stainless steel

6.2 Measurements on Ion-Stimulated Desorption (M-branch)

6.2.1 Thermal Annealing

Ion-stimulated desorption was measured for almost all samples with at least two different ion species. In the following chapters, only the most pronounced effects will be presented, but all results including the calculated errors are summarized in the appendix (chapter 11.5).



Figure 45: Background-subtracted mass spectrum recorded during irradiation of a non-annealed milled OFCu sample with Au²⁵⁺.

Similar to thermal desorption, the gas desorbed under ion irradiation is mainly composed of H_2 , H_2O , CO and CO_2 . The contribution of argon is again very small and therefore not shown in the diagrams. For some selected samples a full mass spectrum up to m/q 100 was recorded, an example is presented in Figure 45. The spectra indicate that there is also a small contribution of low-molecular hydrocarbons. Desorbing masses are in the sequence of their usually abundance: 26, 27, 15, 25, 39, 30 and 41. The masses can probably be related to fractions of CH_4 , C_2H_x and C_3H_x .

Figure 46 presents desorption yields measured in beam time 2021 for OFCu samples with different annealing temperatures and for a sample, which was stored in the vacuum of the load lock of the TDS-setup for about 4 months. Vacuum storage reduces the desorption by approximately a factor of 3. Ex-situ annealing reduces ISD significantly. In the measurements with the calcium ions, the desorption yields decrease with increasing annealing temperature as it is reported in the literature [Ach79; Mah11; Mal20c; War16b]. However, in the gold beam time the measurements do not follow a systematic trend, but the results agree with the results from the thermal desorption measurements (cf. chapter 6.1.1). This inconsistence is probably due to different storage conditions. The samples annealed at 300 and 500 °C were prepared only a few days before the beginning of the gold beam time, while the 400 °C sample was prepared one month before the gold beam time and stored in atmosphere until the beam time. The calcium beam time took place one month after the gold beam time. In between all samples were stored in atmosphere. This may attenuate the effect observed in the gold beam time. Additionally, different durations for the annealing process were applied (300 °C: 8.2 h, 400 °C: 6.9 h, 500 °C: 4.1 h), because at 300 °C it took longer to reach again a pressure in the low 10⁻¹⁰ mbar regime. The extended annealing time of the 300 °C sample probably leads to the observed smaller ISD yield. It can be concluded, that the sample history has a crucial impact. The measuring method is able to see these differences. Due to the limited beam time, it was not possible to measure several identical samples to gain enough statistics.



Figure 46: Desorption yields measured for OFCu samples annealed at different temperatures (beam time 2021). Results marked with an asterisk are mean values of two measurements on the same sample. Note the different scales for the left and the right part of the diagram.

The positive effect of sample annealing can be explained by the depletion of gas atoms from the bulk as shown in the TDS-simulation and probably also by the removal of carbon and oxygen contaminations from the surface. The correlation between ISD yield and carbon and oxygen concentration at the surface was shown by Mahner et al. [Mah11]. During storage, gas from the surrounding environment might diffuse back into the solid. Hydrogen, which is usually the most dominant gas species during ISD, is not available in the atmosphere, so it cannot diffuse back into the sample. Hydrogen can only be produced by dissociation of water. Diffusion of oxygen and formation of an oxide layer is expected. If the samples are protected from contaminations, the carbon content at the surface should stay low.

For beam time 2022, the study was extended by preparing two samples for each treatment. In the diagrams, the mean values of the two identical samples are presented. Usually the standard deviation of the mean values is smaller than the calculated systematic errors. Again, annealing at three different temperatures was conducted. The samples were prepared one week before the calcium beam time, stored in the load lock of the TDS-setup and transported to the M1 beamline with minimal exposure to air. After ISD measurement with calcium ions, the samples were brought back to the TDS load lock, stored there until the gold beam time and transported again to the beamline for the ISD measurement. All samples were annealed for 4 h, but this time the base pressure in the analysis chamber was only in the range between 5E-9 and 2E-8 mbar, because the setup had to be vented before the annealing to fix one of the heater cables. Before the beam time there was not enough time for a vacuum bake-out of the setup. As seen in Figure 47, the annealing process (300–500 °C) reduced the desorption yield by more than one order of magnitude. The base pressure during annealing was still in the UHV range and obviously had no negative influence. The 500 °C sample has a slightly lower desorption than the 300 °C sample, but the differences are in the range of the error bars. Warth [War16a] obtained similar results. He found only minor differences between OFCu samples ex-situ annealed at 300, 400 and 500 °C.



Figure 47: Desorption yields (each a mean values of two identical samples) of OFCu samples without annealing and after annealing at different temperatures.

Furthermore, different storage conditions were tested. Samples were stored in argon, vacuum or atmosphere for three different durations (3, 6 and 9 months before the calcium beam time; 5, 7 and 11 months before the gold beam time). The results are presented in Figure 48 for the calcium beam time and in Figure 49 for the gold beam time. The positive effect of annealing persists for at least 11 months. For comparison, the samples, which were annealed at 400 °C one week before the calcium beam time and stored in the load lock of the TDS-

setup, are also shown. These samples have the lowest desorption, but annealed samples stored in argon have only slightly higher desorption yields. The samples, which were not annealed but stored in argon for 9 or 11 months, have a lower desorption than the non-annealed samples stored in atmosphere. The yields for the different storage durations scatter, no clear dependence on storage duration is observable, even for the samples stored in atmosphere.

Unfortunately, the samples stored in vacuum in the dedicated setup were mixed up during storage. It was not possible to assign the samples to the different storage durations. Therefore, in Figure 48 and Figure 49, the results of the individual samples are shown for the annealed samples stored in vacuum instead of mean values. The untreated samples stored in vacuum have a lower desorption than the non-annealed samples stored in atmosphere, but a higher or comparable desorption than the untreated argon-stored samples. Presumably, this is caused by the repeated venting of the vacuum setup to insert new samples. For the measurement with gold ions, this effect is attenuated because the argon-stored samples were exposed to atmosphere two more times. It is not clear, why in the calcium beam time the annealed samples stored in vacuum have higher desorption yields than the annealed samples stored in atmosphere. During gold beam time, the values are comparable.



Figure 48: Desorption yields of annealed OFCu samples after storage in atmosphere, argon or vacuum for different time intervals. For comparison, also non-annealed samples with the same storage conditions and an annealed sample, which was annealed one week before the ISD measurement and stored under vacuum in the load lock of the TDS-setup (denote as "Annealed, no storage") are shown. ISD measurements were done with Ca¹⁰⁺ ions.



Figure 49: Desorption yields of annealed OFCu samples after storage in atmosphere, argon or vacuum for different time intervals. ISD measurements were done with Au²⁶⁺ ions.

6.2.2 Surface Treatment

Figure 50 presents the ISD results of two series of OFCu and tungsten sheet samples treated with different combinations of lapping, etching and polishing. For each surface treatment, two samples were prepared one without and one with annealing at 400 °C. For the OFCu samples, none of the surface treatments was successful, the lowest desorption has the untreated sample. This sample also exhibits the least textured surface in the SEM images. Etching results in very high desorption yields. In particular, the sample, which was lapped and etched, has a huge desorption yield of approximately 160,000 molecules/ion. Among the treated samples, the lowest desorption has the sample treated by lapping and polishing. For all samples, a subsequent ex-situ annealing process results in a significant reduction of their desorption yield.

For the tungsten samples, the desorption yields are usually more than one order of magnitude smaller than for the corresponding OFCu sample with the same surface treatment. Each treatment step reduces the desorption. The untreated tungsten sample has the highest desorption yield, followed by the lapped sample. The best sample is the one, which was first lapped, then etched and finally polished. This sample also has the smoothest surface according to the AFM measurements. The final etching step increases the surface roughness and simultaneously also the desorption yield. As for the OFCu samples, annealing decreases the desorption of all samples. Among the annealed samples, the lapped and polished sample has the lowest desorption, but this value is close to the sensitivity limit of the mass spectrometer.

The behavior of the OFCu and tungsten samples during ISD is similar to the TDS results. In both cases, the OFCu sample with the highest desorption is the lapped and etched one followed by the lapped sample, while for the tungsten samples, the highest desorption is exhibited by the lapped sample followed by the lapped and etched sample. For the other samples the thermal desorption is similar and for ISD there are some small differences in the desorption yields.

The differences in the desorption behavior between the surface treatments of the copper and the tungsten samples can possibly be explained by the different ductility of the materials. Copper is very ductile, therefore during polishing smoothing is mainly due to plastic deformation and many lapping and polishing grains are introduced into the surface as observed in the SEM images. In contrast, tungsten is less ductile and smoothing is caused by abrasive material removal, which results in a cleaner surface.



Figure 50: Desorption yields of OFCu and tungsten sheet samples treated with different combinations of lapping (lap), etching (etch) and polishing (pol) without and with annealing (ann) at 400 °C. The annealing duration was chosen according to the pressure evolution.

Because of the poor results of the series of OFCu sheet samples, an alternative approach was tried. For the beam times in 2020–2022, 2.35 mm of the surface of all OFCu samples is milled to remove surface impurities. Compared to the untreated sheet sample, desorption of the milled disk sample is reduced by approximately 40 % (Figure 51). The yield of the sample polished with SiC and the plasma electrolytic polished sample is comparable to the milled samples. The samples polished with calcium carbonate or diamond abrasive have desorption yields, which are approximately 50 % lower than the yield of the milled sample. The diamond polished sample also shows the cleanest surface in the SEM images, while on the surface of the calcium carbonate polished sample several areas with increased oxidation were found by EDX. The sample, which was lapped and polished with diamond abrasive, has a slightly higher desorption than the sample, which was only polished with diamond. Figure 51 presents also the desorption yield of a polished copper single crystal. As for thermal desorption, the single crystal shows the lowest desorption yield, which is further reduced by annealing at 400 °C.



Figure 51: Desorption yields of milled and polished OFCu samples and copper single crystals measured with Ca¹⁰⁺ (* mean value of two identical treated samples, ** mean value of two measurements on the same sample).

Figure 52 to Figure 54 present desorption yields of selected samples as a function of the surface properties measured with the atomic force microscope. The surfaces are characterized by the arithmetical mean height Sa (Figure 52), the mean inclination angle δ_m (Figure 53) and the ratio of true surface area to geometrical surface area $A_{relative}$ as defined in equation (76) (Figure 54). The diagrams show tungsten, OFCu sheet, OFCu disk and sputter cleaned OFCu samples. The OFCu sheet samples have the highest yields, followed by the tungsten samples. The OFCu disk samples and the sputtered samples have the lowest desorption yields. Due to the different bulk properties, only samples of the same type are comparable.

For very rough surfaces high desorption yields are observed. However, for rather smooth surfaces the desorption yields differ by up to one order of magnitude even if the surface parameter varies only slightly. It is not possible to find a clear correlation between desorption yield and surface roughness. The same is true for the other surface parameters. The mean inclination angle was considered, because it is a suitable parameter to predict sputter yields of rough surfaces. But for ISD the angle dependence is less pronounced as for sputtering [Mol07]. The mean inclination angle is obviously not an appropriate parameter for the prediction of desorption yields. A larger surface area offers more sites for the adsorption of gas molecules. Therefore, the true surface area compared to the geometric surface area was examined. On trend the desorption yields increase with increasing surface area, but the values scatter too much to derive a clear correlation.


Figure 52: Desorption yields (irradiation with Ca^{10+}) of different sample series as a function of the arithmetical mean height *Sa*. The desorption yields were calculated from the total pressure measurements (nitrogen equivalent).



Figure 53: Desorption yields (irradiation with Ca¹⁰⁺) of different sample series as a function of the mean inclination angle δ_m . The desorption yields were calculated from the total pressure measurements (nitrogen equivalent).



Figure 54: Desorption yields (irradiation with Ca^{10+}) of different sample series as a function of the ratio of true surface area to geometrical surface area $A_{relative}$ as defined in equation (76). The desorption yields were calculated from the total pressure measurements (nitrogen equivalent).

6.2.3 Sputter Cleaning

Figure 55 and Figure 56 present results of the desorption measurements on the sputter cleaned samples (beam time 2021). In both diagrams it is clearly seen that the irradiation of the samples with 5 keV argon ions improve the desorption behavior compared to the milled or polished samples. The samples, which were polished before the sputtering, have higher desorption yields than the milled and sputtered sample (Figure 55). The polished samples, which were not sputtered, also showed higher yields than the milled samples produced for the 2021 beam time. This might be because the polishing was already done for the previous beam time (2020). Additional annealing has for the sputter cleaned samples only a minor effect on the desorption. In contrast to the TDS measurements, no increased argon desorption was observed. Probably, the range of the 5 keV argon ions (3.5 nm [Zie13]) and therefore the implantation depth is larger than the escape depth of the desorbed gas. This is an advantage of sputter cleaning with keV ions from an ion source compared to glow discharge cleaning. Due to the smaller energy of the ions from the glow discharge of only a few 100 eV [Dyl88; Mat87], the ions are implanted very close to the surface and can desorb easily.

Desorption yields for samples sputtered with different ion fluences are shown in Figure 56. The yields seem to decrease with increasing fluence and saturate for higher fluences. Unfortunately, only one measurement per sample was conducted. Hence, there is no statistics. After annealing, the desorption of all sputtered samples is comparable and slightly lower than of the annealed and not sputtered sample. Figure 56 presents a comparison of samples sputtered with three different incidence angles, but from the data no clear statement can be deduced.



Figure 55: Desorption yields for sputter cleaned OFCu samples with different surface treatments before sputter cleaning (beam time 2021). For comparison, samples without sputter cleaning are also shown. All samples were sputtered with 5 keV argon ions under an incidence angle of 30° and with a fluence of 2.9E18 ions/cm².



Figure 56: Desorption yields for OFCu samples sputter cleaned with 5 keV argon ions of different fluences (in ions/cm²) without and with annealing (incidence angle 30°) and for different incidence angles. The ISD measurements were done with Ca^{10+} ions (beam time 2021).



Figure 57: Desorption yields of sputtered OFCu samples as a function of fluence of 5 keV argon ions for various irradiations with calcium and gold ions. Desorption yields were calculated from the total pressure measurements (nitrogen equivalent). The brackets indicate a sample with increased surface oxidation as observed by EDX (further explanation in the text).



Figure 58: Desorption yields of sputtered OFCu samples (3.0E17 ions/cm²) as a function of argon ion energy. Desorption yields were calculated from the total pressure measurements (nitrogen equivalent).

Figure 57 shows results from the beam time in 2022. Again, OFCu samples sputtered with various fluences were investigated. This time the focus was on lower fluences in the range from 1.6E17 to 1.0E18 ions/cm². All samples were milled before the sputtering. The yields scatter very much and therefore no dependence on the fluence can be derived. The sample with a fluence of 2.36E17 ions/cm² exhibits a very large desorption for all measurements. It is even higher than the yield of the untreated samples. In the SEM, many dark spots can be seen on the surface. EDX indicate that the dark areas contain an increased amount of oxygen and also carbon and calcium of different contents. The origin of the spots could not be identified. With the gold beam, the samples were measured twice, once with full beam size of approximately 8 mm diameter and a second time with the beam cut to a size of 4x4.5 mm using the slits. Maybe the samples were not sputtered uniformly, because the beam intensity has a Gaussian shape. This could result in a variation of the desorption yield. The smaller gold beam hits only the sample center, where the area sputter cleaned by the keV-ion irradiation is expected to be uniform. Except for the sample with 2.36E17 ions/cm², which has a very high desorption in all measurements, and two outliers the results scatter less for the small beam size. Surprisingly, the untreated sample has in this measurement a yield comparable to the sputtered samples. In Figure 58, results of samples sputtered with different ion energies between 3–5 keV are presented. In this energy range, no dependence on argon ion energy is observable.

For argon sputtering under 60°, electrostatic deflection plates had to be installed, which increased the distance between ion source and sample from 120 to 300 mm. Figure 59 shows a comparison for three different sputter conditions: (i) perpendicular incidence and short distance, (ii) perpendicular incidence and long distance and (iii) 60° incidence angle and long distance. For each of these conditions, three different fluences were applied. The results show no clear trend. The differences in the results for perpendicular and 60° irradiation are in the range of the error bars. With 60° incidence angle the sputter yield of 5 keV argon ions on copper is 14.8 atoms/ion, while for perpendicular incidence it is only 6.7 atoms/ion as calculated by SRIM (Version SRIM-2013, [Zie13]). A higher sputter yield results in a larger material removal. However, according to the results, this has no influence on the desorption yield. This is in agreement with the outcome that the ion fluence has no significant effect.



Figure 59: Desorption yield of sputtered OFCu samples as a function of fluence for different distances between argon ion source and sample and different incidence angles.

Figure 60 presents desorption yields for sputtered aluminum samples (Al6061) and a copper single crystal. For the aluminum samples, sputter cleaning reduces the desorption yield. In this measurement, the sample with higher fluence has a lower yield. The copper single crystal has a slightly lower desorption yield than the polycrystalline sample sputtered with equal fluence, but the difference is not as distinctive as it could be expected from the SEM images, where the surface of the single crystal is almost perfectly smooth except from very few holes (cf. Figure 31d).



Figure 60: Desorption yields for sputter cleaned aluminum, OFCu and single crystal Cu for various fluences (in ions/cm²) of 5 keV argon ions. Results marked with an asterisk are mean values of measurements on two identical samples.

6.2.4 Aluminum and Tungsten-Copper

Figure 61 presents a comparison of the tungsten-copper (WCu) samples, the two different aluminum grades Al1050 and Al6061 and OFCu samples (beam time 2020). Additionally, results from an untreated and an annealed Al1050 sample recorded in beam time 2021 are shown. The WCu sample without annealing has a very large desorption yield, but the yield is reduced by approximately one order of magnitude by annealing at 400 °C for 4.75 h.

The milled aluminum samples have slightly lower desorption yields than the OFCu sample. Al1050 has a slightly lower desorption compared to Al6061. The effect of the annealing treatment depends on the annealing temperature. Annealing at 100 °C has almost no effect for aluminum, while annealing at 280 or 400 °C reduce the desorption by more than 50 %. The results from beam time 2021 differ from the yields measured in 2020. Reasons are that the measurement conditions change slightly from beam time to beam time and for the gold ions, another charge state was provided (Au²⁵⁺ instead of Au²⁶⁺).



Figure 61: Desorption yield of the WCu and aluminum samples without and with annealing. For comparison, OFCu samples are shown. The last two measurements in both charts are from 2021, while all other measurements were conducted in 2020.

6.2.5 Coatings

Ion-stimulated desorption of stainless steel samples can be reduce by coating with the non-evaporable getter TiZrV as shown in Figure 62. The desorption yield of the non-annealed NEG-coated sample is approximately 75 % smaller than the yield of the uncoated sample. Different heat treatments were applied to the coated samples. The lowest desorption shows the sample, which was annealed ex-situ at 400 °C for 4 h. The ex-situ annealing at 180 °C for about 24 h, which corresponds to a typical NEG activation procedure, however increase the desorption compared to the untreated sample. Even the in-situ annealing at 177 °C is worse than the 400 °C annealing. The problem during in-situ annealing at the M1 beamline is the large desorption from the sample holder. After switching on the heater, a pressure rises up to approximately 1E-7 mbar for the total pressure occurs. Afterwards the pressure stayed constant at 7E-9 mbar for the total pressure and 2.3E-10 mbar for the partial pressure of CO₂. As a result, the NEG film is saturated again. At 10⁻⁹ mbar, some tens of monolayers can be adsorbed on any surface within one day. The sorption capacity of a NEG film is usually one monolayer [Mal09]. High partial pressures of CO and CO₂ cause poisoning of the NEG film. Even short pressure pulses can poison the NEG film. Pressure pulses arise for example by closing or opening of valves or by the movement of the sample holder. They cannot be avoided during the ISD measurements. In consequence, no measurements on activated NEG samples could be conducted. A dedicated setup would be needed to investigate activated NEG films. It requires pressures below 1E-11 mbar and a heater with very little thermal desorption. A possible solution would be to install the TDS-setup at the accelerator, but because of the limited space at the M-branch, this could not be realized.



Figure 62: Desorption yields of the NEG-coated stainless steel samples with different heat treatments. An uncoated stainless steel sample is shown for comparison.



Figure 63: Desorption yields of OFCu samples coated with titanium nitride or carbon with two different layer thicknesses (200 and 500 nm). An uncoated OFCu sample is shown for comparison. Desorption was measured with Au²⁵⁺ ions.

Figure 63 presents desorption yields for OFCu samples coated with titanium nitride or carbon with two different layer thicknesses. Three types of samples were prepared: (i) samples without annealing, (ii) samples where the substrate was annealed before the coating and (iii) samples with annealing after the coating process. The TiN-coated samples have higher desorption yields than the carbon-coated samples, but in general, both types of samples show very high desorption much higher than the uncoated OFCu sample. For both coatings, desorption increases with increasing layer thickness. The annealing has no significant influence on the samples coated with 200 nm TiN. For the 200 nm carbon-coated samples, there is only a weak reduction and no difference when the annealing took place. For both 500 nm coatings, the annealing after the coating is more effective than the annealing of the substrate. Annealing before coating should reduce desorption from the substrate, while annealing after coating should decrease desorption of the coating and may also decrease the desorption from the substrate. If TiN acts as diffusion barrier as it is assumed in the literature [Mam14], no depletion of gas from the substrate is expected. During TDS, the samples with coating of 500 nm thickness exhibit also larger desorption. In contrast to the ISD results, TiN and carbon have equal thermal desorption behavior.

