9.7 cm

Local magnetic moments in $Fe_{3-x}Cr_xSi$ and $Fe_{3-x}Cr_xAl$ alloys

A. Go[a], M. Pugaczowa-Michalska[b], L. Dobrzyński[ac], S. Lipiński[b]

[a]Institute of Experimental Physics, University of Bialystok,
Lipowa 41, 15-424 Bialystok, Poland

[b]Institute of Molecular Physics, Polish Academy of Science,
Smoluchowskiego 17, 60-179 Poznań, Poland

[c]The Soltan Institute for Nuclear Studies,
05-400 Otwock-Świerk, Poland

We present the results of self-consistent spin-polarised TB-LMTO band structure calculations of Fe_3Si and Fe_3Al substituted by chromium. The ordered alloys have DO_3-type crystal structure with two sites of iron that are not equivalent. The aim of the paper is to show an influence of the local environment on the distribution of hyperfine magnetic fields. All the nearest neighbour atomic configurations corresponding to the observed sextets contributing to the Mőssbauer spectra are analysed. Comparing the total energies of the completely ordered systems with the energies of the configurations with partial disorder between iron and silicon or iron and aluminium sublattices we conclude that the ordering tendency in Fe_3Si is stronger than in Fe_3Al alloy.

13.4 cm

Subject category :

7. Computations of Electronic Band Structures

Presentation mode :
poster

Corresponding author :
A. Go

Address for correspondence :
Institute of Experimental Physics,
University of Bialystok,
Lipowa 41, 15-424 Bialystok,
Poland

Email address :
annago@alpha.uwb.edu.pl