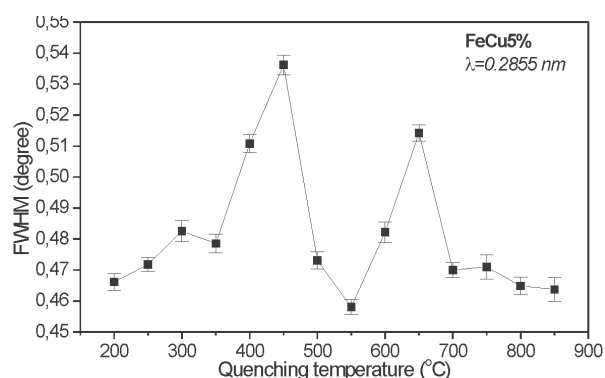


s14.m39.p3 **Stresses on Cu Precipitates in FeCu(5%) Alloy.** L.Kőszegi, *Research Institute for Solid State Physics and Optics, H-1525 Budapest, P.O.Box 49, Hungary. E-mail: koszegi@szfki.hu*

**Keywords: Neutron diffraction; Precipitation; Residual stress**

Precipitation of copper in iron and steels has been studied extensively in the past, especially because of the pressure vessel steels, which are used in nuclear reactors [1,2]. According to the equilibrium phase diagram [3], the highest solubility of Cu  $\alpha$  in iron (1.8 at% at 850°C) divides the Cu precipitates into two branches. The Cu amount above this value precipitates mostly on the boundaries of the Fe grains (PGB) while the remaining portion, after ageing precipitates inside the Fe grains (PIG) [4]. Here we present a detailed investigation on quenched-in stresses in Fe<sub>95</sub>Cu<sub>5</sub> alloy. Identical samples were homogenized (850°C, 3h) to attain precipitation (PGB) above 1.8 at% Cu. The samples were later cooled down (~1°C/min) and were quenched one by one into water after every 50 °C decrease down to 200 °C. Excess precipitations, PIG gradually appear below the solubility limit.  $\lambda=0.2855$  nm neutrons with identical support and slits were used in order to measure the Cu (111) reflection. The differential Bragg law,  $e = \Delta d/d_0 = -\cot\Theta\Delta\Theta$  yields the strains and the stresses were calculated by  $\sigma_{\text{cal}} = E_{111}(191.1 \text{ GPa}) \times e$  [5] and  $d_0=0.2087$  nm [4]. The Cu grains are under increasing tension as the quenching temperature increases. The total stress varies from 355 MPa to 280 MPa. The difference in the thermal expansion coefficients ( $\alpha_{\text{Cu}}-\alpha_{\text{Fe}}\sim 4.5 \times 10^{-6}/^\circ\text{C}$ ) would cause 713



MPa 155 MPa stresses in this quenching region which means that the missing elastic stress probably appear in plastic ones which produce broadening. The sample quenched from 850°C contains only PGB with 2.5 nm average diameter. The 0.21° additional broadening comes from the pumped in plastic deformation. At 200°C quenching temperature beside similar amount of PGB uniformly sized PIG is also present with 0.5nm characteristic diameter. The contributions of PGB and PIG to the broadening, however, are not separable. Between the extrema, PIG start to grow and pass through structures (9R, 3R) and dimensions (<0.1 $\mu\text{m}$ ) which definitely contribute to the broadening. In contrary on PGB one would expect decreasing plastic deformation with decreasing quenching temperature while significant amount on PIG because the constrains of the Fe matrix.