The high desorption of the carbon-coated samples is in agreement with results from Mahner et al. [Mah11]. They found a correlation between carbon and oxygen content of the surface and ISD yield. For TiN coating, no measurement on ISD were found in the literature. All studies on the desorption of TiN coatings focus on thermal outgassing. Possibly the titanium in the TiN acts as a getter material and adsorbs gas molecules [Mam14]. Due to the small coated surface area of the ISD samples, the getter property does not influence the experiments presented here, but it could impair outgassing measurements of large surface areas. Therefore, outgassing rates reported in literature have to be examined carefully. Maybe lower desorption yields could be achieved by a more appropriate coating process. The barrier effect of the TiN layer depends on stoichiometry and crystallinity of the film and is influenced by the coating method [Sai95]. Since the TiN coating was produced by sputtering at room temperature, the TiN layer is expected to be amorphous.

One of the annealed TiN samples with 500 nm layer thickness was irradiated with Au²⁵⁺ ions for approximately 2 h. After the irradiation, the sample was analyzed by scanning electron microscopy. In the SEM images, many cracks were observed in the irradiated part of the coating. The cracks do not appear after short time irradiation of 2 min. In conclusion, the lack of radiation hardness and the huge desorption yields make TiN coatings unsuitable for heavy ion accelerator applications.

6.2.6 Dependence on Energy Loss

To investigate how desorption depends on the energy loss of the ion in the material, samples were irradiated with calcium and gold ions of different charge states (Ca¹⁰⁺, Ca¹⁹⁺, Au²⁶⁺ and Au⁵²⁺). The energy loss dE/dx scales with the square of the charge state, as listed in Table 18 for different target materials. In the following, the ISD results were analyzed according to their dependence on the electronic energy loss. As discussed in chapter 2.3.2, the energy loss scaling follows the power function

$$\eta = \kappa \left(\frac{dE}{dx}\right)_{elec}^{n} \tag{78}$$

with n = 1 - 3. Desorption yields as a function of energy loss are plotted for OFCu samples in Figure 64, for tungsten samples in Figure 65 and for aluminum samples and the copper single crystals in Figure 66. For each sample the four different ISD yields, which correspond to the measurements with the four different ions, were fitted with equation (78). The results of the fits are shown in Table 19. The parameter κ depends on the sample and is large for samples with high desorption. The exponent n depends on the desorption mechanism and is in theory equal for all samples. In this study, the exponent ranges from 0.53 to 2.08 with a mean value of $n = 1.21 \pm 0.07$. This value is smaller than the values reported in the literature. The closest value is reported by Caron et al. [CarO3]. They measured desorption of nitrogen from amorphous carbon stimulated by a large variety of ions (Z: 6–73, q_{ion}: 6–54, energy: 6–13 MeV/u) and 5 keV electrons. They found $n = 1.37 \pm 1.00$

0.07 including the measurement with electrons and $n = 1.66 \pm 0.03$ without the electrons. Kollmus et al. [Kol09] found $n \approx 2.1$ for argon ions (q_{ion}: 8–12, energy: 5–100 MeV/u) and $n \approx 2.9$ for U⁷³⁺ ions (energy: 15–100 MeV/u) on stainless steel. A similar value is reported by Molvic et al. [Mol07]. They found $n \approx 2$ for K⁺ ions (energy: 70–1000 keV) for an incidence angle of approximately 85° on stainless steel.

Table 18: Electronic energy loss dE/dx for different ions, charge states and materials. The values were calculated for 4.8 MeV/u specific energy using the program CasP (version 5.2, model: UCA, screening function: general, [Sch13]).

Torgot motorial	Energy loss [keV/nm]			
l'arget material	Ca ¹⁰⁺	Ca ¹⁹⁺	Au ²⁶⁺	Au ⁵²⁺
Copper	6.22	12.09	34.75	70.64
Tungsten	9.32	17.01	50.96	94.75
Aluminum	2.38	4.64	13.53	27.20

Table 19: Results of the fits of the desorption yields using equation (78)

Sample	к	κ error	n	<i>n</i> error
OFCu milled (1)	4.34E+2	1.90E+2	0.96	0.11
OFCu milled (2)	1.32E+2	3.14E+1	1.38	0.06
OFCu milled + annealed (1)	3.24E+1	6.22E+0	1.22	0.05
OFCu milled + annealed (2)	3.68E+1	3.23E+0	1.15	0.02
OFCu polished (SiC)	8.67E+1	2.31E+1	1.36	0.06
OFCu polished (SiC) + annealed	2.62E+1	7.71E+0	1.19	0.07
OFCu polished (CaCO₃)	3.18E+1	1.35E+1	1.48	0.10
OFCu lapped	1.04E+3	6.74E+2	1.24	0.16
OFCu polished (diamond)	9.77E+1	3.24E+1	1.18	0.08
OFCu lapped + polished (diamond)	2.32E+2	1.38E+2	1.00	0.15
Cu single crystal	4.42E+0	1.45E+0	2.08	0.08
Cu single crystal annealed	1.93E+0	7.20E-1	1.93	0.09
W untreated	3.66E+3	4.62E+3	0.96	0.29
W lapped	3.95E+3	7.56E+3	0.79	0.45
W lapped + etched	7.09E+3	1.61E+4	0.62	0.54
W lapped + polished	8.82E+2	1.55E+3	0.74	0.41
W lapped + polished + annealed	8.96E+1	3.35E+1	1.32	0.08
W lapped + etched + polished	4.48E+2	4.31E+2	1.10	0.22
W lapped + etched + polished + annealed	4.03E+2	5.15E+2	1.00	0.29
W lapped + etched + polished + etched	3.05E+2	3.23E+2	1.09	0.24
W lapped + etched + polished + etched +	5.28E+3	2.03E+4	0.53	0.93
annealed				
Al1050	1.88E+2	7.25E+0	1.46	0.01
Al1050 annealed	3.87E+1	1.30E+1	1.69	0.10
Al6061	1.67E+2	7.83E+0	1.49	0.02
Al6061 annealed	1.89E+2	1.55E+1	1.36	0.03

For the OFCu and aluminum samples, the scaling with $\eta \sim (dE/dx)_{elec}^n$ is well fulfilled. In the double logarithmic scale of Figure 64 and Figure 66, the data points lie on a straight line for both ions and charge states. It can be concluded that the ions reach the equilibrium charge state in a sample depth that is much larger than the escape depth of the desorbed particles, otherwise one would not see a difference in the desorption for the two charge states of the ion. The ions usually reach equilibrium charge state within less than 10 % of their range [Tou06], in the given energy regime this corresponds to several tens of nm [Ass17].

For the tungsten samples, the difference in the desorption yields is less for the two charge states compared to the difference between the two ion species (Figure 65). Furthermore, the exponents derived by the fitting are surprisingly small compared to the other materials and have large uncertainties. Hence, the values of the exponents derived for the tungsten samples are not reliable. When excluding the fit results of the tungsten samples, the mean value of the exponent changes to $n = 1.39 \pm 0.08$, which is in good agreement with the result from Caron et al.



Figure 64: Desorption yields as a function of the electronic energy loss for OFCu samples. The desorption yields were calculated from the total pressure (nitrogen equivalent). The lines show the derived fit functions.



Figure 65: Desorption yields as a function of the electronic energy loss for tungsten samples. The desorption yields were calculated from the total pressure (nitrogen equivalent). The lines show the derived fit functions.



Figure 66: Desorption yields as a function of the electronic energy loss for copper single crystals and aluminum samples. The desorption yields were calculated from the total pressure (nitrogen equivalent). The lines show the derived fit functions.

6.3 Measurements at CRYRING

The fast pressure measurement technique for the desorption experiment at CRYRING worked very well. Figure 67 shows the pressure evolution during one ion pulse. The pressure was calculated with equation (71) from the ion current of the extractor gauge measured with the femtoammeter.



Figure 67: Pressure evolution derived from the ion current of the extractor gauge measured by the femtoammeter during one ion pulse (Au^{78+} , specific energy: 4.8 MeV/u, pulse length: approx. 0.23 µs) for the lapped and etched OFCu sample. The ion pulse arrives at approximately 0.4 s.

In Figure 67 the pressure increase due to the ion pulse arriving at approximately 0.4 s is clearly seen. About 3 s after the arrival of the ion pulse, a valley is observed. This is not related to a pressure drop, but is due to an electromagnetic perturbation during the ramping of the main dipole magnet of the CRYRING. The amplitude of the main dipole is shown in Figure 68. The minimum of the magnet amplitude is reached approximately 3 s after the extraction of the beam. The correlation between the valley in the pressure curve and the magnet ramp was confirmed by a dedicated test measurement without magnet ramping.



Figure 68: Beam intensity as measured by the beam transformer (top) and amplitude of the main dipole (bottom) at CRYRING during one accelerator cycle. The x-axis indicates the time in hh:mm:ss. The beam is extracted at 00:07:17.8. The minimum of the magnet ramp is at about 00:07:20.8. This time interval of approximately 3 s corresponds to the observe time lag in the pressure signal between the arrival of the ion pulse and the minimum.

Figure 69 shows the results of the desorption measurements at CRYRING with Au⁷⁸⁺ ions of 2, 3 and 4.8 MeV/u. The beam intensity decreases with decreasing ion energy, because more ions get lost in the ring during the deceleration process. For the milled OFCu sample, no pressure increase was measurable even during the irradiation with the highest intensity at 4.8 MeV/u. For the OFCu sample coated with TiN, the pressure increase at 2 MeV/u was very small resulting in large error bars. The desorption behavior of the samples follows the same trend as during the measurements at the M-branch, but the yields are more than a factor of 5 smaller compared to the yields determined from the M-branch measurements. From theory, the yields are expected to be larger, because the charge state of the ions used at CRYRING was higher resulting in a larger energy loss.

The statistical errors from the pulse-to-pulse deviations are small, but the measurements have large systematic uncertainties. One source of error is the determination of the number of particles per pulse. At the present state, no data exist about the extraction efficiency for different ions and beam energies. For the data analysis, the extraction efficiency is assumed to be constant, but the results indicate that this is not the case. Additionally, at low intensities it is difficult to determine in the data the exact moment when the extraction takes place and to derive the right particle numbers. The second source of uncertainties is the determination of the number of desorbed molecules. When calculating the desorption yields from the difference between the base pressure and the maximum pressure in the single shot method, the pumping speed is neglected. However, the vacuum vessel at CRYRING has a large pumping speed of \geq 400 l/s. It would be more accurate to

integrate the pressure pulse and multiply it with the effective pumping speed rather than using the product of pressure increase and vessel volume. However, because of the perturbation due to the magnet ramping, it is not possible to define the end of the pressure pulse and thereby the upper integration limit.



Figure 69: Desorption yields measured at CRYRING with Au⁷⁸⁺ ions for different ion energies. Error bars represent statistical errors for different ion pulses.



Figure 70: Desorption yields as a function of the electronic energy loss measured with Au⁷⁸⁺ ions. Error bars represent statistical errors.

To measure desorption as a function of the electronic energy loss, the energy loss was varied by changing the kinetic energy of the ion. The desorption yields as a function of energy loss are shown in Figure 70. The energy loss was calculated by the software CasP (version 5.2, model: UCA, screening function: general, [Sch13]). The scaling of the desorption yields with the electronic energy loss $\eta \sim (dE/dx)_{elec}^n$ is not observed here. There are two possible explanations. As mentioned above, the measurements have large systematic errors including the unknown extraction efficiency, which may result in a wrong determination of the particle numbers. On the other hand, the highly charged ions have large potential energies. Therefore, the ions can pick up electrons very fast, maybe even before penetrating into the solid. This results in lower charge states and smaller energy losses in the surface near regions of the sample, where desorption occurs.

The experiment shows that desorption measurements at CRYRING are possible even at the very low beam intensities. In future beam times more effort has to be spent to gain reliable results. In particular, a method to measure the beam intensity in the extraction beamline has to be implemented. A second important improvement is to remove the ramping of the main dipole magnet from the acceleration cycle. Tests showed that this is possible by adjusting the accelerator settings.

7 Summary and Conclusion

Ion-stimulated desorption yields were measured with calcium and gold ions at 4.8 MeV/u specific energy for copper, tungsten, aluminum and stainless steel samples with different pretreatments. The main desorbing gas species are hydrogen, water, carbon monoxide and carbon dioxide. The lowest desorption showed the copper single crystal, which is ascribed to the high purity and the absence of grain boundaries. Aluminum has slightly lower desorption yields than polycrystalline copper, but aluminum alloys have the disadvantage that they cannot be annealed at high temperatures and pure aluminum has a limited mechanical strength. For tungsten, the surface was smoothed by lapping, etching and polishing to achieve lowest desorption.

The desorption yields show no clear correlation with surface roughness, mean inclination angle or true surface area. Larger surface roughness trends to result in higher desorption yields, but chemical cleanliness and bulk properties are also important contributions. For surface treatments, diamond milling or polishing is recommendable, but the positive effect of polishing depends on the quality of the process. For future experiments, extended surface analysis and a larger amount of samples is needed to achieve better statistics.

Ex-situ thermal annealing was demonstrated to create a pronounced improvement of the desorption behavior. The annealing temperature has to be sufficiently large ($T \ge 300 \,^{\circ}C$), but for OFCu no significant differences were observed after annealing at temperatures between 300 and 500 $^{\circ}C$. For the copper and tungsten samples, a temperature of 400 $^{\circ}C$ and a duration of approximately 4 h have proven to be suitable parameters. However, for larger components the annealing duration have to be adjusted by observing the pressure evolution during annealing. The reduced desorption persists for at least 11 months of storage. When the samples are stored in atmosphere, the desorption yields of the annealed samples are approximately a factor of 3 lower than the yields of the untreated samples. Even lower desorption can be achieved by storage in argon. No distinct relationship to the storage time was observed. This indicates the great advantage of the developed annealing procedure: accelerator components can be annealed ex-situ and stored until their installation. The ex-situ annealing is also applicable for accelerator parts, which cannot be baked in-situ.

NEG-coated stainless steel samples showed lower desorption than uncoated stainless steel. Annealing at 400 °C for 4 h leads to the lowest desorption among the NEG-coated samples. It was not possible to measure ion-stimulated desorption for activated NEG films. It could be expected that the yield of an activated NEG film is even lower. In contrast, titanium nitride and carbon coatings turned out to be not suitable for applications in heavy ion accelerators.

Another approach to reduce ion-stimulated desorption is surface cleaning by sputtering with 3–5 keV argon ions. For sputter cleaning, the fluence, energy and incidence angle of the argon ions were varied, but none of the parameters showed a clear influence on the desorption yield. For sputter cleaned samples, subsequent annealing has only a minor effect. Increased desorption of argon, as reported for argon glow discharge cleaning, was observed only for thermal desorption not for ISD. For ion-stimulated desorption, the implantation depth of argon ions with energies ≥ 3 keV is obviously larger than the escape depth of the desorbing gas particles. The sputter technique could be used in future experiments to clarify from which depth the desorbed gas originates. By varying the ion energy, gas ions can be implanted in different depths. For copper, the measurements indicate that the upper limit for the escape depth is smaller than the range of the 3 keV argon ions, which is approximately 2.5 nm [Zie13].

For several samples, ion-stimulated desorption was measured with calcium and gold ions of two different charge states (Ca¹⁰⁺, Ca¹⁹⁺, Au²⁶⁺ and Au⁵²⁺). For copper and aluminum, the desorption yields are proportional to the electronic energy loss to the power of $n = 1.39 \pm 0.08$. In contrast, for tungsten the desorption yields measured with the two charge states differ less than expected from the power function.

For most of the samples, the results from the thermal desorption measurements are in good agreement with the ion-stimulated desorption measurements. The pressure evolution during thermal desorption spectroscopy

can be simulated by a simple model involving Fick's laws and the Polanyi-Wigner equation. The simulation reproduces the experimental results well and the chosen input parameters are in the range of the values reported in the literature.

In addition to the experiments with continuous ion bombardment at the M-branch, also single shot measurements were conducted at CRYRING. The commissioning experiment demonstrated that ion-stimulated desorption measurements at CRYRING are possible despite the low beam intensities. However, to carry out more precise experiments in the future, a beam current measurement in the extraction beamline is required. It is also necessary to adjust the accelerator setting in order to eliminate the disturbance in the pressure signal from the ramping of the main dipole magnet.

In conclusion, the experimental results clearly indicate that ion-stimulated desorption is not a pure surface effect, but also involve processes from deeper layers. This statement is supported by the fact that the copper single crystal shows lower desorption than polycrystalline copper samples. Moreover, the positive effect of the annealing treatment persists during storage in atmosphere over several months. As the simulation of thermal desorption shows, during annealing at 400 °C gas molecules are removed from very deep layers. During storage in atmosphere, the surface is covered instantaneously with adsorbed gas particles, while the deep layers cannot be refilled with gas. To mitigate ion-stimulated desorption from accelerator components, the surface and the bulk have to be treated. Surfaces can be optimized by diamond milling, polishing or sputter cleaning, while for the bulk treatment, thermal annealing is mandatory.

8 References

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9 List of Symbols

а	fit parameter for the QMS calibration
a_0	radius of the first atomic orbit
a _{jump}	characteristic jump distance
a_{ramp}	slope of the temperature ramp
Α	area
A _{relative}	ratio of true surface area to geometrical surface area
b	fit parameter for the QMS calibration
В	stopping number
С	speed of light
С	particle concentration
<i>c</i> ₀	initial particle concentration
$c_{surface}$	particle concentration in the near-surface layer
С	vacuum conductance
C_{EXT}	calibration factor of the extractor gauge
$C_{e/a}$	specific heat of the electronic or atomic system
d	sample thickness
d_{col}	collision diameter of adatom
D	diffusion coefficient
D_0	pre-exponential factor of the diffusion coefficient
е	elementary charge
Ε	energy
E_B	binding energy
E_{des}	desorption energy
E _{dif}	activation energy of diffusion
E _{dis}	dissociation energy
f	flux term in the partial differential equation
g	coupling constant
h	Planck's constant
h _n	height difference
l	order of desorption reaction
1	mean ionization potential
I _{beam}	ion beam current
I _{emis}	electron emission current in the extractor gauge
I _{ion}	ion current in the extractor gauge
J ;	deservation rate
J des	diffusion rate
Jdif i	particle flux diffusing out of the cample
Jout Iz	Poltzmann constant
ĸ K	thermal conductivity of the electronic or atomic system
me/a	exponent for angle scaling of the desorption yield
m.	molecular mass
m	electron mass
m_{ppp}	symmetry parameter in the partial differential equation
m/a	mass-to-charge ratio
M	molar mass
n	exponent for dE/dx scaling of the desorption vield
n_0	initial volumetric particle concentration in the vacuum
n_e	electron density
-	

\vec{n}	normal vector
\vec{n}_{Λ}	normal vector of the triangle in the AFM measurements
Ň	atomic density
N_{A}	Avogadro constant
Nion	number of impacting ions
Nnirel	number of pixels
Ntot	total number of desorbed particles
p	pressure
$p_{chamber}$	pressure in the vacuum chamber
p_{int}	value of the integral $\int \Delta p(t) dt$
q	gas flow
q_{ion}	charge state
Q	amount of gas
r	radius
\vec{r}	position vector
R	universal gas constant
S	source term in the partial differential equation
<i>s</i> ₀	sticking coefficient
S(E)	stopping power
S	pumping speed
S_0	fit parameter for the pumping speed
S_1	fit parameter for the pumping speed
Sa	arithmetical mean height
S_{eff}	effective pumping speed
t	time
$t_{e/a}$	oscillation time of electrons or atoms
Т	temperature
$T_{e/a}$	temperature of the electronic or atomic system
T _{chamber}	temperature of the vacuum chamber
Tgas	temperature of the gas
T_{max}	final temperature
T_{sample}	temperature of the sample
и	pre-factor in the partial differential equation
v	velocity
v_0	electron velocity in the first atomic orbit / Bohr velocity
V	volume
x	depth coordinate
x_d	depth of the concentration change
$x_{surface}$	thickness of the surface layer for calculation of the areal particle density
Y	sputter yield
Z_{eff}	effective charge state
Z_p	atomic number of the projectile
Z_t	atomic number of the target

- α exponent for fluence scaling of the desorption yield
- δ inclination angle
- δ_m mean inclination angle
- Δp pressure increase
- ϵ_0 vacuum electric permittivity
- η desorption yield
- θ surface coverage
- κ fit parameter for dE/dx scaling of the desorption yield
- ν jump frequency
- u_{dif} average jump frequency of the adatoms on the surface
- v_i pre-exponential factor for desorption
- σ number of adparticles per surface area
- σ_{mono} number of adparticles per surface area in one monolayer
- σ_s number of adsorption sites per surface area
- ho mass density
- au fit parameter for the pumping speed
- au_0 period of the lattice oscillations
- φ incidence angle
- Φ ion fluence

