

Chapter 7

Summary

In this work the influence of hydrogen on the structure and lattice dynamics in different austenitic stainless steels (Fe-25Cr-20Ni and Fe-18Cr-10Ni) was investigated. The experimental data obtained by elastic and inelastic neutron scattering were used to perform a modelling of the phonon density of states.

Firstly the lattice dynamics in non-hydrogenated austenitic stainless steels was investigated. Austenitic stainless steels Fe-18Cr-12Ni-2Mo and Fe-18Cr-16Ni-10Mn show very similar phonon dispersion curves which can be well described by model calculations including interactions of two-neighbour shells plus contributions of conduction electrons on the lattice dynamics. Our results for the elastic constants and engineering elastic moduli are close to the results obtained by ultrasonic studies on polycrystalline samples. For further investigations of alloying effects on elastic constants and moduli, ultrasonic measurements on single crystals would be supportive. The calculations of vibrational densities of states from the modelling of phonon dispersion branches have been confirmed by measurements of the vibrational frequency spectra. Experimental data based on the phonon density of states show, that differences between the samples (Fe-18Cr-12Ni-2Mo, Fe-18Cr-16Ni-10Mn and Fe-18Cr-10Ni) are inside the error bars. The obtained Debye temperature Θ_D gives a minimum at about 40 K and shows good agreement with previous studies on similar fcc systems.

Firstly, the influence of hydrogen on the acoustic modes was introduced into the model, unfortunately, reliable experimental data do not exist to verify the model calculations. Further investigations an accurate measurement of the acoustic modes is required.

The experimental data for the optical modes for samples with high hydrogen content are significantly different from the data of medium and low hydrogen content and therefore the appropriate model is different. Samples with medium and low hydrogen content in the range of ($0.0027 < H/Me < 0.66$) show a very similar density of states .

For the fully hydrogenated system ($H/Me \sim 1$) the Born-von Karman model is used with contributions from the hydrogen-hydrogen interaction and from different alloying elements. From this model hydrogen-hydrogen force constants are obtained by the fitting procedure. Also, the phonon dispersion curves were simulated. For the accurate calculation of the interatomic force constants inelastic neutron scattering on single crystal samples are nec-

essary. To my knowledge, this experiment is not possible due to the extreme conditions (pressure up to the 7 GPa) during hydrogenation, which will destroy the single crystal. The obtained force constants from the fully hydrogenated system are used for the calculation of the phonon density of states in partially hydrogenated systems ($0.3 < H/Me < 0.7$). The simple model presented in ([Rafizadeh 1981]) gave a reasonable agreement with the experimental data. The main difference in the profile of the DOS could be explained by the fact, that hydrogen, due to a differing metal neighbourhood, feels a different potential compared to pure metal-hydrides with distorted interatomic potential. For an improved description of hydrogenated austenitic stainless steels ab-initio calculations will be supportive.

The model for the samples with low hydrogen fit well to the experimental data. Due to the low contribution of the hydrogen-hydrogen bonding to the lattice dynamics it is plausible to apply the same model for samples with low and medium hydrogen contents. The simulations show, that the main contribution to the broadening of the DOS is due to non-central positions of hydrogen in the octahedral interstitial sites.

In the second part the structure and lattice dynamics of $Cu_{2-\delta}Se$ was investigated. Diffraction studies were performed with X-ray and synchrotron radiation in different temperature ranges. From the diffraction experiments reliable data for the high-temperature (α -phase) was obtained. In the α -phase copper atoms are distributed over different interstitial sites of the fcc lattice. Future investigations on single crystals are necessary to obtain structural data for the low-temperature (β -phase). These data will be supportive for ab-initio calculations on $Cu_{2-\delta}Se$ to give a better interpretation of the obtained data for the phonon dispersion curves and the phonon density of states. Ab-initio calculations will also give additional information on the nature of the low energy modes, which are correlated with the diffusion processes.