- [1] F. Maury, *et al.*, *J. Phys. Cond. Matter.* **6** (1994) 569.
- [2] R. Monzen, *et al.*, *Phil. Mag. A* **80** (2000) 137, 711.
- [3] O. Kubaschewski, *Iron Binary Phase Diagram*, Springer, Berlin, 1982.
- [4] L. Kőszegi, G. Mészáros, *Appl. Phys. A* **74** (2002) S1172.
- [5] I. C. Noyan, J. B. Cohen, *Residual Stress*, Springer, Berlin, 1987.

s14.m39.p4 **Lattice Dynamics in Hydrogenated Austenitic Stainless Steels Fe-25Cr-20Ni and Fe-18Cr-10Ni.** Vedran Rajevac,<sup>a</sup> Markus Hoelzel,<sup>a,b</sup> Hartmut Fuess,<sup>a</sup> <sup>a</sup>Darmstadt University of Technology, Institute for Materials Science, Petersenstr. 23, 64287 Darmstadt, Germany, <sup>b</sup>Munich University of Technology, ZWE-FRM-II, Lichtenbergstr. 1, 85747 Garching, Germany. E-mail: rajevac@st.tu-darmstadt.de

**Keywords: Lattice dynamics; Hydrogen-metal system; Austenitic stainless steels**

Hydrogenated austenitic stainless steels Fe/Cr25/Ni20 and Fe/Cr18/Ni10 were investigated by elastic and inelastic neutron scattering. High-pressure treatment was used for the hydrogenation to obtain hydrogen contents of H/Me~0.003-1. The analysis of diffraction studies as well as experimental results of inelastic neutron scattering studies is presented by M. Hoelzel et al. in this issue [1]. In this contribution we report on the modelling of hydrogen vibrational modes obtained by inelastic neutron scattering. The experimental data were corrected for multiphonon contribution using the method of Dawidowski *et al.*[2,3]. The site occupancies of hydrogen atoms were known from the diffraction studies [1]. The modelling of hydrogen vibrations was based on Born-von Karman interactions taking into account the site occupancies of hydrogen atoms, following the approach of Rafizadeh [4], applied on the Pd-H(D) system. Force constants according to metal-metal(3 parameters), metal-hydrogen(2 parameters) and hydrogen-hydrogen interaction(3 parameters) were used as input parameters. Metal-metal force constants were taken from the modelling of measured phonon dispersion curves in hydrogen-free single crystalline austenitic stainless steels, using Born-von Karman interactions [5,6]. These parameters were corrected for the hydrogen-induced lattice expansion using the Grüneisen parameter. Metal-hydrogen force constants were obtained from inelastic neutron scattering studies on Fe-H[8], Cr-H[7] and Ni-H[7] and interpolated to the actual metal-hydrogen interatomic distances. The influence of the various metal elements in Fe/Cr25/Ni20 and Fe/Cr18/Ni10 were taken into account in the way that phonon densities of states were calculated for the eight most probable configurations of Fe, Cr and Ni atoms around hydrogen atoms. Hydrogen-hydrogen force constants were refined from fitting procedures using least-squares algorithms. The obtained phonon densities of states were corrected by the instrumental resolution of the filter-analyser neutron spectrometer. The resulting phonon densities of states fit well to the experimental data. The derived hydrogen-hydrogen force constants are in good agreement with existing data for other metal-hydrates systems [4].

- [1] Hoelzel M., Rajevac V. and Fuess H. this issue.
- [2] Dawidowski J., Bermejo F. J. and Granada J. R. (1998) *Phys. Rev. E* **58**, 706-715.
- [3] Dawidowski J., Cuello G.J., Koza M.M., Blostein J.J., Aurelio G., Fernández Guillermet, A. *et al.* (2002). *Nucl. Instr. and Meth. B* **195**, 389-399.
- [4] Rafizadeh H.A. (1981) *Phys. Rev.* **B23**, 1628-1632.
- [5] Hoelzel M., Danilkin S.A., Hoser A., Ehrenberg H., Wiedner T. and Fuess H., (2002), *Appl. Phys. A* **74**, 1013-1015.
- [6] Rajevac V., Hoelzel M., Danilkin S. A., Hoser A. and Fuess H. (2004), *J. Phys. C: Cond. Matter*, accepted.
- [7] Cornell K., Wipf H., Antonov V.E., Antonova T.E., Kolesnikov A.I., Ponyatovsky E.G., and Dorner B. (1997) *Pol. J. Chem.* **71** 1792-1796.
- [7] Dorner B., Belash I.T., Bokhenkov E. L.,Ponyatovsky E. G., Antonov V. E. and Pronina L. N. (1989) *Solid State Comm.* **69**, 121-124.