Charge and spin density perturbation on iron nuclei by 4d and 5d impurities substituted on the iron sites in alpha-Fe

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Hyperfine field in alpha-Fe is due to the non-vanishing electron spin density on the iron nucleus. The latter density originates from the atomic core polarization and from the itinerant electron polarization. The spin and charge (electron) density on the nucleus is caused predominantly by the s-like electrons belonging either to the atomic core or to the conduction band. Relatively diluted non-magnetic impurity on the iron site generates perturbation in the vicinity of the Fermi level, the latter perturbation having short-range influence on the charge and spin density on the adjacent iron nuclei. The paper is aimed at the review of the charge and spin density perturbation on the iron nucleus in the BCC iron-based binary alloys containing as the impurity either 4d (Nb, Mo, Ru, Rh, Pd) or 5d (Os, Ir, Au) metals [1]. Additionally Ga has been used as such impurity as well. Measurements have been performed by means of the 57Fe transmission Mössbauer spectroscopy at room temperature. Investigations performed versus impurity concentration (randomly distributed over iron sites) indicate additive effect for the charge density perturbation, and additive in the algebraic sense effect for the corresponding spin density perturbation. Hence, the effect of impurity depends solely on the distance between impurity and the iron nucleus. It has been found that impurities being further away than a third or in some cases as the second neighbor shell do not contribute directly to the charge and spin perturbation. On the other hand, they have usually some minor effect on the average charge and spin density. Generally, the perturbation to either charge or spin density has some oscillatory character versus distance from the impurity [2, 3]. The phase and period of the charge oscillation is vastly different from the phase and period of the spin oscillation in the majority of cases. Substitution of the impurities with the increasing number of 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. Subsequent impurities donate more and more d-type electrons to the band, and the latter screen more and more effectively s-like electrons. Hence, the density of the s-like electrons on the iron nucleus diminishes. Impurities with 5d electrons have generally stronger effect on the charge and spin density perturbation than impurities with 4d electrons.


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