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List of abbreviation

AISI	A merican I ron and S teel I nstitute
AS	a xially s ymmetric force constants
bcc	b ody c entred c ubic
BvK	B orn von K arman
DOS	d ensity of s tates
EDX	E nergy D ispersive X -ray spectroscopy
FANS	F ilter A nalysers N eutron S pectrometer
fcc	f ace c entred c ubic
FWHM	F ull W idth H alf M aximum
GF	g eneralised force constants
hcp	h exagonal c losed p acking
ILL	I nstitute L aué- L angevin
INS	I nelastic N eutron S cattering
JINR	J oint I nstitute for N uclear R esearch
LE	L ow - E nergy
NIST	N ational I nstitute of S tandards and T echnology
TAS	T riple A xis S pectrometer
TOF	T ime- o f- f light
TOSCA	T hermal O riginal S pectrometer with C ylindrical A nalysers

List of symbols

α	Cartesian coordinate, linear expansion coefficient
$\alpha_1, \alpha_2, \alpha_3$	force constants in generalised force model
α_{ij}	force constants in generalised force model
β_{ij}	force constants in generalised force model
$\beta_1, \beta_2, \beta_3$	force constants in generalised force model
γ	Grüneisen parameter
δ	displacement
θ	angle
Θ_D	Debye temperature
$\Theta(T)$	Debye temperature as a function of absolute temperature
Θ_0	Debye temperature in the low-temperature limit
Θ_∞	Debye temperature in the high-temperature limit
$\varepsilon_{\alpha\beta}$	strain
$\vec{\varepsilon}(\vec{k})$	polarisation vector
$\varepsilon(\vec{q})$	dielectric function
χ	susceptibility
μ	Poisson ratio
μ'	Lamé coefficient
ϕ	potential
Φ	force constant matrix, angle, potential
ρ	density
$\vec{\tau}$	reciprocal lattice vector
σ	cross section
$\frac{d^2\sigma}{d\omega d\Omega}$	double differential cross section
λ	screening length of Coulomb potential, Lamé coefficient, wavelength
ω	angular frequency
ω_D	Debye frequency
Ω	space angle
$\Delta\omega$	frequency shift
A	Zener anisotropy, force constant in axially symmetrical model
$A(\vec{k})$	Amplitude of oscillation
a	lattice constant

Δa	dilatation of lattice constant
a_0	Bohr radius
b, b_i	scattering lengths
B	force constant in axially symmetrical model, bulk modulus
B_{iso}	isotropic thermal parameter
C	Voigt tensor of elasticity
$c_{\alpha\beta\gamma\delta}$	tensor of elastic constants
c_V	specific heat capacity
C_V	heat capacity
C_{ij}	elastic constants
C_{11}, C_{12}, C_{44}	elastic constants of a cubic system
D	dynamical matrix
G	shear modulus
G_H	Hershy-Kröner-Eshelby average of the shear modulus
G_R	Reiss average of the shear modulus
G_V	Voigt average of the shear modulus
E	energy, Young modulus
E_i, E_f	initial, final energy
E_{hkl}	intensity at the point with indices (hkl)
$\vec{e}(\vec{k})$	polarization vector
F	free energy
F_0	minimum of free energy
$F(\vec{Q})$	form factor
$g(\omega)$	density of states
H	Hamiltonian
h, \hbar	Planck,(reduced) Planck constant
i, j	summation indices
i, j, k	Miller indices
\vec{k}	wave vector
k_B	Boltzmann constant
k_c	inverse screening length
k_e	inverse screening length
k_{TF}	Thomas-Fermi wave number
l	length
m	mass
m_H	mass of hydrogen atom
m_{Me}	mass of metal atom
m_n	mass of neutron
N	number of particles
n	order of maximum
n_e	concentration of electrons
$n(\omega)$	Bose-Einstein distribution