10 List of Acronyms

AFM	Atomic force microscopy
ann.	annealed
CasP	Convolution approximation for swift Particles
deg.	degree
DN	Nominal diameter
ECR	Electron Cyclotron Resonance (ion source)
EDX	Energy-dispersive X-ray spectroscopy
ESD	Electron-stimulated desorption
ESR	Experimental Storage Ring
etch.	etched
FAIR	Facility for Antiproton and Ion Research
FCC	Future Circular Collider
HIAF	High Intensity Heavy-ion Accelerator Facility
ISD	Ion-stimulated desorption
ITO	Indium tin oxide
lap.	lapped
MGR	Menzel-Gomer-Redhead (model for ESD and PSD)
NEG	Non-evaporable getter
OFCu	Oxygen-free copper
PBN	Pyrolytic boron nitride
PG	Pyrolytic graphite
PIG	Penning Ionization Gauge (ion source)
pol.	polished
PSD	Photon-stimulated desorption
QMS	Quadrupole mass spectrometer
SEM	Scanning electron microscopy
SIP	Sputter ion pump
SIS	Schwerionen-Synchrotron / Heavy ion synchrotron
SPIRAL2	Système de Production d'Ions Radioactifs en Ligne de 2e generation
sputt.	sputtered
SRIM	The stopping and range of ions in matter
st.	stainless
TDS	Thermal desorption spectroscopy
TSP	Titanium sublimation pump
UCA	Unitary convolution approximation
UNILAC	Universal linear accelerator
UHV	Ultra-high vacuum
WRG	Wide-range gauge
YAG	Yttrium aluminum garnet

11 Appendix

11.1 Input Parameters for the Thermal Spike Calculations

Table 20 presents the input parameters for the thermal spike calculations. The electronic and nuclear energy loss of the 4.8 MeV/u gold ion was determined with SRIM (Version SRIM-2013, [Zie13]). The oscillation time of the electrons t_e is calculated by

$$t_e = 2\pi \sqrt{\frac{\epsilon_0 m_e}{e^2 n_e}} \tag{79}$$

where n_e is the electron density. For the atoms the oscillation time is determined by

$$t_a = 2\pi \sqrt{\frac{\epsilon_0}{\rho} \left(\frac{M}{eN_A}\right)^2} \tag{80}$$

with ρ as mass density, M as molar mass and N_A as Avogadro constant. The specific heat of the lattice as a function of temperature is described by the following polynomial

$$C_a = C_0 + C_1 T + C_2 T^2 + C_3 T^3$$
(81)

The corresponding polynomial for the thermal conductivity of the lattice is

$$K_a = K_0 + K_1 T + K_2 T^2 + K_3 T^3 + K_4 T^4$$
(82)

The coefficients for the polynomials are listed in Table 21 and Table 23 for copper and in Table 22 and Table 24 for aluminum.

thermal spike model					
	Copper	Aluminum	Reference		
Initial temperature [K]	300	300	-		
Number of valence electrons	1.5	1.5	[Zim19]		
Specific energy [MeV/u]	4.8	4.8	-		
Electronic subsystem					
Oscillation time of electrons [fs]	0.383	0.258	-		
Oscillation time deviation [fs]	0.383	0.258	-		
Electronic energy loss [keV/nm]	60.56	24.84	[Zie13]		
Ionization potential [eV]	7.73	5.99	[Lia23]		
Beam energy radius parameter	1.667	1.667	[Wal86]		
Atomic subsystem					
Oscillation time of atoms [fs]	130	101	-		
Oscillation time deviation [fs]	130	101	-		
Nuclear energy loss [keV/nm]	0.12	0.04	[Zie13]		
Thermal properties					
Molar mass [g/mol]	63.546	26.97	[Wan94]		
Solid mass density [g/cm ³]	8.93	2.7	[Wan94]		
Liquid mass density [g/cm ³]	7.94	2.368	[Wan94]		
Melting temperature [K]	1356	933	[Wan94]		
Evaporation temperature [K]	2840	2740	[Wan94]		
Debye temperature [K]	343	428	[Wan94]		

Table 20: Input parameters for the calculation of the temperature distribution around the ion trajectory with the inelastic thermal spike model

Table 21: Coefficients for the calculation of the lattice specific heat of copper as a function of temperature [Wan94]

Temperature thresholds [K]		Lattice specific heat coefficients [J/(g K)]			
Lower	Upper	C ₀	C ₁	C ₂	C ₃
10	100	0.0058	-0.0015	0.000093	-5.3E-07
100	300	-0.053	0.0046	-0.000017	2.2E-08
300	1356	0.36	0.000086	2.9E-09	0
1356	inf	0.5	0	0	0

Table 22: Coefficients for the calculation of the lattice specific heat of aluminum as a function of temperature [Wan94]

Temperature thresholds [K]		Lattice specific heat coefficients [J/(g K)]								
Lower	Upper	Co	C ₁	C ₂	C ₃					
10	100	0.032	-0.0045	0.00018	-8.70E-07					
100	300	-0.34	0.012	-4.00E-05	5.00E-08					
300	700	0.76	4.60E-04	0	0					
700	inf	1.08	0	0	0					

Table 23: Coefficients for the calculation of the thermal conductivity of copper as a function of temperature [Wan94]

Temperature thresholds [K]		Thermal conductivity coefficients [W/(cm K)]									
Lower	Upper	Ko	K ₁	K ₂	K ₃	K ₄					
4	15	22.6	9.2	1	-0.079	0					
15	100	287	-15	0.31	-0.0029	0.0000097					
100	300	6.7	-0.035	0.00015	-2E-7	0					
300	1356	3.9	0.0013	-0.000003	9.2E-10	0					
1356	2000	0.6	0.0011	-2.6E-7	0	0					
2000	inf	2.1	0	0	0	0					

Table 24: Coefficients for the calculation of the thermal conductivity of aluminum as a function of temperature [Wan94]

Temperature thresholds [K]		Thermal conductivity coefficients [W/(cm K)]									
Lower	Upper	Ko	K ₁	K ₂	K ₃	K ₄					
6	15	-4.04	9.67	-3.2	0	0					
15	100	146.5	-6.8	0.12	-0.001	3.80E-06					
100	300	8.84	-0.11	7.50E-04	-2.20E-06	2.40E-09					
300	933	2.4	0	0	0	0					
933	2740	0.63	3.30E-04	0	0	0					
2740	inf	1.5	0	0	0	0					

11.2 MATLAB Code for the Simulation

11.2.1 Simulation of Diffusion Combined with Desorption

```
Main program:
global T max E dif E des R k h D0 C0 Csurface ramp x d sigma s x surface
%Simulation parameter
d=4e-3; %Sample thickness [m]
xmesh=linspace(0,d,101); %x nodes [m]
dx=xmesh(2)-xmesh(1); %Distance between x nodes [m]
stst=500; %Number of temporal nodes
tspan=linspace(0,14400,stst); %temporal nodes [s]
m PDE=0; %Symmetry parameter 0=planar
%Constants
R=8.3144; %Universal gas constant [J/(mol*K)]
k=1.3806e-23; %Boltzmann constant [J/K]
h=6.626e-34; %Planck's constant [Js]
%TDS parameters
T_max=400; %Final temperature [°C]
ramp=6/60; %Slope of the temperature ramp [K/s]
%Physical parameters
D0=8.5e-6; %[m^2/s]
E_dif=40e3; %Activation energy for diffusion [J/mol]
E des=64e3; %Desorption energy [J/mol]
C0=3e23; %Initial concentration [1/m^3]
Csurface=1e22; %Initial concentration close to surface [1/m^3]
x d=1.0e-4; %Depth of Csurface [m]
sigma_s=1e19; %Number of adsorption sites [1/m<sup>2</sup>]
Seff=0.27; %Effective pumping speed [m^3/s]
x_surface=1e-9; %Depth for surface integration [m]
%Solving of the differential equation
sol=pdepe(m_PDE,@(x,t,c,DcDx) PDE_ramp(x,t,c,DcDx,d,dx,D0,E_dif),...
    @(x) Init_cond(x,d,dx),@Boundary_Des,xmesh,tspan);
%Calculation of particle flux j dif
j dif=zeros(stst,101);
Temp2=zeros(1,stst);
for i=1:stst
    ci=sol(i,:);
    [c,dcdx]=pdeval(m,xmesh,ci,xmesh); %c: concentration [1/m^3],...
        %dc/dx: derivative of the concentration [1/m^4]
    Temp=tspan(i).*ramp+273;
    if tspan(i)<=(T max/ramp)</pre>
        Temp2(i)=Temp;
    else
        Temp2(i)=T_max+273;
    end
    D=D0.*exp(-E dif./(R.*Temp2(i))); %Diffusion coefficient [m^2/s]
```

```
j_dif(i,:)=D.*dcdx; %[1/(s*m^2)]
end
%Calculation of particle flux out of the sample
A=pi.*5e-3.^2; %Sample area [m^2]
j_out=A.*j_dif(:,1); %Particle flux as function of time [1/s]
%Calculation of pressure increase
delta_p=j_out.*k.*300./Seff.*1e-2; %Pressure increase [mbar]
N_tot=trapz(tspan,j_out); %Total number of desorbed particles
Q_tot=N_tot.*k.*300.*10./(pi.*0.5.^2); %Total amount of desorbed gas [mbar*1/cm^2]
```

Definition of the differential equation:

```
function[u,f,s] = PDE_ramp(x,t,c,DcDx,d,dx,D0,E_dif)
global T_max R ramp
T=t.*ramp+273;
if t>=T_max/ramp
    T=T_max+273;
end
D=D0.*exp(-E_dif./(R.*T)); %Diffusion coefficient [m^2/s]
f=D.*DcDx; %Flux term
u=1; %Left part of equation
s=0; %Source term
```

Definition of the initial condition:

```
function cinit = Init_cond(x,d,dx)
global C0 Csurface x_d
if x<=x_d
    cinit=Csurface;
else
    cinit=C0;
end</pre>
```

Definition of the boundary conditions with desorption:

```
function [pl,ql,pr,qr] = Boundary_Des(xl,cl,xr,cr,t)
global T_max E_des R k h ramp sigma_s x_surface
%Left boundary (desorption)
T=t.*ramp+273;
if t>=(T_max/ramp)
    T=T_max+273;
end
sigma=cl*x_surface;
j=k.*T./h./sigma_s.*sigma.^2.*exp(-E_des./(R.*T);
```

pl=j; ql=-1;

%Right boundary (no flux)
pr=0;
qr=1;

Definition of the boundary conditions with constant particle concentration at one side:

function [pl,ql,pr,qr] = Boundary_cconst(xl,cl,xr,cr,t)
global n0

%Left boundary (constant particle concentration n0)
pl=cl-n0;
ql=0;

```
%Right boundary (no flux)
pr=0;
qr=1;
```

11.2.2 Simulation of Desorption from a Partially Covered Surface

Main program:

```
global k h R sigma_mono
%Constants
R=8.3144; %Universal gas constant [J/(mol*K)]
k=1.3806e-23; %Boltzmann constant [J/K]
h=6.626e-34; %Planck's constant [Js]
sigma_mono=1e19; %Number of particles in one monolayer [1/m^2]
%Physical parameters
T0=296; %Temperature for coverage calculation [K]
tau0=h/(k*T0); %Period of the lattice oscillations [s]
s0=0.1; %Sticking coefficient
m_H2=2e-3/6.022e23; %Molecular mass H2 [kg]
E des=64e3; %Desorption energy [J/mol]
p0=3e-9; %Initial chamber pressure [Pa]
Seff=0.27; %Effective pumping speed [m^3/s]
%Calculation of the initial coverage with the Henry adsorption isotherm
theta=s0*tau0*exp(E_des/(R*T0))/(sigma_mono*sqrt(2*pi*m_H2*k*T0))*p0;
sigma0=theta*sigma mono; %[1/m^2]
%Solving of the differential equation
stst=500; %Number of temporal nodes
tspan=linspace(0,14400,stst); %Temporal nodes [s]
sol=ode15s(@(t,n) DGL_Desorption_TDS(t,sigma,E_des),tspan,sigma0);
[sigmai,dsigmadt]=deval(sol,tspan); %sigmai: surface concentration [1/m^2],...
    %dsigmadt: derivative of surface concentration [1/(m^2*s)]
```

%Calculation of pressure increase A=pi.*5e-3.^2; %Sample area [m^2] j_des=-A.*dsigmadt; %Particle flux as function of time [1/s] delta_p=j_des.*k.*300./Seff.*1e-2; %Pressure increase [mbar] N_tot=trapz(tspan,j_des); %Total number of desorbed particles Q_tot=N_tot.*k.*300.*10/(pi.*0.5.^2); %Total amount of desorbed gas [mbar*1/cm^2]

Definition of the differential equation:

function j = DGL_Desorption_TDS(t,sigma,E_des)
global k h R sigma_mono
T=t.*0.1+273; %Temperature [K]
if T>673
 T=673;
end
j=-k./h.*T./sigma_mono.*sigma.^2.*exp(-E_des./(R.*T));

11.3 Surface Roughness Determined by AFM Measurements

Table 25: Surface parameters determined by AFM measurements in tapping mode. Sa denotes the arithmetical mean height, δ_m the mean inclination angle and $A_{relative}$ the ration of true surface area to geometrical surface area as defined in equation (76).

Sample	<i>Sa</i> [nm]	Standard	δ_m	Standard	A _{relative}	Standard
		deviation	[degree]	deviation		deviation
		<i>Sa</i> [nm]		δ_m [deg.]		A _{relative}
OFCu untreated	18.60	3.73	6.55	0.45	0.0108	0.0022
OFCu lap.	77.10	7.38	23.78	0.54	0.1571	0.0094
OFCu lap.+pol.	13.00	3.69	8.64	0.91	0.0210	0.0051
OFCu lap.+etch.+pol.	45.00	19.90	12.70	3.23	0.0581	0.0255
OFCu lap.+etch.+pol.+	79.70	19.60	23.48	4.14	0.2298	0.0801
etch.						
OFCu annealed	44.40	4.55	17.34	1.02	0.0745	0.0105
W untreated	53.40	14.10	15.92	1.88	0.0691	0.0168
W lap.	56.60	3.25	21.87	0.86	0.1216	0.0116
W lap.+etch.	122.00	15.60	27.40	0.18	0.2299	0.0113
W lap.+pol.	11.50	1.74	10.03	0.69	0.0267	0.0040
W lap.+etch.+pol.	7.19	0.45	7.02	0.83	0.0129	0.0024
W lap.+etch.+pol.+etch.	13.20	1.46	11.34	0.84	0.0325	0.0041
NEG untreated	15.30	2.68	6.06	0.36	0.0088	0.0011
NEG 3.6h at 400°C	28.60	6.86	8.89	1.02	0.0182	0.0039
NEG 24.4h at 180°C	45.00	8.10	14.42	1.69	0.0680	0.0171
NEG 60h at 180°C	32.20	6.87	10.68	1.58	0.0430	0.0128
WCu	16.40	1.75	10.74	1.07	0.0314	0.0069
Al1050	4.42	0.61	3.75	0.24	0.0036	4.59E-4
Al6061	3.88	0.88	3.93	0.61	0.0051	0.0017
OFCu lap.	80.60	6.84	27.34	1.60	0.2285	0.0314
OFCu pol. (diamond)	4.78	0.33	5.65	0.42	0.0079	9.96E-4
OFCu lap.+pol.	13.70	4.37	12.60	2.02	0.0641	0.0208
(diamond)						
OFCu pol. (SiC)	4.97	0.39	5.76	0.22	0.0075	5.94E-4
OFCu pol. (CaCO₃)	6.44	0.43	7.88	0.41	0.0143	0.0015
Cu single crystal	5.74	1.01	5.45	0.46	0.0071	0.0013
Cu single crystal ann.	3.10	0.27	5.76	0.61	0.0109	0.0022
OFCu plasma elec. pol. 1	20.20	0.27	9.97	0.48	0.0216	0.0022
OFCu plasma elec. pol. 2	26.80	1.11	9.36	1.06	0.0209	0.0042
OFCu sputt. 2.96e18	16.50	1.08	6.79	0.26	0.0103	6.74E-4
annealed						
OFCu sputt. 1.17e18	7.60	1.50	4.03	0.35	0.0039	7.65E-4
annealed						
OFCu sputt. 2.21E18	10.50	0.36	6.68	0.40	0.0096	0.0012
annealed						
OFCu sputt. 3.67E18	10.80	0.67	4.05	0.21	0.0035	4.00E-4
annealed						
OFCu sputt. 4.35E18	14.50	0.53	7.13	0.52	0.0113	0.0017
annealed						
OFCu sputt. 3.40E18	15.20	1.32	8.74	0.10	0.0186	6.13E-4

11.4 Results of the Thermal Desorption Measurements

Measurement	Sample	Total	Total	H₂	H₂	H₂O	H₂O	со	со	CO2	CO2	Ar	Ar
			Error										
20190328_1313	OFCu lap	1.05E-2	2.97E-3	1.66E-2	5.07E-3	7.82E-3	2.08E-3	2.63E-4	7.16E-5	3.98E-3	3.83E-3	5.17E-6	1.40E-6
_R1-26													
20190328_1953	OFCu lap+etch	5.52E-2	1.56E-2	3.00E-2	9.14E-3	1.31E-2	3.49E-3	1.18E-2	3.19E-3	2.94E-2	2.83E-2	2.49E-5	6.74E-6
_R1-27													
20190329_1009	OFCu lap+pol	1.09E-2	3.08E-3	1.55E-2	4.73E-3	3.30E-3	8.78E-4	8.54E-4	2.32E-4	4.52E-3	4.34E-3	5.51E-6	1.49E-6
_R1-28													
20190401_0941	OFCu lap+etch+	8.65E-3	2.45E-3	1.78E-2	5.42E-3	3.16E-3	8.41E-4	2.38E-4	6.47E-5	2.92E-3	2.80E-3	3.13E-6	8.46E-7
_R1-29	pol												
20190329_1556	OFCu lap+etch+	1.08E-2	3.05E-3	1.11E-2	3.39E-3	3.70E-3	9.85E-4	1.29E-3	3.51E-4	7.48E-3	7.19E-3	3.35E-6	9.06E-7
_R1-30	pol+etch												
20200306_1516	W untreated	8.59E-4	2.43E-4	8.88E-4	2.70E-4	6.25E-4	1.66E-4	9.18E-5	2.50E-5	1.83E-4	1.76E-4	3.81E-7	1.03E-7
_R1-9													
20190401_1902	W lap	2.31E-3	6.54E-4	1.56E-3	4.75E-4	1.27E-3	3.38E-4	2.20E-4	5.97E-5	6.35E-4	6.10E-4	2.35E-7	6.36E-8
_R1-10													
20190402_0940	W lap+etch	1.15E-3	3.25E-4	9.69E-4	2.95E-4	4.21E-4	1.12E-4	2.58E-4	7.01E-5	5.88E-4	5.65E-4	3.77E-7	1.02E-7
_R1-11													
20190402_1634	W lap+pol	1.73E-4	4.91E-5	1.68E-4	5.10E-5	5.14E-5	1.37E-5	6.21E-5	1.69E-5	2.03E-4	1.95E-4	0	
_R1-12													
20190405_0938	W lap+etch+pol	1.53E-4	4.32E-5	2.03E-4	6.17E-5	4.27E-5	1.14E-5	4.67E-5	1.27E-5	1.45E-4	1.39E-4	0	
_R1-13													
20190405_1622	W lap+etch+	1.09E-4	3.09E-5	1.64E-4	4.98E-5	3.46E-5	9.21E-6	3.13E-5	8.51E-6	8.21E-5	7.89E-5	0	
_R1-14	pol+etch												

Table 26: Results of the TDS measurements of the OFCu and tungsten sheet samples

Table 27: Results of the TDS measurements of the copper, aluminum and WCu samples

Measurement	Sample	Total	Total Error	H ₂	H ₂ Error	H ₂ O	H ₂ O Error	со	CO Error	CO2	CO₂ Error	Ar	Ar Error
20200304_1057 _5-1	OFCu milled (1)	1.83E-3	5.18E-4	1.48E-2	4.50E-3	2.31E-4	6.14E-5	3.86E-5	1.05E-5	1.51E-4	1.45E-4	6.55E-8	1.77E-8
	OFCu milled (2)	1.29E-3	3.65E-4	8.36E-3	2.54E-3	1.98E-4	5.26E-5	3.56E-5	9.68E-6	1.46E-4	1.40E-4	1.94E-8	5.25E-9
20200310_0914 _5-18	OFCu polished (SiC)	2.10E-3	5.94E-4	1.26E-2	3.84E-3	7.44E-4	1.98E-4	1.01E-4	2.75E-5	4.41E-4	4.24E-4	2.12E-7	5.73E-8
20200305_0858 _6-1	WCu	2.66E-3	7.53E-4	1.46E-2	4.44E-3	3.70E-4	9.84E-5	4.58E-5	1.25E-5	1.50E-4	1.44E-4	4.37E-8	1.18E-8
20210211_0953 _6-11	Al1050	4.43E-4	1.26E-4	1.81E-3	5.50E-4	4.23E-5	1.13E-5	3.28E-5	8.91E-6	4.91E-5	4.72E-5	2.49E-7	6.74E-8
20200305_1647 _6-8	Cu single crystal	6.31E-4	1.79E-4	1.27E-3	3.88E-4	3.00E-4	7.97E-5	6.66E-5	1.81E-5	2.66E-4	2.56E-4	1.51E-7	4.09E-8
20210303_0811 _8-6_300Grad	OFCu, 300 °C	1.00E-3	2.83E-4	2.97E-3	9.04E-4	1.99E-4	5.29E-5	7.43E-5	2.02E-5	2.36E-4	2.27E-4	0	
20210204_0830 _8-9	OFCu, 400 °C	2.12E-3	6.02E-4	1.16E-2	3.54E-3	8.36E-5	2.22E-5	4.27E-5	1.16E-5	1.31E-4	1.26E-4	1.54E-7	4.17E-8
20210302_0853 _8-5_500Grad	OFCu, 500 °C	1.68E-3	4.76E-4	5.97E-3	1.82E-3	2.16E-4	5.74E-5	6.57E-5	1.78E-5	2.03E-4	1.95E-4	0	
20220404_1536 _10-9	OFCu, 300 °C	2.47E-3	7.00E-4	7.16E-3	4.46E-3	9.19E-4	3.20E-4	9.63E-5	3.42E-5	1.09E-3	3.25E-4	0	
20220405_1509 _10-10	OFCu, 300 °C	2.95E-3	8.37E-4	8.09E-3	5.04E-3	1.05E-3	3.64E-4	8.48E-5	3.01E-5	1.21E-3	3.62E-4	0	
20220331_0948 _10-7	OFCu, 400 °C	3.63E-3	1.03E-3	1.04E-2	6.47E-3	1.55E-3	5.40E-4	4.27E-5	1.52E-5	1.14E-3	3.41E-4	4.71E-7	1.33E-7
20220404_0900 _10-8	OFCu, 400 °C	3.12E-3	8.84E-4	9.67E-3	6.03E-3	7.07E-4	2.46E-4	5.28E-5	1.87E-5	6.69E-4	1.99E-4	3.41E-7	9.65E-8
20220405_0828 _10-11	OFCu, 500 °C	4.33E-3	1.23E-3	1.29E-2	8.03E-3	9.21E-4	3.21E-4	1.06E-4	3.78E-5	1.24E-3	3.71E-4	3.95E-7	1.12E-7
20220406_1522	OFCu, 500 °C	3.66E-3	1.04E-3	9.11E-3	5.68E-3	8.14E-4	2.83E-4	8.92E-5	3.17E-5	1.21E-3	3.61E-4	0	
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_10-12													

