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11.3 Local Magnetic Moments and Hyperfine Fields in $\text{Fe}_{3-x}\text{Cr}_x\text{Al}$

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Self-consistent spin-polarised TB-LMTO band structure calculations of Fe_3Al with Cr substituted for iron were carried out. An influence of the local environment on the distribution of hyperfine magnetic fields were seen. All the nearest neighbours atomic configurations corresponding to the observed sextets contributing to the Mössbauer spectra were analysed. Substitution of a chromium atom in the nearest

neighbourhood causes strong decrease of the hyperfine field.

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11.4 Mössbauer Study of the $\text{Fe}_{1-x}\text{Ni}_x$ Invar Alloys by Monochromatic Circularly Polarized Source

by D.Satuła¹⁾, K.Szymański¹⁾, L.Dobrzyński¹⁾, K.Rećko¹⁾, J.Waliszewski¹⁾

X-ray diffraction measurements and Mössbauer spectroscopy with and without an external magnetic field parallel to the beam direction have been performed for $\text{Fe}_{1-x}\text{Ni}_x$ ($x = 0.25, 0.30, 0.35$) alloys. The compositions of the alloys studied were chosen in order to cover the concentration range where the fcc \leftrightarrow bcc structural transformation appears, as well as where single phase fcc Fe-Ni alloys exhibit the Invar phenomena. Spatial distribution of the iron magnetic moments is discussed. The hyperfine magnetic field (h.m.f.) distribution is analyzed for two models discussed in the literature. In the first model it is assumed that any hyperfine magnetic field vector have the same spatial distribution (the same values of $\langle \cos\theta \rangle$). In the second, the low field component of the

hyperfine magnetic field is ordered antiferromagnetically (or disordered) while the high field component is aligned by an external magnetic field. In order to determine the mean value of the cosine of the angle between γ -rays direction and hyperfine field vector of iron, $\langle \cos\theta \rangle$, a monochromatic circularly polarized Mössbauer source (MCPMS) was used. The analysis of the MCPMS results shows that the shapes of the measured spectra can be explained by single values of $\langle \cos\theta \rangle$.

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11.5 Magnetic Properties of Cr_3Si Doped Fe and Co

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Polycrystalline samples of $\text{Cr}_{3-x}\text{TM}_x\text{Si}$ (where $x = 0.02, 0.1, 0.2, 0.3$; TM = Fe, Co) were prepared from pure elements in an arc furnace. The very weak magnetization of these samples was measured by the VSM method as a function of magnetic field (~ 2 kOe to 12 kOe) and temperature (10 K to 300 K). With increasing iron concentration the $\text{Cr}_{3-x}\text{Fe}_x\text{Si}$ alloys change from the paramagnetic ($x \leq 0.2$) to the

ferromagnetic ($x = 0.3$) ones. In the case of Co impurities the ferromagnetic properties were observed in the most diluted samples ($x = 0.02$). However, these latter alloys for higher Co content exhibit very anomalous magnetic properties.

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11.6 Error Maps in Charge and Momentum Density Studies by the Maximum Entropy Methods

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The uncertainty of the electron charge and momentum densities reconstructed by the Maximum Entropy Method was analyzed. Various sources of uncertainties and errors that can appear in the reconstructions are discussed. In particular, it was shown that small features seen on the maps have to be

treated with caution and analysis of their statistical significance must be particularly well done.

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