\vec{p}	momentum
\vec{q}, \vec{Q}	wave vector
p	pressure
r	radial coordinate
R	universal gas constant, metal-hydrogen distance
\vec{r}_{ij}	radius vector from point (i) to point (j)
r_s	average interatomic distance
S	surface, entropy
$S(\vec{Q}, \omega)$	dynamical structure factor
t	time
T	absolute temperature
u	distance from equilibrium point
$u_\alpha(\mathbf{k})$	component of displacement from equilibrium position
$\langle u_\alpha^2 \rangle$	mean square displacement
U	internal energy
v_L, v_T	longitudinal, transversal velocity of sound
V	potential, volume
V_a	atomic volume
V_0	minimum of potential
W	Debye-Waller exponent
e^{-2W}	Debye-Waller factor

Bibliography

- [Abrikosov 1983] N.H. Abrikosov, V.F. Bankina, M.A. Korzhuev, G.K. Demski, O.A. Teplov: Calorimetric study of the superionic transition in Cu_{2-x}Se , *Sov. Phys.-Solid State* **25**, 1678 (1983).
- [Antonov 1996] V.E. Antonov, T.E. Antonova, N.A. Chirin, E.G. Ponyatovsky, M. Baier, F.E. Wagner: T-P phase diagram of the Mn-H system at pressures to 4.4 GPa and temperatures to 1000 °C , *Scripta Materialia* **34**, 1331 (1996).
- [Antonov 2000] V.E. Antonov, K. Cornell, B. Cornell, V.K. Fedotov, G. Grosse, A.I. Kolesnikov, F.E. Wagner and H. Wipf: Neutron spectroscopy of γ manganese hydride, *Solid state Comm.* **113**, 569 (2000).
- [Ashcroft 1976] N.W. Ashcroft and N.D. Mermin(1976), *Solid state physics*, W.B. Saunders Company.
- [Beskrovni 1999] A. Beskrovni, S.A. Danilkin, H. Fuess, E.L. Jadrowski, M. Neova-Baeva, T. Wieder: Effect of Cr on the crystal structure and lattice dynamics of FCC Fe-Cr-Ni-N austenitic alloys, *J.Alloys Comp.* **291**, 262 (1999).
- [Boyce 1981] J.B. Boyce, T.M. Hayes and J.C. Mikkelsen: EXAFS investigation of mobile-ion density: CuI and Cu_2Se contrasted, *Solid State Ionics* **5**, 497 (1981).
- [Brugger 1964] K. Brugger: Thermodynamic Definition of Higher Order Elastic Coefficients, *Phys. Rev.* **133**, A1611 (1964).
- [Chene 1977] J. Chene, *Metaux, Corrosion, Industrie*, **262**, 623 (1977).
- [Cornell 1997] K. Cornell, H. Wipf, V.E. Antonov, T.E. Antonova, A.I. Kolesnikov, E.G. Ponyatovsky, B. Dorner: The inelastic neutron scattering spectrum of dhcp iron hydride, *Pol. J. Chem.* **71**, 1792 (1997).
- [Danilkin 1997] S.A. Danilkin, E.L.Jadrowski: Phonon dispersion in Fe-18Cr-10Mn-15Ni FCC steel, *Physica B* **234**, 900 (1997).
- [Danilkin 2001] S.A. Danilkin, H. Fuess, T. Wieder, A. Hoser: Phonon dispersion and elastic constants in Fe-Cr-Mn-Ni austenitic steel, *J.Mater.Sci.* **36**, 811 (2001).