Table 28: Results of the TDS measurements of the (OFCu samples prepared fo	r the different storage conditions
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Measurement	Sample	Total	Total	H ₂	H ₂	H₂O	H₂O	со	со	CO2	CO2	Ar	Ar
	(Storage)		Error		Error		Error		Error		Error		Error
20210708_0851	11 months,	1.13E-3	3.19E-4	2.88E-3	8.76E-4	7.69E-5	2.04E-5	2.72E-5	7.40E-6	7.77E-5	7.46E-5	0	
_9-1	atmosphere												
20210710_1618	11 months,	1.21E-3	3.44E-4	3.13E-3	9.52E-4	7.27E-5	1.93E-5	2.70E-5	7.34E-6	7.81E-5	7.50E-5	0	
_9-2	atmosphere												
20210712_0836	11 months,	1.15E-3	3.27E-4	3.03E-3	9.23E-4	7.34E-5	1.95E-5	2.59E-5	7.03E-6	7.42E-5	7.13E-5	0	
_9-3	vacuum												
20210712_1556	11 months,	1.24E-3	3.53E-4	3.48E-3	1.06E-3	6.26E-5	1.67E-5	2.16E-5	5.87E-6	6.21E-5	5.97E-5	0	
_9-4	vacuum												
20210714_0830	11 months,	1.08E-3	3.06E-4	3.00E-3	9.13E-4	5.97E-5	1.59E-5	2.24E-5	6.08E-6	6.76E-5	6.49E-5	0	
_9-5	argon												
20210714_1547	11 months,	1.42E-3	4.03E-4	3.57E-3	1.09E-3	8.63E-5	2.30E-5	3.93E-5	1.07E-5	1.14E-4	1.09E-4	0	
_9-6	argon												
20211006_0827	8 months,	1.07E-3	3.03E-4	3.86E-3	2.41E-3	6.05E-5	2.10E-5	5.15E-6	1.83E-6	7.05E-5	2.10E-5	5.25E-7	1.49E-7
_9-13	atmosphere												
20211006_1748	8 months,	1.22E-3	3.47E-4	4.79E-3	2.99E-3	5.82E-5	2.02E-5	3.79E-6	1.35E-6	6.27E-5	1.87E-5	5.36E-7	1.52E-7
_9-14	atmosphere												
20211007_0837	8 months,	9.85E-4	2.79E-4	3.46E-3	2.16E-3	5.58E-5	1.94E-5	3.66E-6	1.30E-6	6.64E-5	1.98E-5	5.10E-7	1.44E-7
_9-15	vacuum												
20211007_1704	8 months,	1.26E-3	3.57E-4	4.84E-3	3.02E-3	6.59E-5	2.29E-5	4.16E-6	1.48E-6	6.95E-5	2.07E-5	5.62E-7	1.59E-7
_9-16	vacuum												
20211008_0726	8 months, argon	1.27E-3	3.60E-4	4.19E-3	2.61E-3	9.39E-5	3.27E-5	5.81E-6	2.06E-6	9.76E-5	2.91E-5	5.38E-7	1.52E-7
_9-17													
20211008_1433	8 months, argon	1.13E-3	3.20E-4	4.51E-3	2.81E-3	5.26E-5	1.83E-5	3.72E-6	1.32E-6	6.06E-5	1.81E-5	5.38E-7	1.52E-7
_9-18													
20220114_0828	5 months,	1.14E-3	3.24E-4	3.79E-3	2.36E-3	6.26E-5	2.18E-5	9.87E-6	3.51E-6	6.30E-5	1.88E-5	3.09E-7	8.75E-8
_9-19	atmosphere												
20220117_0902	5 months,	1.20E-3	3.40E-4	4.28E-3	2.67E-3	5.32E-5	1.85E-5	7.05E-6	2.51E-6	5.38E-5	1.60E-5	3.25E-7	9.20E-8
_9-20	atmosphere												
20220118_0825	5 months,	1.13E-3	3.20E-4	3.78E-3	2.35E-3	5.95E-5	2.07E-5	6.92E-6	2.46E-6	6.19E-5	1.84E-5	3.13E-7	8.85E-8
_9-21	vacuum												
20220119_0821	5 months,	1.19E-3	3.38E-4	4.58E-3	2.85E-3	4.99E-5	1.74E-5	5.47E-6	1.94E-6	4.64E-5	1.38E-5	3.24E-7	9.16E-8
_9-22	vacuum												
20220120_0826	5 months, argon	1.13E-3	3.21E-4	4.23E-3	2.64E-3	4.89E-5	1.70E-5	6.02E-6	2.14E-6	5.11E-5	1.52E-5	3.28E-7	9.28E-8
_9-23													
20220121_1005	5 months, argon	1.26E-3	3.58E-4	4.48E-3	2.79E-3	6.60E-5	2.30E-5	8.51E-6	3.02E-6	5.67E-5	1.69E-5	3.66E-7	1.03E-7
_9-24													

Table 29: Results of the TDS measurements of the sputter cleaned OFCu samples

Measurement	Sample	Total	Total	H ₂	H ₂	H₂O	H₂O	со	со	CO2	CO ₂	Ar	Ar
			Error		Error		Error		Error		Error		Error
20210308_0036	OFCu pol.	2.99E-3	8.46E-4	1.13E-2	3.43E-3	2.96E-4	7.86E-5	1.13E-4	3.08E-5	3.15E-4	3.03E-4	6.37E-5	1.72E-5
_5-5	(CaCO ₃), sputt.												
	30° 2.97E18												
20210308_1201	OFCu milled,	1.82E-3	5.17E-4	9.17E-3	2.79E-3	1.01E-4	2.69E-5	3.45E-5	9.38E-6	1.02E-4	9.77E-5	4.53E-5	1.23E-5
_8-16	sputt. 30°												
	2.96E18												
20210401_0854	OFCu milled,	1.33E-3	3.78E-4	5.64E-3	1.72E-3	9.30E-5	2.47E-5	6.50E-5	1.77E-5	1.65E-4	1.59E-4	9.14E-5	2.47E-5
_8-17	sputt. 30°												
	1.17E18												
20210401_1618	OFCu milled,	1.34E-3	3.79E-4	5.75E-3	1.75E-3	7.84E-5	2.09E-5	5.10E-5	1.39E-5	1.51E-4	1.45E-4	1.02E-4	2.76E-5
_8-18	sputt. 30°												
	2.21E18												

	_												
20210401_2316	OFCu milled,	1.30E-3	3.69E-4	5.43E-3	1.65E-3	7.20E-5	1.91E-5	4.66E-5	1.27E-5	1.36E-4	1.31E-4	9.88E-5	2.67E-5
_8-19	sputt. 30°												
	3.67E18												
20210402_1054	OFCu milled,	1.28E-3	3.63E-4	5.50E-3	1.67E-3	6.53E-5	1.74E-5	4.22E-5	1.15E-5	1.25E-4	1.20E-4	8.84E-5	2.39E-5
_8-20	sputt. 30°												
	4.35E18												

Table 30: Results of the TDS measurements of the coated samples

Measurement	Sample	Total	Total	H ₂	H ₂	H₂O	H₂O	со	со	CO2	CO2	Ar	Ar
			Error		Error		Error		Error		Error		Error
20210202_0912	OFCu TiN-	7.47E-3	2.12E-3	1.72E-2	5.23E-3	1.78E-3	4.74E-4	4.10E-4	1.12E-4	4.86E-4	4.67E-4	8.00E-6	2.16E-6
_7-20	coated 200nm												
20210203_0855	OFCu TiN-	9.93E-3	2.81E-3	2.29E-2	6.98E-3	2.86E-3	7.60E-4	6.82E-4	1.85E-4	6.61E-4	6.35E-4	2.27E-5	6.14E-6
_7-17	coated 500nm												
20210206_1005	OFCu carbon-	4.46E-3	1.26E-3	1.76E-2	5.37E-3	4.18E-4	1.11E-4	4.88E-4	1.33E-4	5.67E-4	5.44E-4	4.86E-6	1.32E-6
_7-13	coated 200nm												
20210205_0837	OFCu carbon-	7.09E-3	2.01E-3	2.36E-2	7.18E-3	8.90E-4	2.37E-4	9.55E-4	2.60E-4	1.28E-3	1.23E-3	2.00E-5	5.40E-6
_7-16	coated 500nm												
20210212_0815	Stainless steel,	2.22E-4	6.29E-5	1.47E-3	4.47E-4	6.09E-6	1.62E-6	1.11E-5	3.01E-6	1.29E-5	1.24E-5	1.27E-7	3.44E-8
_R1-16	NEG-coated												

11.5 Results of the Ion-Stimulated Desorption Measurements at M-branch

11.5.1 ISD Results from Beam Time 2019

Table 31: ISD results fr														
Measurement	Sample	Total	Total	H ₂	H ₂ Error	H ₂ O	H ₂ O	со	со	CO2				
			Error				Error		Error					
20190401_1901_R1-18	OFCu lap	1.31E4	2.37E3	6.34E3	2.70E3	7.25E2	3.23E2	1.32E3	3.79E2	2.20E3				
20190401_1832_R1-19	OFCu lap+etch	1.59E5	2.87E4	2.42E4	8.07E3	3.65E4	1.45E4	2.63E4	7.43E3	4.86E4				
20190401_1813_R1-20	OFCu lap+pol	1.03E4	1.85E3	1.92E4	6.56E3	1.02E3	4.27E2	1.09E3	3.12E2	2.68E3				
20190401_1759_R1-21	OFCu	4.61E4	8.32E3	1.62E4	6.08E3	7.11E3	2.84E3	5.12E3	1.44E3	8.88E3				
	lap+etch+pol													
20190401_1746_R1-22	OFCu	7.33E4	1.32E4	2.50E4	8.53E3	1.52E4	6.04E3	9.52E3	2.69E3	1.85E4				
	lon, atch, nol, atch									1				

CO2 Error

7.30E2

1.61E4

8.86E2

2.94E3

6.10E3

time 2010 for C_2^{10+} - I-- I 24.100 Τa

Table 32: ISD results from beam time 2019 for Ca¹⁹⁺

lap+etch+pol+etch

Measurement	Sample	Total	Total	H₂	H ₂ Error	H ₂ O	H₂O	со	СО	CO2	CO2
			Error				Error		Error		Error
20190401_1420_R1-17	OFCu untreated	3.07E3	5.55E2	0.00E0	0.00E0	1.04E3	4.19E2	5.05E2	1.45E2	4.29E2	1.43E2
20190401_1507_R1-18	OFCu lap	1.49E4	2.69E3	5.33E3	1.89E3	3.06E3	1.22E3	1.37E3	3.86E2	1.79E3	5.93E2
20190403_1206_R1-18	OFCu lap	1.52E4	2.74E3	6.08E3	2.04E3	3.80E3	1.51E3	1.24E3	3.50E2	1.97E3	6.52E2
20190403_1226_R1-26	OFCu lap,	9.84E3	1.78E3	2.81E3	9.48E2	4.19E3	1.67E3	8.72E2	2.46E2	2.04E3	6.74E2
	annealed										
20190401_1533_R1-19	OFCu lap+etch	2.20E5	3.97E4	1.64E4	5.53E3	9.49E4	3.77E4	3.09E4	8.70E3	3.91E2	2.68E2
20190403_1241_R1-19	OFCu lap+etch	1.70E5	3.08E4	3.68E4	1.22E4	5.85E4	2.33E4	1.08E4	3.06E3	5.29E4	1.75E4
20190403_1310_R1-27	OFCu lap+etch,	2.77E4	5.00E3	5.34E3	1.79E3	1.17E4	4.67E3	1.03E3	2.91E2	6.38E3	2.11E3
	annealed										
20190401_1615_R1-20	OFCu lap+pol	9.42E3	1.70E3	0.00E0	0.00E0	2.21E3	8.94E2	8.35E2	2.40E2	2.26E3	7.48E2
20190403_1325_R1-20	OFCu lap+pol	1.27E4	2.29E3	3.96E3	1.33E3	4.30E3	1.71E3	8.07E2	2.28E2	2.64E3	8.72E2
20190403_1339_R1-28	OFCu lap+pol,	6.57E3	1.19E3	8.18E2	3.05E2	2.64E3	1.05E3	6.13E2	1.73E2	1.37E3	4.54E2
	annealed										
20190401_1636_R1-21	OFCu lap+etch+	3.83E4	6.91E3	1.47E3	6.16E2	1.09E4	4.32E3	2.86E3	8.09E2	6.20E3	2.05E3
	pol										

	-	-	-	-			-				
20190403_1401_R1-21	OFCu lap+etch+	3.28E4	5.93E3	6.17E3	2.07E3	1.02E4	4.06E3	2.58E3	7.28E2	6.84E3	2.26E3
	pol										
20190403_1417_R1-29	OFCu lap+etch+	6.55E3	1.18E3	9.31E2	3.69E2	1.64E3	6.54E2	5.37E2	1.52E2	1.52E3	5.02E2
	pol, annealed										
20190401_1656_R1-22	OFCu lap+etch+	6.52E4	1.18E4	9.85E3	3.43E3	2.21E4	8.81E3	4.49E3	1.27E3	1.17E4	3.86E3
	pol+etch										
20190403_1835_R1-22	OFCu lap+etch+	6.97E4	1.26E4	7.84E3	2.61E3	2.04E4	8.10E3	2.93E3	8.32E2	1.53E4	5.07E3
	pol+etch										
20190403_1855_R1-30	OFCu lap+etch+	9.12E3	1.65E3	6.54E2	3.40E2	2.06E3	8.20E2	4.19E2	1.19E2	1.72E3	5.69E2
	pol+etch,										
	annealed										
20190403_1909_R1-2	W lap	1.71E4	3.09E3	5.47E2	2.76E2	2.20E3	8.81E2	1.17E3	3.31E2	2.17E3	7.17E2
20190403_2002_R1-10	W lap, annealed	3.46E3	6.25E2	2.55E2	1.64E2	2.86E2	1.16E2	6.69E2	1.89E2	5.87E2	1.94E2
20190404_1129_R1-3	W lap+etch	4.25E3	7.67E2	5.22E2	1.88E2	5.91E2	2.36E2	3.75E2	1.06E2	9.57E2	3.17E2
20190404_1203_R1-11	W lap+etch,	1.47E3	2.65E2	3.78E2	1.39E2	2.45E2	9.81E1	1.90E2	5.38E1	1.97E2	6.51E1
	annealed										
20190406_1513_R1-4	W lap+pol	1.94E3	3.50E2	1.79E2	1.05E2	1.55E2	6.45E1	3.00E2	8.50E1	2.71E2	8.99E1
20190406_1530_R1-12	W lap+pol,	4.95E2	8.94E1	0.00E0	0.00E0	0.00E0	0.00E0	7.88E1	2.30E1	7.73E1	2.60E1
	annealed										
20190406_1549_R1-5	W lap+etch+pol	1.82E3	3.28E2	0.00E0	0.00E0	1.71E2	7.05E1	2.35E2	6.67E1	1.65E2	5.47E1
20190406_1608_R1-13	W lap+etch+pol,	4.55E2	8.22E1	1.17E2	1.28E2	5.91E1	3.10E1	6.60E1	1.99E1	7.81E1	2.64E1
	annealed										
20190406_1625_R1-6	W lap+etch+pol+	8.79E2	1.59E2	6.75E2	2.39E2	1.92E2	7.87E1	1.16E2	3.36E1	1.14E2	3.80E1
	etch										
20190406_1644_R1-14	W lap+etch+pol+	3.41E2	6.16E1	1.17E2	6.67E1	1.35E2	5.82E1	4.66E1	1.50E1	6.62E1	2.26E1
	etch, annealed										

Table 33: ISD results from beam time 2019 for $\mathrm{Au}^{^{26+}}$

Measurement	Sample	Total	Total	H ₂	H ₂ Error	H ₂ O	H ₂ O	со	со	CO ₂	CO ₂
			Error				Error		Error		Error
20190322_1634_R1-17	OFCu untreated	7.00E4	1.26E4	1.59E4	7.58E3	4.02E3	2.06E3	8.85E3	2.51E3	7.24E3	2.41E3
20190322_1926_R1-17	OFCu untreated	5.13E4	9.27E3	1.62E4	1.20E4	9.58E3	3.94E3	6.43E3	1.84E3	5.31E3	1.78E3
20190322_1612_R1-18	OFCu lap	1.60E5	2.89E4	4.33E4	1.94E4	2.61E4	1.05E4	1.96E4	5.55E3	2.23E4	7.40E3
20190322_1940_R1-18	OFCu lap	1.40E5	2.53E4	2.31E4	1.15E4	2.70E4	1.08E4	1.66E4	4.73E3	1.97E4	6.54E3
20190322_1550_R1-19	OFCu lap+etch	2.02E6	3.65E5	2.70E5	8.98E4	8.79E5	3.50E5	2.14E5	6.11E4	3.35E5	1.11E5
20190322_1858_R1-19	OFCu lap+etch	1.76E6	3.19E5	3.20E5	1.17E5	5.68E5	2.26E5	1.62E5	4.59E4	2.99E5	9.88E4
20190322_1703_R1-20	OFCu lap+pol	3.87E5	6.99E4	6.36E4	2.31E4	7.87E4	3.13E4	3.30E4	9.36E3	4.66E4	1.54E4
20190322_1837_R1-20	OFCu lap+pol	2.18E5	3.94E4	6.80E4	2.42E4	3.79E4	1.51E4	2.71E4	7.68E3	3.81E4	1.26E4
20190322_1958_R1-21	OFCu lap+etch+	1.38E5	2.50E4	2.96E4	1.25E4	1.62E4	6.56E3	2.10E4	5.96E3	1.53E4	5.08E3
20190322_1911_R1-22	OFCu lap+etch+ pol	3.02E5	5.45E4	1.04E5	3.75E4	6.83E4	2.73E4	1.74E4	4.98E3	3.97E4	1.32E4
20190322_2220_R1-1	W untreated	1.64E5	2.97E4	5.13E4	2.04E4	8.47E3	3.51E3	2.54E4	7.16E3	1.25E4	4.13E3
20190322_2129_R1-2	W lap	5.58E4	1.01E4	0.00E0	0.00E0	1.37E4	5.58E3	6.49E3	1.86E3	5.62E3	1.87E3

11.5.2 ISD Results from Beam Time 2020

Measurement	Sample	Total	Total	H ₂	H ₂ Error	H₂O	H ₂ O	СО	со	CO2	CO ₂
			Error				Error		Error		Error
20200321_0127_5-3	OFCu milled (1)	8.40E2	1.52E2	8.25E1	2.28E1	2.17E1	4.52E0	2.88E1	6.27E0	2.17E1	4.45E0
20200321_0117_5-4	OFCu milled (2)	1.20E3	2.17E2	1.07E2	2.89E1	3.67E1	7.71E0	4.22E1	9.19E0	3.07E1	6.37E0
20200321_0058_5-1	OFCu milled,	2.62E2	4.72E1	1.12E1	4.53E0	4.77E0	1.11E0	5.48E0	1.22E0	7.35E0	1.51E0
	annealed (1)										
20200321_0137_5-2	OFCu milled,	3.32E2	6.00E1	2.62E1	7.68E0	9.08E0	1.94E0	1.67E1	3.58E0	7.59E0	1.56E0
	annealed (2)										
20200321_0208_5-22	OFCu pol. (SiC)	8.63E2	1.56E2	7.16E1	1.84E1	4.17E1	8.72E0	2.76E1	6.21E0	2.24E1	4.67E0

