HYPERFINE PARAMETERS OF THE HEUSLER TYPE $Fe_{2+x}V_{1-x}$ ALLOYS

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9.7 cm

The hyperfine parameters (isomer shift and hyperfine magnetic field) for ^{57}Fe nucleus in the Heulser-type $Fe_{2+x}V_{1-x}$ ($x \geq 0$) alloys were calculated by means of the *ab initio* electronic structure calculation methods. The calculations performed for these alloys have shown that the Fe anti-site (AS) atoms (Fe at V positions of the Heulser Fe_2VAl) characterizes the stable (independent on concentration x) magnetic moment of magnitude of 2.2—2.5 μ_B. On the other hand the Mössbauer experimental investigations of the $Fe_{2+x}V_{1-x}$ ($x \geq 0$) alloys have indicated the presence of Fe atoms with intermediate value of hyperfine magnetic field (∼15 T). The experimental data interpreted within the simple model of linear scaling (HF∼ μ_{Fe}) have predicted the presence of the Fe atoms with the medium sized magnetic moment (∼1.5 μ_B) which number varies with temperature and concentration. The results of calculations for the hyperfine magnetic field (HF) have explained the experimental data in the following way. The calculated magnitude of HF on Fe-AS atoms depends sensitively on the magnetization of the nearest neighborhs. The transferred part of the HF, usually small as compared the local part, reaches relatively large values and points toward opposite direction compared the local HF. The both parts of HF (local and transferred) reduce each other on Fe-AS atoms leading to the medium sized magnitude of HF despite the high value of magnetic moment of these atoms.

13.4 cm

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