- [Dawidowski 1998] J.Dawidowski, F.J.Bermejo, J.R.Granada: Efficient procedure for the evaluation of multiple scattering and multiphonon corrections in inelastic neutron-scattering experiments, *Phys. Rev. E* **58**, 706 (1998).
- [Dawidowski 2002] J.Dawidowski, G.J.Cuello, M.M.Koza, J.J.Blostein, G.Aurelio, A.Fernández Guillermet, P.G.Donato: Analysis of multiple scattering and multiphonon contributions in inelastic neutron scattering experiments, *Nucl. Instr. and Meth. B* **195**, 389 (2002).
- [Dorner 1989] B. Dorner, I.T. Belash, E.L. Bokhenkov, E.G. Ponyatovsky, V.E. Antonov, L.N. Pronina: Inelastic incoherent neutron scattering spectra from fcc Ni_{1.05}, hcp Cr_{1.0} and Mo_{1.2} at 15 K., *Solid State Comm.* **69**, 121 (1989).
- [Fukai 1981] Y. Fukai, H. Sugimoto: On the optical-mode excitation energy of interstitial hydrogen in metals, *J. Phys. F: Metal Phys.* **11**, L137 (1981).
- [Fullprof 2002] T. Roisnel and J. Rodrigues-Carvajal, Winplotr December 2002 <http://www-llb.cea.fr/fullweb/winplotr/winplotr.htm>
- [Gairola 1981] B.K.D. Gairola: A simple formula for calculating the bounds and the self-consistent value of the shear modulus of a polycrystalline aggregate of cubic crystals, *E. Kröner Internat. J. Engng. Sci.* **19**, 865 (1981).
- [Hallman 1969] E.D. Hallman, B.N. Brockhouse: Crystal dynamics of nickel-iron and copper-zinc alloys, *Can.J.Phys.* **47**, 1117 (1969).
- [Heyding 1976] R.D. Heyding and R.M. Murray: Crystal structures of Cu_{1.8}Se, Cu₃Se₂, α - and γ -CuSe, CuSe₂, and CuSe₂ II, *Can. J. Chem.* **54**, 841 (1976).
- [Hoelzel 2002] M. Hoelzel, S.A. Danilkin, A. Hoser, H. Ehrenberg, T. Wieder, H. Fuess *J.Appl.Phys. A* **75** 1-3 (2002), Supplement of the ICNS 2001.
- [Hoelzel 2004] M. Hoelzel, *Struktur und Gitterdynamik wasserstoffbeladener austenitischer Edeltähle*, Doctoral thesis (2004).
- [Hooper 1978] A. Hooper, *Contemp. Phys.* **19**, 147 (1978).
- [Jackman 1986] J.A. Jackman, T.M. Holden, W.J.L. Buyers, P.de V. DuPlessis, O. Vogt, and J. Genossar: Systematic study of the lattice dynamics of the uranium rocksalt-structure compounds, *Phys. Rev.* **B33**, 7144 (1986).
- [Kádár 1999] G.Kádár and L.Rosta(1999), Introductory Course to the 2nd European Conference on Neutron Scattering.
- [Keen 1995] D.A. Keen and S. Hull: The high-temperature structural behaviour of copper(I) iodide, *J. Phys.: Condens. Matter.* **7**,5793 (1995).