Table 34: ISD results from beam time 2020 for Ca^{10+}

		1			1	1	1	1	1	1	
20200321_0200_5-18	OFCu pol. (SiC),	1.92E2	3.47E1	2.65E1	7.30E0	1.17E0	6.35E-1	1.82E0	4.65E-1	6.14E0	1.28E0
	annealed										
20200319_2334_6-16	OFCu pol. (CaCO ₃)	4.29E2	7.74E1	5.44E1	1.33E1	1.34E1	2.88E0	8.15E0	1.85E0	7.72E0	1.62E0
20200321_0148_5-16	OFCu lapped	7.03E3	1.27E3	5.84E2	1.40E2	1.79E3	3.66E2	2.83E2	6.33E1	5.50E2	1.14E2
20200321_0219_5-24	OFCu pol.	5.38E2	9.71E1	3.86E1	1.08E1	1.75E1	3.68E0	1.68E1	3.69E0	1.34E1	2.75E0
	(diamond)										
20200321_0108_5-15	OFCu lap.+pol.	6.88E2	1.24E2	5.50E1	1.46E1	2.19E1	4.58E0	1.88E1	4.24E0	2.21E1	4.60E0
20200319_2155_6-7	Cu single crystal	3.44E2	6.22E1	1.46E1	5.71E0	6.72E0	1.45E0	1.20E1	2.66E0	4.50E0	9.31E-1
20200321_0038_6-7	Cu single crystal	2.83E2	5.10E1	5.08E0	3.26E0	4.65E0	1.07E0	7.52E0	1.72E0	5.51E0	1.13E0
20200319_2212_6-8	Cu single crystal,	3.84E1	7.20E0	3.46E0	3.01E0	1.22E0	3.84E-1	9.82E-1	2.51E-1	3.32E0	6.95E-1
	annealed										
20200321_0048_6-8	Cu single crystal,	1.16E2	2.10E1	4.98E0	3.03E0	9.54E-1	2.87E-1	1.07E0	2.69E-1	3.87E0	7.99E-1
	annealed										
20200319_2347_R1-17	OFCu sheet,	1.89E3	3.41E2	6.62E1	1.91E1	9.39E1	1.98E1	5.71E1	1.35E1	9.14E1	1.93E1
	untreated										
20200319_2357_R1-25	OFCu sheet,	2.47E3	4.46E2	1.25E2	3.34E1	1.23E2	2.58E1	1.17E2	2.80E1	1.29E2	2.73E1
	annealed										
20200320_0010_R1-20	OFCu sheet	7.63E3	1.38E3	9.59E2	2.10E2	8.50E2	1.75E2	4.39E2	9.93E1	7.53E2	1.56E2
	lap+pol										
20200320_0027_R1-28	OFCu sheet	1.04E4	1.88E3	7.27E2	1.76E2	1.25E3	2.58E2	8.04E2	1.79E2	1.08E3	2.25E2
	lap+pol, annealed										
20200320_0842_R1-1	W untreated	1.87E4	3.37E3	2.29E3	5.33E2	1.42E3	2.93E2	1.87E3	4.89E2	1.23E3	2.72E2
20200320_0826_R1-2	W lap	1.07E4	1.93E3	4.55E2	1.03E2	1.17E3	2.40E2	5.22E2	1.56E2	7.67E2	1.69E2
20200320_0800_R1-3	W lap+etch	1.33E4	2.40E3	7.42E2	1.71E2	1.46E3	3.02E2	6.89E2	2.42E2	1.76E3	4.04E2
20200320_0743_R1-4	W lap+pol	1.78E3	3.22E2	9.53E1	2.45E1	1.01E2	2.09E1	8.39E1	1.84E1	8.32E1	2.11E1
20200320_0916_R1-12	W lap+pol,	1.51E3	2.72E2	6.64E1	1.80E1	5.74E1	1.19E1	4.45E1	9.86E0	6.72E1	1.47E1
	annealed										
20200320_0726_R1-5	W lap+etch+pol	3.42E3	6.18E2	3.47E2	8.06E1	2.46E2	5.06E1	2.48E2	5.34E1	1.54E2	3.16E1
20200320_0929_R1-13	W lap+etch+pol,	1.23E3	2.22E2	6.73E1	1.80E1	3.00E1	6.25E0	6.51E1	1.37E1	4.45E1	9.08E0
	annealed										
20200320_0700_R1-6	W lap+etch+pol+	1.89E3	3.42E2	1.08E2	2.79E1	1.38E2	2.84E1	6.32E1	1.46E1	9.13E1	1.89E1
	etch										
20200320_0943_R1-14	W lap+etch+pol+	1.25E3	2.26E2	4.01E1	1.24E1	4.69E1	9.73E0	2.77E1	6.39E0	6.06E1	1.24E1
	etch, annealed										
20200319_2224_6-2	WCu	2.98E3	5.38E2	2.90E2	7.27E1	1.95E2	4.07E1	1.74E2	3.85E1	9.65E1	2.02E1
20200319_2237_6-1	WCu, annealed	6.22E2	1.12E2	2.59E1	8.08E0	1.76E1	3.74E0	2.13E1	4.70E0	9.92E0	2.07E0
20200319_2248_6-10	Al1050	5.74E2	1.04E2	5.54E1	1.61E1	1.46E1	3.11E0	1.66E1	3.65E0	7.82E0	1.63E0
20200319_2259_6-9	Al1050, annealed	2.81E2	5.07E1	2.60E1	7.74E0	5.38E0	1.38E0	6.02E0	1.36E0	3.98E0	8.32E-1
20200319_2311_6-18	Al6061	6.25E2	1.13E2	8.79E1	2.29E1	1.07E1	2.31E0	1.64E1	3.69E0	1.05E1	2.20E0
20200319_2322_6-17	Al6061, annealed	6.55E2	1.18E2	7.45E1	2.08E1	1.47E1	3.13E0	3.03E1	6.63E0	1.25E1	2.60E0

Table 35: ISD results from beam time 2020 for Ca¹⁹⁺

Measurement	Sample	Total	Total	H ₂	H ₂ Error	H₂O	H ₂ O	со	со	CO2	CO2
			Error				Error		Error		Error
20200320_2208_5-3	OFCu milled (1)	5.52E3	9.98E2	4.94E2	1.31E2	1.59E2	3.37E1	1.84E2	4.12E1	1.52E2	3.12E1
20200320_2147_5-4	OFCu milled (2)	5.02E3	9.07E2	3.39E2	9.54E1	1.74E2	3.69E1	1.95E2	4.36E1	1.17E2	2.44E1
20200320_2056_5-1	OFCu milled, annealed (1)	7.98E2	1.44E2	5.87E1	1.81E1	2.98E1	6.40E0	1.20E1	2.91E0	1.93E1	4.04E0
20200320_2233_5-2	OFCu milled, annealed (2)	6.07E2	1.10E2	5.59E1	1.51E1	1.71E1	3.78E0	1.75E1	3.92E0	1.16E1	2.40E0
20200320_2257_5-22	OFCu pol. (SiC)	1.92E3	3.47E2	7.80E1	2.44E1	9.09E1	1.93E1	7.07E1	1.44E1	4.11E1	8.58E0
20200320_2307_5-18	OFCu pol. (SiC), annealed	3.98E2	7.19E1			3.65E0	1.16E0	5.73E0	1.38E0	8.20E0	1.73E0
20200319_1928_6-16	OFCu pol. (CaCO ₃)	1.88E3	3.39E2	8.58E1	2.89E1	7.02E1	1.50E1	4.65E1	1.07E1	2.53E1	5.35E0
20200320_2317_5-16	OFCu lapped	1.07E4	1.94E3	8.37E2	1.89E2	3.21E3	6.60E2	2.12E2	5.03E1	6.01E2	1.24E2
20200320_2245_5-24	OFCu pol. (diamond)	1.50E3	2.70E2	8.60E1	2.61E1	4.62E1	9.84E0	5.53E1	1.24E1	3.18E1	6.61E0
20200320_2136_5-15	OFCu lap.+pol.	2.08E3	3.76E2	1.55E2	4.01E1	6.65E1	1.42E1	6.39E1	1.47E1	5.63E1	1.18E1
20200319_2038_6-7	Cu single crystal	2.35E3	4.24E2	1.08E2	3.19E1	1.88E1	4.43E0	1.30E2	2.88E1	1.30E1	2.75E0
20200320_2108_6-7	Cu single crystal	1.32E3	2.38E2	7.24E1	2.08E1	2.57E1	5.63E0	6.18E1	1.37E1	1.30E1	2.69E0

20200319_2049_6-8	Cu single crystal,	7.54E2	1.36E2	3.18E1	1.67E1	1.65E1	3.88E0	3.77E1	8.01E0	7.30E0	1.56E0
	annealed										
20200320_2119_6-8	Cu single crystal,	3.84E2	6.94E1	3.34E1	1.37E1	4.27E0	1.37E0	5.59E0	1.32E0	6.62E0	1.40E0
	annealed										
20200319_1942_R1-17	OFCu sheet,	7.39E3	1.33E3	2.46E2	6.63E1	4.63E2	9.81E1	2.91E2	6.90E1	3.46E2	7.30E1
	untreated										
20200319_1954_R1-25	OFCu sheet,	7.67E3	1.38E3	2.18E2	6.45E1	4.07E2	8.56E1	3.33E2	7.91E1	3.85E2	8.12E1
	annealed										
20200319_2007_R1-20	OFCu sheet	1.74E4	3.15E3	1.63E3	3.52E2	2.03E3	4.20E2	6.17E2	1.50E2	1.41E3	2.93E2
	lap+pol										
20200319_2019_R1-28	OFCu sheet	2.04E4	3.69E3	1.19E3	2.76E2	2.73E3	5.64E2	8.92E2	2.09E2	1.62E3	3.36E2
	lap+pol, annealed										
20200320_1539_R1-1	W untreated	2.18E4	3.93E3	1.34E3	3.97E2	3.53E2	7.90E1	1.29E3	2.84E2	4.03E2	8.35E1
20200320_1529_R1-2	W lap	1.06E4	1.92E3	1.27E2	1.02E2	2.64E2	5.78E1	3.26E2	7.46E1	2.51E2	5.22E1
20200320_1515_R1-3	W lap+etch	1.43E4	2.59E3	2.61E2	1.24E2	5.10E2	1.07E2	5.43E2	1.27E2	6.02E2	1.25E2
20200320_1458_R1-4	W lap+pol	3.35E3	6.05E2	5.14E0	3.65E1	5.20E1	1.43E1	9.53E1	2.27E1	6.72E1	1.44E1
20200320_1551_R1-12	W lap+pol,	2.69E3	4.85E2	1.91E2	1.14E2	3.44E1	1.16E1	7.62E1	1.81E1	4.34E1	9.74E0
	annealed										
20200320_1446_R1-5	W lap+etch+pol	4.56E3	8.24E2	3.49E2	1.38E2	2.54E1	9.16E0	1.64E2	3.71E1	8.39E1	1.75E1
20200320_1602_R1-13	W lap+etch+pol,	3.06E3	5.52E2	3.13E2	1.30E2	2.23E1	7.81E0	1.11E2	2.39E1	5.29E1	1.09E1
	annealed										
20200320_1433_R1-6	W lap+etch+pol+	2.82E3	5.09E2			9.32E1	2.13E1	7.84E1	1.80E1	4.18E1	8.79E0
	etch										
20200320_1614_R1-14	W lap+etch+pol+	2.87E3	5.19E2	2.47E2	1.17E2	3.16E1	9.63E0	5.73E1	1.39E1	5.24E1	1.12E1
	etch, annealed										
20200319_1811_6-2	WCu	9.78E3	1.77E3	7.25E2	1.87E2	6.28E2	1.32E2	5.44E2	1.21E2	2.37E2	4.93E1
20200319_1828_6-1	WCu, annealed	1.44E3	2.60E2	3.75E1	1.81E1	4.19E1	9.04E0	4.59E1	1.00E1	1.58E1	3.30E0
20200319_1842_6-10	Al1050	1.83E3	3.31E2	9.81E1	3.19E1	4.02E1	8.67E0	5.15E1	1.15E1	1.67E1	3.52E0
20200319_1853_6-9	Al1050, annealed	8.05E2	1.45E2	1.74E1	1.47E1	2.08E1	4.99E0	1.92E1	4.33E0	7.20E0	1.56E0
20200319_1905_6-18	Al6061	1.75E3	3.17E2	1.43E2	4.11E1	3.81E1	8.49E0	4.78E1	1.07E1	1.94E1	4.07E0
20200319_1916_6-17	Al6061, annealed	1.67E3	3.01E2	1.25E2	3.90E1	4.31E1	9.29E0	7.67E1	1.69E1	1.86E1	3.89E0
										3	

Table 36: ISD results from beam time 2020 for $\mathrm{Au}^{^{26+}}$

Measurement	Sample	Total	Total	H ₂	H ₂ Error	H₂O	H₂O	со	СО	CO2	CO ₂
			Error				Error		Error		Error
20200314_0838_5-3	OFCu milled (1)	1.53E4	2.77E3	1.86E3	1.36E3	6.78E2	2.13E2	1.24E3	2.82E2	4.72E2	1.05E2
20200314_2307_5-3	OFCu milled (1)	1.33E4	2.40E3	2.33E3	6.51E2	5.42E2	1.24E2	1.44E3	2.97E2	4.69E2	9.49E1
20200314_0906_5-4	OFCu milled (2)	2.32E4	4.20E3	1.72E3	1.09E3	1.40E3	3.58E2	2.31E3	4.99E2	7.61E2	1.60E2
20200314_2253_5-4	OFCu milled (2)	1.70E4	3.07E3	5.07E3	1.27E3	6.51E2	1.56E2	1.93E3	3.98E2	6.89E2	1.41E2
20200314_0746_5-1	OFCu milled,	2.43E3	4.41E2	5.50E3	2.15E3	3.65E2	2.16E2	3.16E2	1.01E2	2.02E2	5.29E1
	annealed (1)										
20200314_2336_5-1	OFCu milled, annealed (1)	2.42E3	4.38E2	3.61E3	1.05E3	7.96E1	5.50E1	1.64E2	4.65E1	1.31E2	2.79E1
20200314_0815_5-2	OFCu milled,	2.21E3	3.99E2	4.03E3	1.95E3	2.19E1	1.57E1			2.14E2	8.15E1
	annealed (2)										
20200314_2322_5-2	OFCu milled,	2.23E3	4.02E2	4.48E2	2.69E2			1.67E2	4.06E1	1.77E2	4.01E1
	annealed (2)										
20200314_1112_5-22	OFCu pol. (SiC)	1.28E4	2.31E3	1.79E4	4.43E3	6.18E2	1.85E2	1.09E3	2.45E2	3.67E2	7.64E1
20200314_1435_5-22	OFCu pol. (SiC)	1.11E4	2.00E3	3.45E3	8.70E2	8.70E2	1.87E2	1.26E3	2.62E2	4.72E2	9.65E1
20200314_1053_5-18	OFCu pol. (SiC),	2.02E3	3.66E2			2.92E2	1.49E2	1.48E2	5.76E1	1.74E2	6.27E1
	annealed										
20200314_2133_5-18	OFCu pol. (SiC),	1.89E3	3.41E2	8.94E1	1.68E2	4.93E0	1.35E1	1.32E2	3.03E1	9.83E1	2.04E1
	annealed										
20200314_0954_6-16	OFCu pol. (CaCO ₃)	7.04E3	1.27E3	7.56E3	2.62E3	3.63E2	1.65E2	3.86E2	1.12E2	4.89E2	1.20E2
20200314_2224_6-16	OFCu pol. (CaCO ₃)	5.78E3	1.04E3	1.08E3	4.45E2	3.65E2	8.61E1	4.20E2	8.90E1	2.86E2	5.82E1
20200314_1035_5-16	OFCu lapped	1.15E5	2.08E4	1.14E4	3.45E3	3.35E4	6.92E3	7.73E3	1.60E3	1.52E4	3.05E3
20200314_2148_5-16	OFCu lapped	9.30E4	1.68E4	1.14E4	2.39E3	4.76E4	9.73E3	1.09E4	2.23E3	1.85E4	3.71E3
20200314_0927_5-24	OFCu pol.	6.90E3	1.25E3	9.01E3	2.80E3	3.46E2	1.54E2	6.35E2	1.62E2	2.42E2	6.45E1
	(diamond)										

20200314_2241_5-24	OFCu pol.	6.88E3	1.24E3	2.23E3	6.99E2	3.12E2	7.69E1	6.05E2	1.25E2	2.93E2	6.12E1
	(diamond)										
20200314_1011_5-15	OFCu lap.+pol.	9.69E3	1.75E3	4.48E3	1.85E3	3.43E2	1.57E2	6.36E2	1.39E2	4.62E2	9.82E1
20200314_2211_5-15	OFCu lap.+pol.	9.22E3	1.66E3	1.76E3	5.44E2	4.07E2	9.17E1	1.01E3	2.09E2	4.80E2	9.78E1
20200316_0251_6-7	Cu single crystal	6.92E3	1.25E3	1.31E3	2.88E2	3.75E2	7.91E1	1.20E3	2.46E2	3.07E2	6.16E1
20200316_0302_6-8	Cu single crystal, annealed	1.76E3	3.19E2	6.08E2	1.46E2	6.32E1	1.58E1	1.25E2	2.59E1	1.64E2	3.30E1
20200316_0446_R1-17	OFCu sheet, untreated	3.03E4	5.47E3	6.00E3	1.24E3	7.08E3	1.45E3	5.21E3	1.06E3	6.80E3	1.36E3
20200316_0500_R1-25	OFCu sheet, annealed	3.30E4	5.97E3	7.91E3	1.60E3	4.72E3	9.67E2	7.70E3	1.57E3	7.45E3	1.49E3
20200316_0518_R1-20	OFCu sheet lap+pol	1.35E5	2.44E4	5.78E4	1.16E4	3.68E4	7.53E3	2.48E4	5.06E3	2.97E4	5.92E3
20200316_0529_R1-28	OFCu sheet lap+pol, annealed	1.96E5	3.54E4	4.71E4	9.41E3	4.09E4	8.38E3	3.28E4	6.69E3	5.35E4	1.07E4
20200315_0355_R1-1	W untreated	1.97E5	3.56E4	6.64E4	1.35E4	2.66E4	5.46E3	5.41E4	1.10E4	1.91E4	3.82E3
20200315_0431_R1-2	W lap	1.31E5	2.37E4	1.35E4	2.76E3	2.89E4	5.93E3	1.85E4	3.85E3	2.29E4	4.59E3
20200315_0502_R1-3	W lap+etch	1.40E5	2.53E4	2.43E4	4.99E3	3.50E4	7.18E3	2.54E4	5.28E3	4.35E4	8.72E3
20200315_0523_R1-4	W lap+pol	2.42E4	4.37E3	5.29E3	1.12E3	3.32E3	6.85E2	5.26E3	1.08E3	2.50E3	5.00E2
20200315_0717_R1-12	W lap+pol, annealed	1.69E4	3.05E3	3.34E3	7.91E2	1.44E3	3.17E2	2.53E3	5.18E2	1.26E3	2.54E2
20200315_0540_R1-5	W lap+etch+pol	4.01E4	7.25E3	1.04E4	2.13E3	6.64E3	1.37E3	9.20E3	1.88E3	3.77E3	7.54E2
20200315_0701_R1-13	W lap+etch+pol, annealed	2.58E4	4.66E3	6.61E3	1.44E3	1.28E3	2.73E2	8.01E3	1.64E3	1.78E3	3.59E2
20200315_0611_R1-6	W lap+etch+pol+ etch	2.62E4	4.73E3	4.37E3	1.01E3	5.16E3	1.06E3	4.12E3	8.45E2	1.84E3	3.69E2
20200315_0639_R1-14	W lap+etch+pol+ etch, annealed	9.90E4	1.79E4	2.14E4	4.37E3	8.94E3	1.85E3	4.07E4	8.29E3	8.82E3	1.76E3
20200316_0313_6-2	WCu	4.04E4	7.30E3	1.33E4	2.68E3	9.02E3	1.85E3	9.46E3	1.93E3	4.17E3	8.34E2
20200316_0325_6-1	WCu, annealed	8.07E3	1.46E3	2.39E3	4.94E2	8.78E2	1.81E2	1.90E3	3.87E2	6.31E2	1.26E2
20200316_0336_6-10	Al1050	8.47E3	1.53E3	4.49E3	9.08E2	7.87E2	1.62E2	1.38E3	2.81E2	4.39E2	8.81E1
20200316_0401_6-9	Al1050, annealed	3.03E3	5.46E2	1.11E3	2.40E2	1.99E2	4.23E1	3.79E2	7.78E1	2.14E2	4.30E1
20200316_0413_6-18	Al6061	8.04E3	1.45E3	4.89E3	9.86E2	6.01E2	1.24E2	1.71E3	3.49E2	4.84E2	9.71E1
20200316_0424_6-17	Al6061, annealed	6.38E3	1.15E3	3.82E3	7.75E2	4.24E2	8.78E1	1.53E3	3.11E2	4.12E2	8.26E1

