MAGNETIC AND HYPERFINE PROPERTIES OF ORDERED AND DISORDERED Fe-Al ALLOYS

J.E. Frackowiak and J. Deniszczyk
Institute of Physics and Chemistry of Metals, University of Silesia
40-007 Katowice, Bankowa 12, Poland

9.7 cm

The magnetic moment (μ), hyperfine field (B_{hf}) and isomer shift (IS) of the Fe atoms in bcc Fe-Al alloys were calculated from first principle. The super-cell including 16 atoms (8xB2 formula unit) was constructed and several possible environments of Al atoms around iron sites in the alloy have been considered in order to study magnetic and hyperfine properties. Different contributions to hyperfine field and isomer shift were calculated separately. The variation of the μ, B_{hf} and IS at iron atoms due to presence of aluminum nearest and next-nearest neighbors was analyzed. The effect of the lattice parameter variation on the above mentioned quantities was also investigated. With increasing pressure the transition from the parallel to anti-parallel alignment of Fe-magnetic moments was found for Al concentration of 30 at.%. The transferred hyperfine field, resulted from the spin-polarization of outer 4s electrons by surrounding magnetic moments, exhibit significant dependence on the number of Al atoms in the first and the second coordination sphere of an Fe atom. The average $< \mu >$, $< B_{hf} >$ and $< IS >$ was calculated for disordered and ordered Fe-Al alloys with B2 and DO_3 superstructure by Monte Carlo simulation method. The very good agreement with experiments was found.

13.4 cm

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Corresponding author :
J.E. Frackowiak

Address for correspondence :
Institute of Physics and Chemistry of Metals
University of Silesia
40-007 Katowice, Bankowa 12

Email address :
jfrack@us.edu.pl