- [Keen 1998] D.A. Keen and S. Hull: Determination of structural disorder in Ag_2Te superionic by neutron total scattering *J. Phys.:Condens. Matter.* **10**, 8217 (1998).
- [Kim 1994] S.A. Kim, H.M. Ledbetter, Y.Y. Li: Elastic constants of four Fe-Cr-Ni-Mn alloys, *J.Mater.Sci.* **29**, 5462 (1994).
- [Kittel 1963] C. Kittel, *Quantum theory of solids(1963)*, J. Wiley& Sons, Inc.
- [Kolesnikov 1991] A.I. Kolesnikov, I. Natkaniec, V.E. Antonov, I.T. Belash, V.K. Fedotov, J. Krawczyk, J. Mayer, E.G. Ponyatovsky: Neutron spectroscopy of $\text{MnH}_{0.86}$, $\text{NiH}_{1.05}$, $\text{PdH}_{0.99}$ and harmonic behaviour of their optical phonons, *Physica B* **174**,257 (1991).
- [Korzhuev 1989] M.A. Korzhuev: Mixed conduction and ultrafast chemical diffusion in superionic Cu_{2-x}Se , *Sov. Phys. - Solid State* **31**,1666 (1989).
- [Koto 1980] K. Koto, H. Schulz and R.A. Huggins: Anion disorder and ionic motion in lead fluoride ($\beta\text{-PbF}_2$), *Solid State Ionics* **1**, 355 (1980).
- [Krebs 1965] K.Krebs: Dispersion curves and lattice frequency distribution of metals, *Phy.Rev.***138**, A143 (1965).
- [Landau 1970] L.D. Landau and E.M. Lifshitz(1970), *Theory of elasticity*, 2nd edn. Oxford: Pergamon
- [Ledbetter 1981] H.M. Ledbetter: Predicted single-crystal elastic constants of stainless steel 316,*Brit. J. Non-Destructive Testing* **34**, 286 (1981).
- [Ledbetter 1984] H.M. Ledbetter: Monocrystal-polycrystal elastic constants of a stainless steel, *Phys.Stat.Sol.(a)* **85**, 89 (1984).
- [Ledbetter 1985] H.M. Ledbetter: Effects of carbon and nitrogen on the elastic constants of AISI type 304 stainless steel, *J.Mater.Sci.* **20**, 2923 (1985).
- [Ledbetter 1988] H.M. Ledbetter, S.A. Kim: Low-temperature manganese contributions to the elastic constants of face-centred-cubic Fe-Cr-Ni stainless steel, *J.Mater.Sci.* **23**, 2129 (1988).
- [Milat 1987] O. Milat, Z. Vucic, B. Rubčić: Superstructural ordering in low-temperature phase of superionic Cu_2Se , *Solid State Ionics* **23**, 37 (1987).
- [Milat 1987b] Ref. 1-11 supplied in [Milat1987].
- [Mohammed 1984] K. Mohammed, M.M. Shukla, F. Milstein, J.L. Merz: Lattice dynamics of face-centered-cubic metals using the ionic Morse potential immersed in the sea of free-electron gas, *Phy.Rev.B.* **29**, 3117 (1984).

- [Oliveria 1988] M. Oliveria, R. K. McMullan and B. J. Wuensch: Single crystal neutron diffraction analysis of the cation distribution in the high-temperature phases α -Cu_{2-x}S, α -Cu_{2-x}Se, and α -Ag_{2-x}Se, *Solid State Ionics* **28-30**,1332 (1988).
- [Rafizadeh 1981] H.A. Rafizadeh: Lattice dynamics of metal hydrides, *Phys.Rev. B* **23**, 1628 (1981).
- [Rahlfis 1936] P. Rahlfs: Über die kubischen Hochtemperaturmodifikationen der Sulfide und Telluride des Silbers und des einwertigen Kupfers, *Z.Physik, Chem.B* **31**,157 (1936).
- [Reuss 1929] A. Reuss *Z. Angew. Math. Mech* **9**, 49 (1929).
- [Sakuma 1989] T. Sakuma, K. Sugiyama, E. Matsubara and Y. Waseda: Determination of the Crystal Structure of Superionic Phase of Cu₂Se *Materials Transactions, JIM* **30**, 365 (1989).
- [Sakuma 1995] T. Sakuma: Structural and dynamical properties of solid state ions *Bulletin of Electrochemistry* **11**, 57 (1995).
- [Salamon 1979] M.B.Salamon (Ed.): *Physics of Superionic Conductors*, Springer-Verlag, Berlin (1979).
- [Sjölander 1958] A.Sjölander: Multi-phonon processes in slow neutron scattering by crystals, *Ark. Fys.* **14**, 315 (1958).
- [Stassis 1982] C. Stassis, C.-K. Loong, C. Theisen, and R.M. Nicklow: Lattice dynamics of fcc Yb, *Phys. Rev. B* **26**, 4106 (1982).
- [Stassis 1983] C. Stassis, J. Zaretsky, D.K. Misemer, H.L. Skriver, B.N. Harmon, and R.M. Nicklow: Lattice dynamics of fcc Ca, *Phys. Rev. B* **27**, 3303 (1983).
- [Svensson 1967] E.C. Svensson, B.N. Brockhouse, J.M. Rowe: Crystal dynamics of copper, *Phys.Rev.* **155**, 619 (1967).
- [Ulmer 1993] D.G. Ulmer, C.J. Altstetter: Phase relations in the hydrogen - austenite system, *Acta metal. mater.* **41 (7)**, 2235 (1993).
- [Vitos 2003] L.Vitos, P.A. Korzhavyi, B. Johansson: Stainless steel optimization from quantum mechanical calculations, *Nat. Mat.***2**, 25 (2003).
- [Voigt 1889] W. Voigt *Ann. Phys.* **38**, 573 (1889).
- [Weber 1973] W. Weber: Lattice Dynamics of Transition-Metal Carbides, *Phys.Rev. B* **8**, 5082 (1973).
- [Willis 1975] B.T.M. Willis and A.W. Pryor(1975), *Thermal vibration in Crystallography*, Cambridge University Press.