Table 37: ISD results from beam time 2020 for Au^{52+}

Measurement	Sample	Total	Total Error	H ₂	H ₂ Error	H₂O	H₂O Error	со	CO Error	CO ₂	CO₂ Error
20200314_0105_5-3	OFCu milled (1)	2.54E4	4.58E3	9.69E3	2.56E3	1.54E3	4.08E2	1.99E3	4.17E2	7.62E2	1.62E2
20200314_0153_5-4	OFCu milled (2)	4.62E4	8.35E3	1.17E4	2.84E3	3.50E3	7.56E2	5.21E3	1.09E3	1.45E3	3.00E2
20200313_2158_5-1	OFCu milled, annealed (1)	5.94E3	1.08E3	4.76E3	3.42E3	4.22E2	3.47E2	4.61E2	1.80E2	4.06E2	1.08E2
20200313_2319_5-1	OFCu milled, annealed (1)	5.93E3	1.07E3	1.62E3	1.41E3	9.46E2	3.19E2	3.44E2	1.02E2	3.07E2	8.03E1
20200314_0030_5-2	OFCu milled, annealed (2)	5.00E3	9.03E2	4.80E3	1.80E3	8.15E2	2.70E2	4.73E2	1.22E2	2.87E2	7.30E1
20200314_0445_5-22	OFCu pol. (SiC)	2.78E4	5.01E3	6.71E3	2.29E3	2.86E3	6.35E2	3.08E3	6.35E2	9.58E2	1.99E2
20200314_0429_5-18	OFCu pol. (SiC), annealed	4.15E3	7.49E2	6.56E2	8.94E2	2.97E2	1.54E2	5.26E2	1.25E2	1.72E2	4.20E1
20200314_0313_6-16	OFCu pol. (CaCO ₃)	1.75E4	3.15E3	4.71E3	1.84E3	1.87E3	4.48E2	1.66E3	3.87E2	7.05E2	1.56E2
20200314_0404_5-16	OFCu lapped	1.99E5	3.60E4	1.48E4	3.51E3	1.07E5	2.20E4	9.23E3	1.90E3	2.68E4	5.36E3
20200314_0237_5-24	OFCu pol. (diamond)	1.49E4	2.69E3	2.31E3	1.21E3	8.58E2	2.33E2	1.75E3	3.76E2	5.29E2	1.14E2
20200314_0340_5-15	OFCu lap.+pol.	1.62E4	2.93E3	3.55E3	1.55E3	1.00E3	2.73E2	1.57E3	3.48E2	6.34E2	1.32E2
20200315_2257_6-7	Cu single crystal	3.10E4	5.59E3	6.53E3	1.49E3	9.94E2	2.25E2	5.62E3	1.14E3	7.31E2	1.48E2
20200315_2314_6-8	Cu single crystal, annealed	7.16E3	1.29E3	5.04E2	3.98E2	5.38E2	1.44E2	1.12E3	2.31E2	3.45E2	7.36E1
20200316_0037_R1-17	OFCu sheet, untreated	9.72E4	1.76E4	1.86E4	4.12E3	8.66E3	1.80E3	1.73E4	3.53E3	1.01E4	2.02E3

20200316_0049_R1-25	OFCu sheet,	7.77E4	1.40E4	1.14E4	2.79E3	5.52E3	1.18E3	1.46E4	2.99E3	1.01E4	2.02E3
	annealed										
20200316_0101_R1-20	OFCu sheet	2.01E5	3.64E4	5.95E4	1.24E4	3.52E4	7.31E3	2.61E4	5.33E3	3.13E4	6.25E3
	lap+pol										
20200316_0124_R1-28	OFCu sheet	3.37E5	6.09E4	4.25E4	8.92E3	3.91E4	8.09E3	5.75E4	1.17E4	7.97E4	1.59E4
	lap+pol, annealed										
20200315_1827_R1-1	W untreated	2.67E5	4.83E4	6.88E4	1.42E4	8.61E3	1.89E3	6.77E4	1.38E4	1.40E4	2.81E3
20200315_1236_R1-2	W lap	1.27E5	2.29E4	1.05E4	3.41E3	1.18E4	2.50E3	1.90E4	3.90E3	8.30E3	1.68E3
20200315_1541_R1-3	W lap+etch	9.47E4	1.71E4	2.38E4	7.85E3	8.74E3	2.07E3	1.75E4	3.68E3	1.03E4	2.16E3
20200315_1715_R1-4	W lap+pol	2.27E4	4.10E3	5.76E3	3.23E3	7.50E2	3.78E2	2.84E3	6.30E2	1.51E3	3.94E2
20200315_1842_R1-12	W lap+pol,	3.63E4	6.55E3	3.10E3	1.94E3	1.16E3	3.53E2	5.26E3	1.09E3	1.40E3	2.97E2
	annealed										
20200315_1807_R1-5	W lap+etch+pol	6.63E4	1.20E4	1.24E4	3.59E3	1.68E3	5.34E2	1.23E4	2.53E3	3.59E3	7.40E2
20200315_1907_R1-13	W lap+etch+pol,	3.64E4	6.57E3	3.31E3	1.71E3	2.72E3	6.26E2	5.87E3	1.22E3	1.95E3	4.14E2
	annealed										
20200315_1818_R1-6	W lap+etch+pol+	4.19E4	7.57E3	4.74E3	2.14E3	3.59E3	8.56E2	5.59E3	1.16E3	1.93E3	3.99E2
	etch										
20200315_1920_R1-14	W lap+etch+pol+	3.14E4	5.67E3	2.63E3	1.40E3	2.81E2	1.40E2	3.36E3	6.96E2	2.03E3	4.18E2
	etch, annealed										
20200315_2341_6-2	WCu	1.30E5	2.35E4	3.06E4	6.71E3	1.54E4	3.26E3	2.78E4	5.67E3	8.37E3	1.68E3
20200315_2329_6-1	WCu, annealed	1.62E4	2.92E3			1.05E3	2.99E2	2.28E3	4.75E2	8.36E2	1.86E2
20200315_2353_6-10	Al1050	2.35E4	4.25E3	1.31E4	2.94E3	7.51E2	2.24E2	8.38E2	1.81E2	8.24E2	1.82E2
20200316_0003_6-9	Al1050, annealed	1.03E4	1.87E3	6.00E3	1.78E3	5.81E2	1.95E2	1.64E3	3.44E2	4.24E2	9.43E1
20200316_0014_6-18	Al6061	2.30E4	4.14E3	1.53E4	3.50E3	6.99E2	2.40E2	2.89E3	6.01E2	7.15E2	1.56E2
20200316_0027_6-17	Al6061, annealed	1.67E4	3.02E3	7.96E3	2.27E3	1.11E2	1.34E2	2.37E3	5.00E2	8.08E2	2.00E2

11.5.3 ISD Results from Beam Time 2021

Table 38: ISD results from beam time 2021 for Ca^{10+}

Measurement	Sample	Total	Total	H₂	H ₂	H₂O	H₂O	со	со	CO2	CO2	Ar	Ar
			Error		Error		Error		Error		Error		Error
20210401_0013	NEG 22h@180°C +	4.42E2	7.98E1	1.67E2	1.24E2	7.34E-2	9.99E-2	2.67E1	1.54E1	1.48E1	7.60E0	1.54E1	3.06E0
_R1-32	14h@177°C +												
	in-situ 25h@177°C												
20210402_1634	NEG untreated	6.80E2	1.23E2	1.98E2	1.44E2	2.09E1	1.37E1	4.89E1	2.85E1	8.57E1	4.43E1	6.84E0	1.43E0
_R1-8													
20210403_1647	NEG 4h@400°C	4.64E2	8.38E1	3.21E1	2.45E1	3.18E0	2.12E0	1.65E1	9.61E0	6.44E1	3.34E1	7.89E0	1.76E0
_R1-16													
20210403_2312	NEG 24h@180°C	1.81E3	3.26E2	8.07E2	5.85E2	5.42E1	3.54E1	2.02E2	1.17E2	2.23E2	1.15E2	1.27E1	3.37E0
_R1-24													
20210331_2349	OFCu milled,	2.65E2	4.78E1	6.28E1	4.91E1	1.38E0	9.48E-1	7.82E0	4.55E0	1.06E1	5.49E0	6.86E0	1.37E0
_8-9	annealed @400 °C												
20210401_0001	OFCu milled,	4.76E2	8.60E1	1.60E2	1.18E2	5.95E0	3.96E0	4.01E1	2.32E1	1.58E1	8.28E0	5.40E0	1.20E0
_8-6	annealed @300 °C												
20210401_0137	OFCu milled,	2.06E2	3.72E1	4.75E0	7.61E0	4.29E-1	3.28E-1	4.36E0	2.56E0	9.34E0	4.88E0	4.18E0	9.28E-1
_8-5	annealed @500 °C												
20210401_0218	OFCu pol. (CaCO ₃)	1.53E3	2.76E2	3.14E2	2.30E2	2.70E1	1.77E1	5.41E1	3.13E1	1.08E2	5.56E1	1.36E1	2.89E0
_5 -6													
20210401_0231	OFCu pol. (SiC)	3.44E3	6.21E2	7.12E2	5.17E2	1.66E2	1.09E2	2.46E2	1.42E2	2.60E2	1.34E2	2.22E1	5.01E0
_5-21													
20210402_1338	OFCu stored in	3.06E2	5.53E1	6.16E1	4.70E1	3.84E0	2.51E0	2.10E1	1.22E1	2.52E1	1.30E1	5.30E0	1.03E0
_8-10	vacuum												
20210403_0029	OFCu milled	1.00E3	1.81E2	2.32E2	1.70E2	4.85E1	3.17E1	6.32E1	3.66E1	1.37E2	7.13E1	6.83E1	1.24E1
_8-3													
20210403_2302	OFCu milled,	7.96E2	1.44E2	3.67E2	2.67E2	1.37E1	8.95E0	1.08E2	6.27E1	4.31E1	2.22E1	8.59E0	1.73E0
_8-6	annealed @300 °C												
20210403_2350	OFCu milled,	1.99E2	3.60E1	2.43E1	1.92E1	7.46E-1	5.18E-1	6.08E0	3.52E0	9.79E0	5.05E0	3.72E0	7.51E-1
_8-5	annealed @500 °C												

20210404_0004 8-9	OFCu milled, annealed @400 °C	2.59E2	4.68E1	1.44E1	1.23E1	2.13E0	1.41E0	8.55E0	4.95E0	1.34E1	6.88E0	6.40E0	1.35E0
20210402_1403	OFCu plasma elec.	4.30E2	7.77E1	7.65E1	5.62E1	7.73E0	5.07E0	2.40E1	1.39E1	3.41E1	1.75E1	8.12E0	1.57E0
20210402_1424	OFCu plasma elec.	4.92E2	8.88E1	1.03E2	7.51E1	8.71E0	5.69E0	5.04E1	2.92E1	4.46E1	2.30E1		
 20210402_1503	OFCu pol. (SiC) +	6.18E2	1.12E2	1.70E2	1.25E2	2.28E1	1.49E1	5.19E1	3.01E1	5.51E1	2.84E1	4.74E0	1.20E0
_5-19 20210401_0027	plasma elec. pol. OFCu milled +	5.39E2	9.74E1	1.14E2	8.60E1	4.76E0	3.15E0	2.96E1	1.71E1	2.04E1	1.05E1	6.48E0	2.53E0
_8-17	sputt. 1.17E18	4 0050	2 4254	7.0054		7.075.4		4 4350	2 5 2 5 2	0.4050	1 1050	4 2054	2 2050
_8-18	sputt. 2.21E18	1.89E2	3.42E1	7.00E1	5.32E1	7.07E-1	5.29E-1	4.43E0	2.58E0	8.48E0	4.40E0	1.28E1	2.38E0
20210401_0055 _8-19	OFCu milled + sputt. 3.67E18	1.59E2	2.86E1	3.70E1	3.08E1	1.60E0	1.15E0	2.81E0	1.64E0	7.17E0	3.72E0	1.10E1	2.46E0
20210401_0112 8-20	OFCu milled +	2.31E2	4.17E1	3.97E1	3.24E1	9.59E-1	6.74E-1	2.83E0	1.65E0	1.02E1	5.38E0	6.16E0	1.33E0
_8-20 20210401 0124	OFCu milled +	5.06F2	9.13F1	1.52F2	1.14F2	1.95F0	1.34F0	3.62F1	2.10F1	1.95F1	1.01F1	1.92F1	3.66F0
_8-16	sputt. 2.96E18 + annealed												
20210401_0150	OFCu pol. (CaCO ₃)	1.20E2	2.17E1	3.80E1	3.07E1	4.86E-1	3.47E-1	2.74E0	1.59E0	6.76E0	3.50E0	5.65E0	1.16E0
_5-5	+ sputt. 2.94E18 + annealed												
20210401_0205 5-20	OFCu pol. (SiC) + sputt. 2.92E18	5.67E2	1.02E2	1.41E2	1.06E2	6.58E0	4.36E0	2.13E1	1.24E1	2.65E1	1.36E1	7.14E0	1.63E0
	OFCu milled +	1.74E2	3.15E1	2.95E1	2.21E1	5.50E0	3.60E0	5.39E0	3.12E0	1.27E1	6.54E0	7.62E0	1.43E0
20210402 2355	OFCu milled +	8.29E2	1.50E2	7.76E2	5.70E2	3.72E1	2.42E1	2.00E2	1.16E2	6.10E1	3.15E1	5.74E0	1.16E0
_8-21	sputt. 45°, 3.29E18 (1)												
20210403_0013	OFCu milled +	2.90E2	5.24E1	6.34E1	4.61E1	1.73E1	1.13E1	1.46E1	8.43E0	1.67E1	8.57E0	4.44E0	9.19E-1
_8-22	sputt. 45°, 3.29E18 (2)												
20210403_2201	OFCu milled +	2.17E2	3.91E1	1.62E1	1.34E1	1.26E0	8.43E-1	3.38E0	1.97E0	1.13E1	5.83E0	9.56E0	1.94E0
_8-17	sputt. 1.17E18, annealed												
20210403_2213	OFCu milled +	1.96E2	3.53E1	9.52E0	7.85E0	1.13E0	7.42E-1	5.43E0	3.15E0	9.45E0	4.86E0	1.18E1	2.13E0
_8-18	sputt. 2.21E18, annealed												
20210403_2236	OFCu milled +	1.34E2	2.43E1	3.10E1	2.37E1	1.27E0	8.41E-1	2.58E0	1.50E0	1.01E1	5.21E0	3.91E0	7.89E-1
_8-19	sputt. 3.67E18, annealed												
20210403_2250	OFCu milled +	1.94E2	3.49E1	1.96E1	1.66E1	1.42E0	9.43E-1	3.28E0	1.91E0	1.24E1	6.42E0	5.84E0	1.10E0
_8-20	annealed												
20210403_2327	OFCu pol. (CaCO ₃)	1.69E2	3.05E1	2.78E1	2.15E1	8.94E-1	6.18E-1	3.09E0	1.80E0	7.24E0	3.74E0	6.81E0	1.43E0
_5-5	+ sputt. 2.94E18 + annealed												
20210403_2339	OFCu milled +	2.30E2	4.16E1	3.02E1	2.32E1	1.45E0	9.59E-1	5.62E0	3.27E0	1.21E1	6.26E0	1.04E1	2.24E0
_8-16	sputt. 2.96E18 + annealed												
20210403_0041 6-10	Al1050	6.26E2	1.13E2	2.19E2	1.58E2	5.15E1	3.36E1	5.05E1	2.93E1	5.09E1	2.62E1	4.80E0	1.17E0
	Al1050, annealed	3.24E2	5.85E1	1.22E2	8.95E1	2.26E1	1.48E1	1.73E1	1.01E1	1.48E1	7.61E0	4.59E0	1.17E0
20210403_1436	TiN 200nm,	7.33E3	1.32E3	4.88E3	3.54E3	5.28E2	3.44E2	1.17E3	6.74E2	7.88E2	4.08E2	3.06E1	1.53E1
_/-8	coating												
20210403_1526 _7-21	TiN 200nm	4.53E3	8.19E2	3.04E3	2.20E3	4.29E1	2.80E1	1.05E3	6.09E2	2.04E2	1.05E2	3.07E1	1.56E1
20210403_1558	TiN 200nm,	1.54E4	2.79E3	5.81E3	4.21E3	8.66E2	5.65E2	2.50E3	1.45E3	8.49E2	4.38E2	8.45E1	3.97E1
_7-20	annealed after coating												

20210403_1610	TiN 500nm,	2.86E4	5.16E3	2.24E4	1.63E4	1.58E3	1.03E3	6.08E3	3.52E3	2.66E3	1.38E3	1.22E2	8.37E1
_7-9	annealed before												
	coating												
20210403_1621	TiN 500nm	3.28E4	5.92E3	2.76E4	2.00E4	1.84E3	1.20E3	6.63E3	3.84E3	2.90E3	1.50E3	1.47E2	9.70E1
_7-18													
20210403_1633	TiN 500nm,	2.70E4	4.87E3	2.16E4	1.58E4	1.59E3	1.04E3	5.09E3	2.95E3	2.71E3	1.40E3	1.81E2	8.46E1
_7-17	annealed after												
	coating												
20210402_1531	Carbon 200nm,	1.17E3	2.11E2	1.10E3	8.00E2	7.34E1	4.79E1	1.86E2	1.07E2	2.07E2	1.07E2	5.12E0	1.17E0
_7-13	annealed before												
	coating												
20210402_1546	Carbon 200nm	1.32E3	2.38E2	1.59E3	1.15E3	1.03E2	6.71E1	3.15E2	1.82E2	1.61E2	8.26E1	5.12E0	1.37E0
_7-14													
20210402_1601	Carbon 200nm,	1.25E3	2.27E2	2.00E3	1.45E3	9.70E1	6.33E1	2.96E2	1.71E2	1.53E2	7.87E1	3.45E0	1.36E0
_7-1	annealed after												
	coating												
20210402_2302	Carbon 500nm,	2.43E3	4.39E2	2.52E3	1.82E3	3.38E2	2.20E2	4.93E2	2.85E2	3.96E2	2.04E2	7.97E0	1.67E0
_7-16	annealed before												
	coating												
20210402_2315	Carbon 500nm	5.12E3	9.24E2	5.53E3	4.00E3	7.48E2	4.88E2	1.62E3	9.36E2	9.83E2	5.05E2	1.48E1	4.72E0
_7-23													
20210402_2336	Carbon 500nm,	2.07E3	3.73E2	4.38E3	3.16E3	2.46E2	1.61E2	6.08E2	3.51E2	2.80E2	1.44E2	3.91E0	1.96E0
_7-4	annealed after												
	coating												

Table 39: ISD results from beam time 2021 for $\mathrm{Au}^{^{25+}}$

Measurement	Sample	Total	Total	H ₂	H ₂	H₂O	H₂O	со	со	CO2	CO2	Ar	Ar
			Error		Error		Error		Error		Error		Error
20210305_2342 _R1-24	NEG 24h@180°C	1.31E4	2.36E3	5.02E3	3.64E3	2.93E1	1.93E1	2.22E3	1.28E3	5.69E2	2.92E2	2.17E2	4.78E1
20210306_0143 _R1-8	NEG untreated	6.13E3	1.11E3	5.96E2	4.72E2	8.58E0	6.07E0	3.46E2	2.00E2	3.27E2	1.68E2	9.56E1	1.98E1
	NEG 4h@400°C	2.91E3	5.25E2	3.45E2	2.71E2	4.96E0	3.52E0	1.52E2	8.77E1	2.60E2	1.34E2	1.58E2	2.90E1
20210306_0237 _R1-32	NEG 22h@180°C	6.70E3	1.21E3	1.38E3	1.02E3	7.35E0	5.17E0	6.85E2	3.96E2	3.22E2	1.67E2	9.88E1	2.60E1
20210308_1958 _R1-32	NEG 22h@180°C + in-situ 14h@177°C	3.53E3	6.38E2	1.67E3	1.26E3	5.41E-1	7.00E-1	5.56E2	3.22E2	1.04E2	5.37E1	6.25E1	1.51E1
20210309_0054 _Sst	Stainless steel, untreated	1.20E4	2.17E3	2.93E3	2.14E3	2.40E2	1.57E2	1.26E3	7.39E2	6.72E2	3.46E2		
20210306_1924 _8-9	OFCu milled, annealed @ 400 °C	2.92E3	5.27E2	7.27E2	5.34E2	1.53E1	1.00E1	1.03E2	5.96E1	2.01E2	1.03E2	7.87E1	1.56E1
20210306_2250 _8-3	OFCu milled	8.73E3	1.58E3	1.15E3	8.34E2	3.38E2	2.21E2	7.24E2	4.18E2	6.24E2	3.21E2	1.12E2	2.18E1
20210306_2303 _ ⁸⁻⁶	OFCu milled, annealed @ 300 °C	1.04E3	1.87E2	2.61E2	2.00E2	1.45E0	1.04E0	2.39E1	1.39E1	6.14E1	3.17E1	4.87E1	9.14E0
20210306_2317 _ ⁸⁻⁵	OFCu milled, annealed @ 500 °C	1.11E3	2.01E2	5.75E2	4.24E2	2.00E0	1.42E0	3.43E1	1.99E1	6.23E1	3.22E1	4.56E1	9.16E0
20210306_2331 _8-10	OFCu stored in vacuum	4.04E3	7.30E2	3.94E2	2.94E2	2.71E1	1.78E1	2.81E2	1.63E2	2.40E2	1.23E2	8.20E1	1.68E1
20210308_2023 _5-6	OFCu pol. (CaCO ₃)	1.55E4	2.79E3	3.95E3	2.87E3	9.32E2	6.10E2	1.66E3	9.58E2	1.15E3	5.92E2	1.24E2	3.12E1
20210308_2037 _5-21	OFCu pol. (SiC)	2.88E4	5.21E3	8.40E3	6.10E3	2.68E3	1.75E3	5.72E3	3.31E3	3.14E3	1.61E3	1.14E2	3.63E1
20210306_2341 _5-10	OFCu plasma elec. pol. (1)	6.11E3	1.10E3	9.95E2	7.29E2	8.33E1	5.44E1	4.56E2	2.64E2	2.79E2	1.43E2	1.12E2	2.19E1

