INFLUENCE OF THE LOCAL ENVIRONMENT ON THE MAGNETIC PROPERTIES OF THE $Fe_{1-x}Al_x$ ALLOY

J. Deniszczyk

Institute of Physics and Chemistry of Metals, Silesian University, Katowice, POLAND

9.7 cm

The electronic and magnetic properties of the ordered binary $Fe_{1-x}Al_x$ alloy with the B_2 crystal structure have been investigated by the self-consistent TB-LMTO method. The effect of the alloying was simulated using the super-cell with eight FeAl formula units with antisite Fe (Fe-AS) atoms at Al positions. The calculations were performed for the number of Fe-AS atoms equal to 0, 1, 2, 3 and 4 what corresponds to the concentration of Al atoms x=0, 0.4375, 0.375, 0.3125 and 0.25. The electronic and magnetic structures as a function of lattice parameter was examined for all crystallographically non-equivalent configurations of Fe-AS atoms within the super-cell. The calculations have shown that the electronic and magnetic structures of calculated systems strongly depend on both lattice parameters and configuration of Fe-AS atoms within the super-cell. For the FeAl compound calculations have shown that the ground state is the magnetic one with the abrupt transition to the paramagnetic state when the lattice parameter is reduced. Also for the Fe_9Al_7 structure the abrupt change of the magnetic moment is observed when the lattice constant is changed. The most striking magnetic behaviour was found for some configurations within concentrations x$\simeq$0.3125 and x$\simeq$0.25 % of Al, where in some positions the Fe-AS magnetic moments show anti-parallel alignment. The similar anomalous behaviour of the magnetic state was observed experimentally for $Fe_{1-x}Al_x$ alloy for concentrations x around 0.3.

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Corresponding author :
J. Deniszczyk

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

Email address :
jdeni@us.edu.pl