- [Yakshibaev 1984] R.A. Yakshibaev, B.N. Konev and M.H. Balapanov: Ionic conductivity and diffusion in superionic conductor in α -Cu_{2-x}Se, Sov. Phys.-Solid State **26**, 2189 (1984).
- [Yamamoto 1991] K. Yamamoto and S. Kashida: X-ray study of the cation distribution in Cu₂Se, Cu_{1.8}Se and Cu_{1.8}S; analysis by the maximum entropy method, J. Solid State Chem. **48**, 241 (1991).
- [Zarestky 1987] J. Zarestky, C. Stassis: Lattice Dynamics of γ -Fe, Phys.Rev.B **35**, 4500 (1987).

Eidesstattliche Erklärung

Hiermit erkläre ich an Eides statt, dass ich meine Dissertation selbstständig und nur mit den angegebenen Hilfsmitteln angefertigt habe. Ich habe zu keinem früheren Zeitpunkt den Versuch einer Promotion unternommen.

Darmstadt, 5. Juli, 2004

Vedran Rajevac

Curriculum vitae

Vedran Rajevac

64295 Darmstadt, Kronstädter Weg 2

Phone: 06151/16-6003;06151/319-489 (private)

E-mail: rajevac@st.tu-darmstadt.de; vrajevac_hr@yahoo.com(private)

Personal data

Place and date of birth	1 st May 1974 in Zagreb, Croatia
Citizenship	Croatian
Religion	Roman-catholic
Family status	single

Education

August 1981 till July 1989	Elementary school in Zagreb
August 1989 till July 1993	Mathematical Gymnasium in Zagreb

Computer Skills

Operating system	Windows, Unix
Packages	Latex, Origin, Mathematica, Microsoft Office
Professional software	Fullprof, Diamond

Skills

Powder diffraction course
Introductory course of neutron scattering, HMI(Berlin)

Study

October 1993 till June 1999	University of Zagreb, Physic department
May 1997	Rector award University of Zagreb for "Electron spectroscopy of plasmon excitation in fulleren molecule"
June 1999	Graduate with average mark 4.77 Defense of thesis: "Dispersive Relations in Phonons in Crystal and Thin Films" with mark: 4
December 2000-2004	PhD thesis in Darmstadt University of Technology, Institute for Materials Science, under the supervision of Prof. Dr. Hartmut Fueß