20210307_0000	OFCu plasma	5.30E3	9.58E2	9.57E2	7.01E2	5.32E1	3.48E1	3.51E2	2.03E2	2.84E2	1.47E2	8.30E1	1.78E1
_5-11	elec. pol. (2)												
20210307_0011 5-19	OFCu pol. (SiC) + plasma elec. pol	8.00E3	1.45E3	1.57E3	1.15E3	1.21E2	7.87E1	7.46E2	4.31E2	3.68E2	1.89E2	7.25E1	1.72E1
20210207 0022		6 7253	1 21F2	1 10F3	8 07F2	1 22F2	8 68F1	6.01E2	3 /8F2	2 58F2	1 8/F2	1 20F2	2 50F1
6-15	\pm nlasma elec	0.7215	1.2105	1.1015	0.0712	1.5562	0.0011	0.0122	J.40L2	5.5012	1.04L2	1.2322	2.5501
_0-15	pol.												
20210307 1813	OFCu milled +	9.66E2	1.74E2	2.92E2	2.15E2	1.10E0	7.67E-1	2.91E1	1.68E1	3.86E1	1.99E1	6.73E1	1.27E1
_8-16	sputt. 2.96E18												
20210307 1826	OFCu pol (SiC) +	3.24E3	5.85E2	8.70E2	6.43E2	2.01E1	1.33E1	2.65E2	1.53E2	1.47E2	7.56E1	1.02E2	2.01E1
5-20	sputt. 2.92E18												
20210307 1842	OFCu pol. (CaCO ₂)	2.51E3	4.53E2	6.16E2	4.64E2	4.42E0	2.97E0	1.52E2	8.78E1	1.12E2	5.75E1	8.44E1	1.90E1
5-5	+ sputt. 2.94E18					_		-					
20210309 0001	OFCu pol. (CaCO ₂)	8.72F2	1.58F2	1.58F2	1.26F2	3.76F0	2.64F0	2.39F1	1.41F1	4.25F1	2.19F1	3.68F1	1.25F1
5-5	+ sputt 2 94F18 +	0				0010						0.00011	
	annealed												
20210309 0016	OFCu milled +	8 29F2	1 50F2	2 /2F2	1 89F2	2 //5E0	1 68F0	2 23E1	1 30F1	6 11F1	3 15F1	5 51F1	1 00F1
8-16	snutt 2 96F18 +	0.2522	1.5022		1.0522	2.4520	1.0010	2.2521	1.5011	0.11111	5.1521	5.5121	1.0011
_0-10	annealed												
20210206 1952		E 66E2	1 0252	1 5152	1 1052	2 1 0 5 1	2 0951	2 5052	2 0252	2 6052	1 2452	0 7651	1 0251
20210300_1855 6 10	A11050	5.00L5	1.0215	1.5115	1.1013	5.10L1	2.00L1	5.50L2	2.0212	2.0012	1.54LZ	0.70L1	1.03L1
20210206 1000	Al1050 appealed	2 2052	4 2052	2 6652	2 0252	7 9/50	5 1950	7 2751	4 2651	1 2152	6 2461	2 0251	7.0650
6-11	AI1050 annealeu	2.3013	4.2922	2.0012	2.0212	7.04LU	5.1010	/.3/L1	4.20L1	1.2112	0.24L1	5.05L1	7.0010
20210206 0002	TIN 500pm	1 0554	7 2252	1 0251	2 5054	1 2652	9 24E2	1 205/	1 0054	0 8252	5 0552	1 2452	1 1152
7 0	annoaled before	4.05L4	1.52L5	4.03L4	5.50L4	1.2015	0.24L2	1.09L4	1.0914	9.02L2	5.05L2	1.24L2	1.1112
_/-5													
20210206 0210	TIN FOOrm	1 0255	2 1051	1 2005	1 0055	2 6052	1 7052	0.2054	E 27E4	2 0052	1 0052	E 12E2	E 62E2
20210306_0210	TIN SUUTITI,	1.9355	3.4854	1.3865	1.0055	2.00E3	1.7063	9.2964	5.3764	3.0003	1.9953	5.13EZ	5.03E2
_/-1/	annealeu arter												
20210206 0222	TIN 500nm	2 01 5	5 2554	2 1255	2 4755	6 5052	1 2052	1 2/65	7 1 9 5 /	5 9752	2 0252	6 5552	9 6752
7 10		2.9115	J.2JL4	J.42LJ	2.4715	0.5525	4.3013	1.24LJ	7.1014	J.07LJ	5.02L5	0.5522	0.0712
20210206 0252	TiN 200nm	1 1 2 5	2 0254	6 1754	1 1651	2 2452	1 4652	1 5 2 5 4	2 61 5 4	2 5752	1 2252	2 0/52	2 0/52
7-20	annealed after	1.12LJ	2.0214	0.1724	4.4024	2.24L3	1.4013	4.5214	2.0114	2.5725	1.52L5	J.J4LZ	2.94LZ
_/-20	coating												
20210306 0306	TiN 200nm	1 0255	1 86F/	8 64F4	6 24F4	2 78F3	1 82E3	2 87F1	2 24F4	2 /2E3	1 2/F3	2 /QE2	2 6352
7-21		1.05L5	1.00L4	0.04L4	0.2414	2.7615	1.02LJ	5.0724	2.2414	2.4215	1.24LJ	2.4922	2.03L2
20210306 0318	TiN 200nm	1 2/F5	2 2/F/	1 13F5	8 16F/	2 9/F3	1 92F3	5 18F/	2 99F1	3 86F3	1 99F3	2 75F2	3 2/F2
7-8	annealed before	1.2405		1.1525	0.1024	2.5425	1.5215	5.1024	2.5524	5.0025	1.5525	2.7522	5.2462
_, 0	coating												
20210308 2338	TiN 500nm	2 49F5	4 49F4	2 52F5	1 82F5	7 85F3	5 23F3	9 44F4	5 46F4	5 12F3	2 69F3	3 31F2	8 30F2
7-9	annealed before				1.0110	1.0010	0.2020			0.110		0.0122	0.0011
	coating												
20210306 1704	Carbon 200nm	1 82F4	3 29F3	3 64F3	2 66F3	3 20F2	2 09F2	6 31F3	3 65F3	1 22F3	6 25F2	7 97F1	3 99F1
7-1	annealed before	1.0221	0.2323	5.0125	2.0025	5.2022	2.0522	0.5125	5.0525	1.2203	0.2322	/	5.5521
_/ _	coating												
20210306 1722	Carbo 200nm	2 66F4	4 81F3	6 29F3	4 55F3	6 81F2	4 45F2	1 10F4	6 37F3	1 95F3	1 00F3	1 37F2	3 69F1
7-14		2.0024	4.0125	0.2525	4.5525	0.0122		1.1024	0.5725	1.5525	1.0025	1.5722	5.0521
20210306 1741	Carbon 200nm.	2.19F4	3.96F3	3.98F3	2.89F3	3.21F2	2.10F2	8.05F3	4.65F3	1.72F3	8.87F2	1.32F2	2.74F1
7-13	annealed after	2.1321	5.5025	5.5025	2.0525	5.2122		0.0525	1.0525	1.7213	0.0722	1.5222	
	coating												
20210306 1758	Carbon 500nm	6.15F4	1.11F4	1.74F4	1.26F4	1.55F3	1.01F3	3.74F4	2.16F4	5.44F3	2.80F3	1.28F2	7.51F1
7-4	annealed before												
	coating												
20210306 1817	Carbon 500nm	8.08F4	1.46F4	2.35F4	1.70F4	2.87F3	1.87F3	4.95F4	2.86F4	8.27F3	4.25F3	2.23F2	8.62F1
7-23													
20210306 1836	Carbon 500nm.	1.63F4	2.94F3	2.84F3	2.05F3	1.08F2	7.06F1	7.16F3	4.14F3	1.16F3	5.95F2	5.93F1	1.25F1
7-16	annealed after												
_	coating												

11.5.4 ISD Results from Beam Time 2022

Measurement	Sample	Total	Total Error	H₂	H ₂ Error	H₂O	H ₂ O Error	со	CO Error	CO2	CO ₂
20220410 0050 0 11	OFCu untroated	6 0252	1 2252	2 0952	1 5152	E 62E0	4 1250	2 1 / E 1	1 5251	1 2051	1 2251
20220410_0050_5-11	argon storage (1)	0.0212	1.2322	2.0012	1.5112	5.03L0	4.13L0	2.14L1	1.35L1	1.30L1	1.2311
20220410 0108 9-5	OFCu annealed.	2.20F2	3.98F1	6.06F1	4.40F1	1.50F0	1.12F0	4.65F0	3.31F0	4.89F0	4.33F0
	argon storage 9										
	months (1)										
20220410_0128_9-6	OFCu annealed,	3.25E2	5.86E1	1.28E2	9.30E1	1.38E0	1.04E0	9.26E0	6.59E0	7.22E0	6.40E0
	argon storage 9										
	months (2)										
20220410_0147_9-17	OFCu annealed,	1.92E2	3.47E1	4.74E1	3.46E1	9.95E-1	7.60E-1	2.83E0	2.02E0	4.29E0	3.80E0
	argon storage 6										
20220440 0202 0 40	months (1)	4 4052	2.0054	2.0054	2.0454	4 4 0 5 4	2 4 0 5 4	2 2250	4 5050	4.0050	2 5550
20220410_0202_9-18	OFCU annealed,	1.48E2	2.68E1	3.89E1	2.84E1	4.10E-1	3.19E-1	2.22E0	1.59E0	4.00E0	3.55E0
	argon storage 6										
20220410 0214 9-23	OFCu annealed	2 80F2	5.06E1	7 8/JF1	5 70F1	1 3/FO	1 02E0	6 08F0	4 33E0	5 63E0	1 98F0
20220410_0214_5-25	argon storage 3	2.0012	5.0011	/.04L1	5.7011	1.540	1.0210	0.0010	4.5520	5.0520	4.5020
	months (1)										
20220410_0226_9-24	OFCu annealed,	2.28E2	4.11E1	4.40E1	3.21E1	1.05E0	7.83E-1	4.07E0	2.90E0	5.34E0	4.73E0
	argon storage 3										
	months (2)										
20220410_1246_9-12	OFCu untreated,	8.60E2	1.55E2	2.82E2	2.04E2	4.11E0	3.03E0	1.94E1	1.38E1	1.30E1	1.15E1
	argon storage (2)										
20220410_2249_9-9	OFCu untreated,	1.46E3	2.64E2	1.14E3	8.26E2	1.48E1	1.08E1	8.35E1	5.94E1	3.45E1	3.05E1
	vacuum storage (1)										
20220410_2312_9-10	OFCu untreated,	9.17E2	1.66E2	5.24E2	3.82E2	2.62E1	1.92E1	2.95E1	2.10E1	2.44E1	2.16E1
	vacuum storage (2)	6 7050	4.2452	5 0050	4.2.452	0.4050	6.0450		4.4254	4.0554	4 4 9 5 4
20220411_0007_Cu1	OFCu annealed,	6.73E2	1.21E2	5.98E2	4.34E2	8.19E0	6.01E0	5.79E1	4.12E1	1.25E1	1.10E1
20220411 0025 002		6 7/52	1 2252	4 1052	2 0052	1 0050	1 /050	1 2051	0 5050	1 5051	1 2/151
20220411_0025_Cu2	vacuum storage (2)	0.74LZ	1.2212	4.1012	5.00L2	1.9910	1.4010	1.2011	0.30LU	1.30L1	1.34L1
20220411 0039 Cu3	OFCu annealed.	6.89F2	1.25E2	5.81F2	4.27F2	3.53E0	2.59F0	1.56F1	1.11F1	1.60F1	1.43F1
	vacuum storage (3)										
20220411_0056_Cu4	OFCu annealed,	7.59E2	1.37E2	4.97E2	3.63E2	3.24E0	2.39E0	2.32E1	1.66E1	1.54E1	1.36E1
	vacuum storage (4)										
20220411_0113_Cu5	OFCu annealed,	4.87E2	8.79E1	2.18E2	1.58E2	2.15E0	1.58E0	1.07E1	7.60E0	8.07E0	7.15E0
	vacuum storage (5)										
20220411_0126_Cu6	OFCu annealed,	5.82E2	1.05E2	4.01E2	2.94E2	2.87E0	2.13E0	1.12E1	7.99E0	1.33E1	1.19E1
	vacuum storage (6)	ļ	ļ		ļ	ļ	ļ	ļ	ļ		
20220410_0027_9-7	OFCu untreated (1)	1.74E3	3.14E2	8.82E2	6.41E2	4.72E1	3.45E1	9.56E1	6.80E1	6.13E1	5.43E1
20220410_0609_9-13	OFCu annealed,	4.67E2	8.44E1	7.51E1	5.46E1	8.61E0	6.31E0	1.19E1	8.45E0	1.20E1	1.06E1
	atm. storage 6										
20220410 0629 9-14	OFCu annealed	4 50F2	8 12F1	6 7/F1	/ 90F1	8 38F0	6 1/F0	1 13F1	8 07F0	1 0/F1	9 16F0
20220410_0029_9-14	atm storage 6	4.3012	0.1211	0.7411	4.3011	0.3010	0.1410	1.1311	0.0710	1.04L1	9.1010
	months (2)										
20220410 0648 9-19	OFCu annealed,	4.18E2	7.54E1	9.29E1	6.74E1	4.88E0	3.58E0	1.09E1	7.79E0	1.03E1	9.14E0
	atm. storage 3										
	months (1)										
20220410_0704_9-20	OFCu annealed,	7.47E2	1.35E2	2.64E2	1.91E2	1.49E1	1.09E1	5.77E1	4.11E1	1.77E1	1.57E1
	atm. storage 3										
	months (2)										
20220410_1341_9-8	OFCu untreated (2)	1.75E3	3.15E2	1.05E3	7.59E2	5.95E1	4.35E1	1.64E2	1.17E2	5.73E1	5.07E1
20220410_2331_9-1	OFCu annealed,	8.59E2	1.55E2	2.52E2	1.83E2	1.16E1	8.53E0	2.79E1	1.98E1	2.26E1	2.00E1
	atm. storage 9 months (1)										

Table 40: ISD results from beam time 2022 for Ca^{10+}

20220410 2255 0 2		1 1152	2 0052	2 7252	2 6052	1 21 51	0 5950	4 4451	2 1651	2 9651	2 5251
20220410_2355_9-2	atm storage 9	1.1105	2.0022	5.72EZ	2.0922	1.5101	9.5620	4.44C1	5.1001	2.0001	2.551
	months (2)										
20220410_0239_11-3	Al6061 (1)	1.64E3	2.96E2	8.90E2	6.46E2	1.51E1	1.11E1	8.39E1	5.97E1	4.69E1	4.16E1
20220410 0254 11-4	Al6061 (2)	1.65E3	2.98E2	9.88E2	7.20E2	1.56E1	1.14E1	9.04E1	6.46E1	5.44E1	4.81E1
 20220410_1414_11-5	Al6061 sputt. 3.02E17	8.63E2	1.56E2	5.40E2	3.93E2	1.01E1	7.39E0	2.89E1	2.06E1	2.22E1	1.96E1
20220410_1437_11-6	Al6061 sputt.	3.97E2	7.16E1	1.01E2	7.34E1	6.96E0	5.10E0	1.53E1	1.09E1	1.05E1	9.31E0
20220410_2213_11-1	Al6061 vacuum	1.09E3	1.97E2	7.86E2	5.78E2	1.10E1	8.08E0	4.74E1	3.38E1	3.71E1	3.29E1
20220410_2234_11-2	Al6061 vacuum	1.41E3	2.55E2	1.11E3	8.18E2	1.28E1	9.38E0	6.04E1	4.31E1	4.67E1	4.14E1
20220409 2322 12-24	Cu single crystal	2 89F2	5 21F1	5 83F1	4 24F1	3 67F0	2 70F0	5 64F0	4 02F0	7 41F0	6 57E0
	sputt. 3.02E17	2.0522	5.2121	5.0521		5.0720	2.7020	5.0120		/	0.5720
20220410 0906 8-20	OFCu sputt. 30°.	9.00E2	1.63E2	1.88E2	1.36E2	1.52E1	1.11E1	3.51E1	2.50E1	3.42E1	3.02E1
	4.35E18, annealed										
20220410_0927_8-23	OFCu sputt. 3.40E18	7.26E2	1.31E2	1.58E2	1.15E2	1.75E1	1.29E1	2.49E1	1.78E1	2.20E1	1.95E1
20220410_1500_12-3	OFCu sputt. 1.57E17	4.88E2	8.81E1	1.60E2	1.16E2	1.05E1	7.73E0	2.10E1	1.50E1	1.21E1	1.07E1
20220410_1528_12-2	OFCu sputt. 2.36E17	5.16E3	9.31E2	5.44E3	3.96E3	4.04E1	2.96E1	1.94E2	1.38E2	2.83E2	2.52E2
20220410_1543_12-4	OFCu sputt. 2.95E17	5.86E2	1.06E2	2.44E2	1.77E2	2.21E1	1.62E1	2.99E1	2.13E1	1.56E1	1.38E1
20220410_1606_12-9	OFCu sputt. 2.99E17	7.25E2	1.31E2	3.53E2	2.56E2	2.61E1	1.91E1	3.53E1	2.51E1	1.77E1	1.57E1
20220410_1633_12-6	OFCu sputt. 3.90E17	3.66E2	6.61E1	9.88E1	7.18E1	7.50E0	5.50E0	1.26E1	8.95E0	1.16E1	1.03E1
20220410_1708_12-7	OFCu sputt. 4.68E17	6.36E2	1.15E2	2.39E2	1.74E2	2.74E1	2.01E1	2.71E1	1.93E1	1.64E1	1.45E1
20220410_1739_12-1	OFCu sputt. 1.03E18	7.79E2	1.41E2	3.98E2	2.88E2	2.44E1	1.79E1	3.71E1	2.64E1	1.92E1	1.70E1
20220410_1759_12-11	OFCu sputt. 3 keV, 3.02E17	3.75E2	6.77E1	1.14E2	8.28E1	7.16E0	5.26E0	1.51E1	1.08E1	1.04E1	9.17E0
20220410_1852_12-10	OFCu sputt. 4 keV, 3.02E17	3.53E2	6.37E1	1.12E2	8.18E1	5.90E0	4.33E0	1.07E1	7.61E0	9.21E0	8.16E0
20220410_0725_10-7	OFCu annealed 400°C, vacuum storage (1)	1.44E2	2.59E1	2.80E1	2.07E1	2.33E-1	1.86E-1	1.81E0	1.29E0	4.12E0	3.65E0
20220410_0746_10-8	OFCu annealed 400°C, vacuum	1.52E2	2.74E1	2.18E1	1.60E1	2.64E-1	2.09E-1	1.65E0	1.18E0	3.87E0	3.43E0
	storage (2)					ļ					
20220410_0802_10-9	OFCu annealed 300°C, vacuum storage (1)	1.05E3	1.89E2	5.53E2	4.04E2	1.91E1	1.40E1	1.58E2	1.12E2	2.82E1	2.50E1
20220410 0820 10-10	OFCu annealed	1.98E2	3.57E1	6.33E1	4.60E1	8.17E-1	6.08E-1	7.19E0	5.12E0	5.17E0	4.58E0
	300°C, vacuum storage (2)										
20220410_0834_10-11	OFCu annealed 500°C, vacuum storage (1)	1.45E2	2.63E1	2.65E1	1.94E1	1.82E-1	1.49E-1	1.57E0	1.12E0	4.02E0	3.56E0
20220410_0850_10-12	OFCu annealed 500°C, vacuum storage (2)	1.55E2	2.80E1	1.53E1	1.14E1	1.53E-1	1.29E-1	1.80E0	1.29E0	4.49E0	3.98E0
20220411_1306_10-7	OFCu annealed 400°C, vacuum storage (1)	1.39E2	2.50E1	2.78E1	2.07E1	3.58E-1	2.99E-1	1.45E0	1.03E0	2.66E0	2.35E0
20220411_1318_10-8	OFCu annealed 400°C, vacuum storage (2)	1.46E2	2.63E1	2.12E1	1.57E1	2.24E-1	1.78E-1	1.61E0	1.15E0	2.89E0	2.56E0
20220411_1330_10-9	OFCu annealed 300°C, vacuum storage (1)	2.46E2	4.44E1	5.51E1	4.03E1	3.94E-1	2.96E-1	8.43E0	6.00E0	4.69E0	4.16E0
20220411_1341_10-10	OFCu annealed 300°C, vacuum storage (2)	2.05E2	3.70E1	4.97E1	3.64E1	7.19E-1	5.45E-1	5.79E0	4.12E0	4.09E0	3.62E0
20220411_1352_10-11	OFCu annealed 500°C, vacuum storage (1)	1.34E2	2.43E1	2.38E1	1.76E1	1.82E-1	1.47E-1	1.54E0	1.10E0	3.23E0	2.86E0

20220411_1404_10-12	OFCu annealed	1.40E2	2.53E1	2.80E1	2.06E1	6.44E-2	6.36E-2	1.89E0	1.36E0	3.43E0	3.04E0
	500°C, vacuum										
	storage (2)										

