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**Anomalous equilibrium volume change of magnetic Fe-Al crystals**

MARTIN FRIÁK, JÖRG NEUGEBAUER, Max-Planck Institute for Iron Research, Max-Planck-Strasse 1, 40237 Düsseldorf, Germany — Iron aluminides represent a very promising class of intermetallic materials with great potential for substituting stainless steels at elevated and high temperatures. Experiments observed an anomalous equilibrium volume behaviour as a function of concentration in Fe-rich compounds [1]. This effect has been tentatively assigned to be due to an order-disorder transition. We have studied the role of magnetism in Fe-Al crystals employing density functional theory (DFT) within the generalized gradient approximation (GGA). The excess energies, equilibrium lattice parameters and magnetic states have been determined for a dense set of different iron concentrations and a large variety of atomic configurations. Both external and internal relaxations were allowed. The spin-polarized calculations for *ordered* ferromagnetic Fe-rich compounds nicely reproduce the anomalous volume behaviour, i.e. the effect is *not* related to an order-disorder transition. Analyzing different magnetic states we identified the change in magnetism to be the driving force. In fact, performing the same calculations but switching off magnetism removed the anomalous volume dependence and showed a clear linear dependence. Based on these results the importance of order-disorder transition in Fe-Al systems is revisited. [1] R. A. Buckley and S. Kaviani, Mat. Sci. Eng. A258, 173 (1998).

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