Hyperfine magnetic fields at nuclei in disordered and partly disordered metal - metalloid alloys

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9.7 cm

Binary and ternary alloys on the basis of Fe, Si and Sn are considered in the paper. Numerous experimental data available in the literature are interpreted with the help of the "first-principles" calculations made by the LAPW method. The investigation revealed the following features of the hyperfine magnetic field (HFF) formation. To describe the HFF in the alloys three main contributions should be taken into account: the polarizations of the core and valence electrons (the Fermi-contact contribution) and the orbital contribution. Particular attention is given in this paper to the polarization of the valence electrons. The polarization dependence on the kind of metalloid atom and the local lattice distortion is studied. For example, it is shown that the lattice relaxation can be neglected for the valence electron polarization at Fe nuclei, whereas at Sn the local distortions result in the significant change in HFF. An analysis of phenomenological models that are every so often used for the HFF description in disordered metal - metalloid alloys is conducted. In particular, it showed inadequacy of the additivity used in description of the alterations of the valence electron polarization at Fe caused by the metalloid atoms of the nearest spheres. At the same time the polarization change caused by the atoms of the third or more distant spheres may be considered as additive contributions and constant in the concentration range 5-8 at.%.

13.4 cm

Subject category :
3. Transition Metals, Alloys and Compounds

Presentation mode :
oral

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