Table 41: ISD results from beam time 2022 for $\mathrm{Au}^{^{26+}}$

Measurement	Sample	Total	Total	H ₂	H ₂ Error	H ₂ O	H₂O	со	CO	CO2	CO ₂
			Error	0.0050			Error	0.0750	Error		Error
20220602_0152_11-5	AI6061 (1)	4.77E3	8.63E2	9.26E2	6.77E2	4.33E1	3.18E1	2.25E2	1.61E2	7.69E1	6.81E1
20220602_0204_11-6	Al6061 (2)	2.91E3	5.26E2	4.64E2	3.45E2	4.13E1	3.04E1	1.46E2	1.05E2	5.70E1	5.05E1
20220602_0518_11-3	Al6061 sputt.	7.68E3	1.39E3	1.08E3	8.15E2	8.26E1	6.08E1	6.26E2	4.51E2	1.62E2	1.44E2
20220602 0620 44 4	3.02E17	7.6452	4 2052	4.0452	4 4252	4 4 5 5 2	0 4754	4 7550	2 2052	4 4052	4 2 4 5 2
20220602_0629_11-4	A16061 Sputt.	7.64E3	1.38E3	1.94E3	1.42E3	1.15E2	8.47E1	4.75E2	3.39E2	1.40E2	1.24E2
20220602 2246 11 1	1.03E18	1.0654	1.0152	2 2052	1 6152	6 9251	F 00F1	6 1652	4 2052	2 2152	1.0652
20220602_2246_11-1	Albubi vacuulli	1.0024	1.9105	2.2025	1.0105	0.0201	5.00E1	0.1022	4.5962	2.2162	1.9022
20220602 2257 11 2		6 01 5 2	1 2552	1 0252	1 2/52	4 7051	2 /551	2 0052	2 8552	1 1552	1 0252
20220002_2257_11-2	storage (2)	0.9113	1.2323	1.03L3	1.54L5	4.70L1	5.45L1	5.99LZ	2.05LZ	1.1362	1.0212
20220602 0610 9 6		2 7052	1 0052	2 7757	2 7252	0 1750	6 9250	0.9751	7.0651	1 2051	2 91 5 1
20220602_0610_9-0	orcu annealeu,	2.70E5	4.00EZ	5.72EZ	2.7562	9.1720	0.02EU	9.0701	7.00E1	4.50E1	5.01E1
	months (2)										
20220602 0642 9-11	OFCu untreated	9 20F3	1 66F3	1 99F3	1 45F3	8 17F1	5 99F1	4 12F2	2 94F2	1 42F2	1 26F2
20220002_0042_0 11	argon storage (1)	5.2025	1.0025	1.5525	1.4525	0.1711	5.5521	7.1202	2.3462	1.7262	1.2022
20220602 0700 9-12	OFCu untreated.	1.04F4	1.88F3	3.47F3	2.56F3	7.79F1	5.72F1	4.30F2	3.06F2	1.71F2	1.52F2
	argon storage (2)		1.0020	011720							
20220602 0715 9-5	OFCu annealed.	2.94E3	5.31E2	3.84E2	2.82E2	1.04E1	7.81E0	9.33E1	6.66E1	3.68E1	3.26E1
	argon storage 11				_						
	months (1)										
20220602_0731_9-17	OFCu annealed,	2.14E3	3.87E2	2.98E2	2.18E2	7.05E0	5.29E0	4.21E1	3.01E1	2.78E1	2.47E1
	argon storage 8										
	months (1)										
20220602_0813_9-23	OFCu annealed,	2.98E3	5.39E2	4.12E2	3.03E2	7.34E0	5.46E0	8.42E1	6.01E1	4.09E1	3.62E1
	argon storage 5										
	months (1)										
20220602_0826_9-24	OFCu annealed,	2.53E3	4.57E2	2.82E2	2.08E2	1.90E1	1.46E1	7.52E1	5.36E1	3.77E1	3.34E1
	argon storage 5										
	months (2)										
20220603_0152_9-17	OFCu annealed,	4.20E3	7.62E2	5.38E2	3.95E2	3.51E1	2.59E1	1.32E2	9.44E1	6.74E1	5.97E1
	argon storage 8										
20220602 0242 0.40	months (1)	6 6252	4 2052	4 2052	1.0452	4 7054	2 4654	4 2252	2.0252	4 0052	0.6454
20220603_0213_9-18	OFCU annealed,	6.63E3	1.20E3	1.38E3	1.01E3	4.72E1	3.46E1	4.23E2	3.03E2	1.09E2	9.64E1
	argon storage 8										
20220602 0216 0.8	$\frac{11011115(2)}{0ECu untroated(2)}$	1 105/	2 1252	2 2152	1 6252	2 7252	2 0052	1 5 2 5 2	1.0052	2 7152	2 2052
20220602_0210_9-8	OFCu untreated (2)	1.10E4	2.1555	2.21E5	2 2552	2.7262	2.0022	1.5265	7 3652	5.71EZ	5.29E2
20220002_0835_5-7		0.18F3	1.66E3	2 2752	1.68F3	0 10F1	6 7/F1	1.0323	2 56F2	2 3252	2.06E2
20220002_1344_9-20	atm storage 5	9.1015	1.0015	2.2715	1.0015	9.1911	0.7411	4.5522	5.50L2	2.5212	2.0012
	months (2)										
20220602 1416 9-19	OFCu annealed.	1.29E4	2.33E3	3.50E3	2.56E3	8.45E1	6.19E1	5.81E2	4.15E2	2.32E2	2.05E2
	atm. storage 5										
	months (1)										
20220602 1617 9-1	OFCu annealed,	7.66E3	1.38E3	8.46E2	6.19E2	9.33E1	6.84E1	6.76E2	4.85E2	2.88E2	2.55E2
	atm. storage 11										
	months (1)										
20220602_1641_9-2	OFCu annealed,	6.94E3	1.26E3	7.54E2	5.51E2	7.95E1	5.83E1	2.22E2	1.59E2	2.57E2	2.28E2
	atm. storage 11										
	months (2)										
20220602_1656_9-13	OFCu annealed,	7.34E3	1.33E3	1.19E3	8.72E2	7.91E1	5.81E1	3.90E2	2.79E2	1.88E2	1.67E2
	atm. storage 8										
	months (1)										

20220602_1707_9-14	OFCu annealed,	7.18E3	1.30E3	1.05E3	7.67E2	8.92E1	6.54E1	5.53E2	3.95E2	2.25E2	1.99E2
	atm. storage 8										
	months (2)										
20220603 0229 9-8	OFCu untreated (2)	8.23E3	1.49E3	9.27E2	6.80E2	2.84E2	2.08E2	5.61E2	4.01E2	2.43E2	2.15E2
20220603_0310_9-8	OFCu untreated (2),	4.36E3	7.88E2	4.42E2	3.26E2	1.84E1	1.37E1	1.93E2	1.38E2	6.18E1	5.49E1
_7x7	beam 7x7mm										
20220603_0344_9-8	OFCu untreated (2),	4.87E3	8.79E2	5.96E2	4.35E2	1.88E1	1.40E1	1.82E2	1.30E2	5.44E1	4.82E1
_4x4.5	beam 4x4.5mm										
20220603_1014_9-8	OFCu untreated (2),	4.49E3	8.11E2	4.47E2	3.34E2	1.28E1	9.61E0	1.17E2	8.32E1	3.56E1	3.16E1
_4x4.5	beam 4x4.5mm										
20220602_1455_10-7	OFCu annealed	1.28E3	2.31E2	1.23E2	9.16E1	2.70E0	2.06E0	2.53E1	1.81E1	2.27E1	2.01E1
	400°C, vacuum										
	storage (1)										
20220602_1512_10-8	OFCu annealed	1.21E3	2.18E2	1.84E2	1.35E2	1.36E0	1.07E0	2.18E1	1.56E1	2.47E1	2.19E1
	400°C, vacuum										
	storage (2)										
20220602_1525_10-9	OFCu annealed	1.25E3	2.26E2	1.57E2	1.16E2	2.40E0	1.85E0	2.85E1	2.04E1	2.58E1	2.29E1
	300°C, vacuum										
	storage (1)										
20220602_1538_10-10	OFCu annealed	1.40E3	2.53E2	1.32E2	9.77E1	1.80E0	1.43E0	3.06E1	2.18E1	2.07E1	1.84E1
	300°C, vacuum										
	storage (2)										
20220602_1551_10-11	OFCu annealed	1.15E3	2.08E2	1.08E2	8.09E1	1.15E0	9.67E-1	2.27E1	1.63E1	1.99E1	1.77E1
	500°C, vacuum										
	storage (1)										
20220602_1608_10-12	OFCu annealed	1.22E3	2.20E2	7.53E1	5.66E1	2.76E0	2.16E0	2.58E1	1.84E1	2.36E1	2.10E1
	500°C, vacuum										
	storage (2)										
20220602_2114_9-9	OFCu untreated,	8.17E3	1.48E3	1.84E3	1.34E3	7.27E1	5.33E1	5.71E2	4.10E2	1.62E2	1.43E2
	vacuum storage (1)										
20220602_2125_9-10	OFCu untreated,	1.04E4	1.89E3	2.53E3	1.85E3	8.35E1	6.13E1	7.10E2	5.08E2	1.46E2	1.29E2
	vacuum storage (2)										
20220602_2135_Cu1	OFCu annealed,	4.29E3	7.76E2	1.77E3	1.33E3	1.17E1	8.61E0	1.18E2	8.41E1	7.39E1	6.56E1
	vacuum storage (1)										
20220602_2146_Cu2	OFCu annealed,	4.15E3	7.50E2	1.01E3	7.39E2	2.24E1	1.67E1	1.29E2	9.22E1	6.02E1	5.33E1
	vacuum storage (2)										
20220602_2159_Cu3	OFCu annealed,	4.31E3	7.80E2	8.72E2	6.37E2	2.19E1	1.64E1	1.39E2	9.88E1	5.73E1	5.07E1
	vacuum storage (3)		_								-
20220602_2210_Cu4	OFCu annealed,	4.32E3	7.82E2	8.35E2	6.11E2	1.28E1	9.43E0	1.29E2	9.22E1	5.78E1	5.12E1
	vacuum storage (4)	6 7050	4 9959	4.0650	7 74 50	2 2054	4 7654	2.4052	4 7959	7.0254	7.0454
20220602_2220_Cu5	OFCu annealed,	6.78E3	1.23E3	1.06E3	/./1E2	2.39E1	1.76E1	2.40E2	1.72E2	7.92E1	7.01E1
20220602 2222 6.6	vacuum storage (5)	4.0552	0.0552	2 4552	4 0252	2 4 2 5 4	4 5054	2 2252	4 5052	7 2054	C 4754
20220602_2232_Cub	OFCU annealed,	4.95E3	8.95E2	2.45E3	1.82E3	2.12E1	1.56E1	Z.ZZEZ	1.58E2	7.30E1	6.47E1
20220601 4040 42 44	Vacuum storage (6)	2.0552	E E 4 E 2	2.0152	2.0052	1 0001	1 2551	0.0551	C 10F1	4 7754	4 2254
20220601_1848_12-14	OFCU sputt. 1.96E16	3.05E3	5.54E2	2.81E2	2.06E2	1.68E1	1.25E1	8.65E1	0.18E1	4.//EI	4.23E1
20220601_1902_12-19	OFCU sputt. 3.90E16	3.14E3	5.6/EZ	2.5/E2	1.88E2	1./1E1	1.27E1	1.33E2	9.51E1	5.42E1	4.80E1
20220601_1913_12-18	OFCU sputt 1 17517	4.33E3	7.82EZ	5.29EZ	3.94EZ	2.40E1	1.82E1	2.02E2	1.44EZ	8.33E1	7.30E1
20220601_1937_12-17	OFCU sputt. 1.1/E1/	3.16E3	5.72E2	3.49E2	3.11EZ	2.50E1	1.84E1	1.82E2	1.32E2	7.93E1	7.14E1
20220601_1950_12-13	OFCU Sputt.	3.61E3	0.52E2	6.43EZ	4.71E2	2.24E1	1.65E1	1.32E2	9.42E1	7.58E1	6.72E1
	1.90E10, IONg										
20220601 2002 12 20		4 7552	0 5050	1 5152	1 11 5 2	2 2751	1 6051	1.0652	1 4052	0 1051	7 25 51
20220001_2003_12-20	1 17E17 Jong	4.7553	0.30E2	1.3153	1.1153	2.2/11	1.0011	1.9022	1.40EZ	0.1961	1.2361
	distance										
20220601 2015 12 22		2 0752	E 2652	2 2552	2 4552	1 7251	1 2751	1.0452	1 2052	E 67F1	E 0251
20220001_2015_12-22	3 90F16 Jong	2.9/63	J.50E2	3.33EZ	2.43EZ	1.7261	1.2/11	1.9462	1.5962	3.0/E1	3.02E1
	distance										
20220601 2025 12 12		5 1252	0 2752	1 2152	0 7052	2 6/51	2 6051	1 6552	1 1753	1 1552	1 2052
20220001_2025_12-12	1 17E17 Jong	3.1253	5.2/CZ	1.5163	9.79EZ	3.0461	2.0001	1.0562	1.1/62	1.4562	1.2962
	distance										
	andunice	1	1	1	1	1	1	1	1	1	1

20220601_2038_12-15	OFCu sputt.	3.81E3	6.88E2	3.68E2	2.73E2	2.96E1	2.18E1	1.76E2	1.25E2	9.74E1	8.63E1
	7.79E16, long										
	distance										
20220601_2050_12-16	OFCu sputt.	3.78E3	6.83E2	3.99E2	2.92E2	2.62E1	1.93E1	1.40E2	1.00E2	8.39E1	7.43E1
	3.91E16, long										
	distance										
20220601_2102_12-24	Cu single crystal	5.01E3	9.06E2	1.12E3	8.21E2	5.26E1	3.89E1	3.46E2	2.46E2	1.24E2	1.10E2
	sputt. 3.02E17							4 0050	1 0 0 7 0	0.0050	
20220601_2338_12-2	OFCu sputt. 2.36E17	2.55E4	4.62E3	1.46E4	1.06E4	4.01E2	2.94E2	1.82E3	1.30E3	8.39E2	7.43E2
20220601_2357_12-3	OFCu sputt. 1.5/E1/	5.09E3	9.20E2	7.94E2	5.83E2	1.05E2	7.80E1	2.85E2	2.03E2	1.55E2	1.38E2
20220602_0017_12-4	OFCu sputt. 2.95E17	6.00E3	1.08E3	1.16E3	8.46E2	1.31E2	9.60E1	4.73E2	3.37E2	1.64E2	1.45E2
20220602_0035_12-6	OFCu sputt. 3.90E17	4.09E3	7.38E2	3.84E2	2.81E2	6.92E1	5.09E1	2.07E2	1.48E2	1.05E2	9.26E1
20220602_0053_12-7	OFCu sputt. 4.68E17	6.58E3	1.19E3	9.65E2	7.05E2	2.08E2	1.53E2	3.96E2	2.83E2	1.65E2	1.46E2
20220602_0110_12-9	OFCu sputt. 2.99E17	6.75E3	1.22E3	1.16E3	8.43E2	1.18E2	8.69E1	3./1E2	2.64E2	1.54E2	1.36E2
20220602_0125_12-10	3.02E17	6.19E3	1.12E3	1.14E3	8.32E2	1.06E2	7.77E1	4.53E2	3.23E2	1.32E2	1.17E2
20220602_0138_12-11	OFCu sputt. 3kV, 3.02E17	5.35E3	9.67E2	1.05E3	7.69E2	1.32E2	9.68E1	2.71E2	1.93E2	1.12E2	9.93E1
20220602_0230_12-1	OFCu sputt. 1.03E18	9.66E3	1.75E3	1.70E3	1.25E3	1.36E2	1.00E2	9.40E2	6.71E2	2.55E2	2.26E2
20220602_0548_12-21	OFCu sputt. 60°,	3.63E3	6.56E2	2.49E2	1.85E2	2.01E2	1.47E2	1.96E2	1.40E2	7.97E1	7.05E1
	7.79E16, long										
	distance										
20220602_2308_8-20	OFCu sputt. 30°,	9.03E3	1.63E3	1.66E3	1.21E3	2.02E2	1.48E2	9.75E2	6.95E2	3.45E2	3.05E2
	4.35E18, annealed										
20220602_2319_8-23	OFCu sputt. 3.40E18	7.60E3	1.38E3	9.06E2	6.63E2	8.45E1	6.20E1	4.41E2	3.15E2	2.29E2	2.03E2
20220603_0414_12-14	OFCu sputt. 1.96E16	4.69E3	8.48E2	4.59E2	3.36E2	1.28E1	9.42E0	1.77E2	1.26E2	4.71E1	4.17E1
_4x4.5	050	5 5052	0.0452	7.0452	5 7052	2 5054	4.0454	2.0252	4 4452	6.0754	6 4 0 5 4
20220603_0432_12-19	OFCU Sputt. 3.90E16	5.50E3	9.94E2	7.91E2	5.78E2	2.59E1	1.94E1	2.02E2	1.44E2	6.97E1	6.18E1
_4X4.5		F 10F2	0.2052	F 22F2	2 0252	2 6251	1.0551	2 2052	1 6252		4.9451
20220603_0445_12-18	OFCU Spull. 7.85E16	2.19E3	9.3862	5.23EZ	3.83EZ	2.03E1	1.9561	2.2962	1.0362	5.47E1	4.84E1
_4x4.5 20220603_0459_12-17	OFCu sputt 1 17F17	1 09F/	1 97F3	1 70F3	1 2/F3	6 50E1	/ 79F1	5 //7F2	3 90F2	1 86F2	1.65E2
4x4.5		1.0524	1.5725	1.7025	1.2425	0.5021	4.7 521	5.4722	5.5022	1.0012	1.0322
20222603 0510 12-3	OFCu sputt. 1.57E17	4.52E3	8.17E2	4.80E2	3.52E2	1.18E1	8.95E0	1.47E2	1.05E2	4.99E1	4.42E1
4x4.5											
	OFCu sputt. 2.36E17	2.29E4	4.15E3	3.94E3	2.88E3	8.58E1	6.30E1	1.37E3	9.76E2	3.44E2	3.05E2
20220603 0531 12-4	OFCu sputt. 2.95F17	4.88F3	8.82F2	4.36F2	3.21F2	2.51F1	1.88F1	1.79F2	1.28F2	6.05F1	5.37F1
4x4.5											
20220603 0544 12-9	OFCu sputt. 2.99E17	3.20E3	5.80E2	6.18E2	4.83E2	2.64E0	2.52E0	7.20E1	5.21E1	1.73E1	1.54E1
4x4.5											
20220603_1034_12-13	OFCu sputt.	1.20E4	2.17E3	1.56E3	1.14E3	2.89E1	2.14E1	7.01E2	4.99E2	1.45E2	1.28E2
_4x4.5	1.96E16, long										
	distance										
20220603_1103_12-16	OFCu sputt.	4.49E3	8.11E2	3.58E2	2.69E2	1.08E1	8.25E0	1.30E2	9.25E1	4.50E1	3.99E1
_4x4.5	3.91E16, long										
	distance			-							
20220603_1134_12-15	OFCu sputt.	4.97E3	8.98E2	5.46E2	4.00E2	1.82E1	1.35E1	1.79E2	1.27E2	5.14E1	4.55E1
_4x4.5	7.79E16, long										
	distance	F 2552	0.4052	6 7052	4.0052	1 5 6 5 4	1 1 (5 1	1 0252	1 2052	F 2554	4.0554
20220603_1152_12-12	OFCU sputt.	5.25E3	9.49E2	6.78E2	4.96E2	1.56E1	1.16E1	1.83E2	1.30E2	5.25E1	4.65E1
_4x4.5	distance										
20220603 1206 12 ₋ 7	OFCU sputt / 68E17	7 80E5	8 8363	4 9562	3 6252	1 6/F1	1 21F1	1 5162	1 0852	5 2251	4 63F1
4x4.5	5, cu sputt. 4.00L17	7.0JLJ	0.05L2		5.0222	1.04L1	1.21L1	1.5112	1.00L2	5.2211	7.03L1
20220603 1311 12-6	OFCu sputt. 3.90F17	4.57F3	8.26F2	5.80F2	4.24F2	9.71F0	7.28F0	1.30F2	9.29F1	3.78F1	3.35E1
4x4.5											
_ 20220603 1357 12-20	OFCu sputt. 60°,	4.26E3	7.70E2	3.60E2	2.71E2	7.21E0	5.54E0	1.24E2	8.82E1	4.34E1	3.85E1
_4x4.5	1.17E17, long	_				_	_				
	distance										

20220603_1409_12-21	OFCu sputt. 60°,	4.24E3	7.67E2	2.97E2	2.24E2	8.30E0	6.22E0	1.26E2	9.01E1	3.92E1	3.48E1
_4x4.5	7.79E16, long										
	distance										
20220603_1422_12-22	OFCu sputt. 60°,	4.15E3	7.50E2	6.00E2	4.42E2	1.17E1	8.95E0	1.09E2	7.77E1	3.57E1	3.17E1
_4x4.5	3.90E16, long										
	distance										
20220603_1436_12-11	OFCu sputt. 3kV,	4.21E3	7.62E2	5.31E2	3.96E2	1.31E1	1.04E1	1.17E2	8.32E1	4.03E1	3.58E1
_4x4.5	3.02E17										
20220603_1451_12-10	OFCu sputt. 4 keV,	8.46E3	1.53E3	1.28E3	9.27E2	4.14E1	3.04E1	3.94E2	2.80E2	7.76E1	6.87E1
_4x4.5	3.02E17										

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