Conference contributions

Poster presentation

1. M.Hoelzel, V.Rajevac, S.A. Danilkin, A.Hoser, T.Wieder, H.Fuess, Phonon dispersion in austenitic stainless steels. International conference on neutron scattering, München 9-13 September 2001
2. S.A. Danilkin, A.N. Skomorokhov, A. Hoser, V. Rajevac, H. Fuess, N.N. Bickulova, Lattice dynamics of superionic conductor $\text{Cu}_{2-\delta}\text{Se}$. Proceedings of the European Spallation Source Conference, 16-17 May 2002. Bonn, Germany
3. S.A. Danilkin, A.N.Skomorokhov, V. Rajevac, H. Fuess, A. Hoser, N.N. Bickulova, Crystal structure and lattice dynamics of superionic conductor $\text{Cu}_{2-\delta}\text{Se}$, 5th International Conference "Solid State Chemistry 2002", Bratislava, July 7-12, 2002.
4. A.N. Skomorokhov, S.A. Danilkin, V.A. Semenov, N.N. Bickulova, V. Rajevac, H. Fuess, A.V. Puchkov, G.N. Asylguzhina, Phonon Density of States in Superionic and non-Superionic $\text{Li}_{0.25}\text{Cu}_{1.75}\text{Se}$, XIIth International Conference on Selected Problems of Modern Physics, Dubna, June 8-11, 2003.
5. A.N. Skomorokhov, N.N. Bickulova, G.N. Asylguzhina, A.I. Beskrovnyj, M. Knapp, V. Rajevac, S.A. Danilkin, H. Fuess, Average Structure in Stoichiometry Dependent α - $\text{Cu}_{2-\delta}\text{Se}$ XIIth International Conference on Selected Problems of Modern physics, Dubna, June 8-11, 2003.
6. V.Rajevac, M.Hoelzel, S.A. Danilkin, A.Hoser, H.Fuess, Lattice dynamics in austenitic stainless steels., XIIth International Conference on Selected Problems of Modern physics, Dubna, June 8-11, 2003.
7. V.Rajevac, M.Hoelzel, S.A. Danilkin, A.Hoser, H.Fuess, Lattice dynamics in austenitic stainless steels Fe-18Cr-12Ni-2Mo and Fe-18Cr-16Ni-10Mn. 3rd European conference on neutron scattering, Montpellier 3-6 September 2003.
8. M.Hoelzel, S.A. Danilkin, T.J. Udovic, A.J. Ramirez-Cuesta V.Rajevac, H.Wipf H.Fuess, Neutron spectroscopy on high-pressure austenitic stainless steels. 3rd European conference on neutron scattering, Montpellier 3-6 September 2003.
9. V. Rajevac, M. Hoelzel, S.A. Danilkin, A.Hoser H. Fuess, Lattice dynamics in austenitic stainless steels. German-JINR User Meeting, Dubna 12-16 June, 2004.
10. V. Rajevac, M. Hoelzel, S. A. Danilkin, T. J. Udovic H. Fuess, Lattice dynamics in hydrogenated austenitic stainless steels. German-JINR User Meeting, Dubna 12-16 June, 2004.
11. D.M. Trots, K.G. Bramnik, H. Ehrenberg, A.N. Skomorokhov, V. Rajevac, R. Theissmann, M. Knapp H. Fuess, Synthesis and X-ray. diffraction studies of $\text{Cu}_{2-\delta}\text{Se}$. German-JINR User Meeting, Dubna 12-16 June, 2004.

Oral contribution

1. Lattice dynamics in hydrogenated austenitic stainless steels. Turkish-German Workshop on Diffraction Techniques, Ankara 19-23 May, 2004.
2. Lattice dynamics in hydrogenated austenitic stainless steels. German-JINR User Meeting, Dubna 12-16 June, 2004.

Publications

1. S.A. Danilkin, A.N. Skomorokhov, A. Hoser, H. Fuess, V. Rajevac and N.N. Bickulova, Crystal structure and lattice dynamics of superionic conductor $\text{Cu}_{2-\delta}\text{Se}$, *J. Alloys and Compounds*, **361**(2003) 57-61.
2. V. Rajevac, M. Hoelzel, S. A. Danilkin, A. Hoser, H. Fuess, Lattice dynamics in austenitic stainless steels Fe-18Cr-12Ni-2Mo and Fe-18Cr-16Ni-10Mn, *J. Phys. Condens. Matt.* **16**(2004) 2609-2616.