VOLUME EFFECT AND ELECTRON BAND MODIFICATION IN α-Fe BY
SUBSTITUTIONAL IMPURITIES

A.Błachowski¹, U.D.Wdowik² and K.Ruebenbauer¹
¹Mössbauer Spectroscopy Division, Institute of Physics, Pedagogical University
PL-30-084 Cracow, ul. Podchorążych 2, Poland; sfblacho@cyf-kr.edu.pl
²Applied Computer Science Division, Institute of Technology, Pedagogical University
PL-30-084 Cracow, ul. Podchorążych 2, Poland

A contribution is aimed at the review of the charge and spin density perturbation on the iron nucleus in the BCC iron-based binary alloys due to various impurities randomly substituting Fe atoms. The iron average hyperfine field is proportional to the average electron spin density on the iron nucleus. Variation of the average total shift for Mössbauer spectra has been interpreted as due to the average electron charge density variation on the iron nucleus. It has been found that individual impurities perturb iron charge and spin density to the third or in some cases to the second neighbor shell [1-3].

Fig. 1 shows correlation between change of the average iron hyperfine field per at.% of impurity and corresponding change of the average electron density on the iron nucleus. Substitution of the impurities with the increasing number of 3d, 4d or 5d electrons leads to the lowering of the electron density on the iron nucleus and causes decreased band spin density on this nucleus. Impurities with d electrons have generally stronger effect on the charge and spin density perturbation with the increasing principal quantum number of the d electrons.

Generally there are two major contributions to the charge and spin density perturbation, i.e., the volume effect and electron band modification, respectively. We have performed ab initio calculations of the volume effect for the ground state of the α-Fe varying lattice constant. Calculations have been performed using the full potential linearized augmented plane-wave method (FLAPW) within the framework of the density functional theorem (DFT) [4]. The variation of the electron density on the iron nucleus in the pure α-Fe was found as ~5.18 electron a.u.⁻³ Å⁻¹, while the corresponding variation of the hyperfine field amounts to 32.7 T Å⁻¹.

Upon having corrected for the volume effect (Vegard law is satisfied for all systems investigated) one obtains another correlation shown in Fig. 2. All d-like impurities form a linear correlation between electron charge and spin density on the iron nucleus. Addition of any d electrons due to the varying atomic number of the impurity leads to decreasing electron density on iron with the simultaneous lowering of the transferred electron spin density. A reduction of the electron density on the iron nucleus is particularly strong for impurities making strong covalent bonds with iron like P and As. On the other hand, enhancement of the transferred electron spin density on iron is much weaker for such impurities in comparison with impurities having more metallic character like Sn or Sb. Beryllium seems somewhat special due to the very soft and of the low-density electron core.

Figure 1. Correlation between average hyperfine magnetic field change per at.% of impurity and corresponding change of the isomer shift.

Figure 2. Correlation between average hyperfine magnetic field change per at.% of impurity and corresponding change of the isomer shift and electron density on the iron nucleus upon having corrected for the volume effect.