

**Ab-initio study of an influence of transition metal doping on  
electronic structure and ordering degree in Fe<sub>3</sub>Al alloy**

**A. Go<sup>1</sup> and L. Dobrzyński<sup>1,2</sup>**

<sup>1</sup>Faculty of Physics, University of Białystok, Lipowa 41, 15-424 Białystok, Poland

<sup>2</sup>The Soltan Institute for Nuclear Studies, 05-400 Otwock-Świerk, Poland

Fe<sub>3</sub>Al alloy crystallizes in DO<sub>3</sub>-type structure. In the perfectly ordered alloy there are two nonequivalent sublattices (A,C) and B, which are occupied by Fe atoms, whereas all D sites are taken by metalloid. However, experimental results indicate, that there is some disorder between B-D as well as (A,C)-D sublattices. This disorder modifies strongly electronic structure and magnetic properties. The aim of this contribution is to investigate total energy dependence of atomic exchange between B-D and (A,C)-D positions in the Fe<sub>3</sub>Al as well as in alloys doped with transition metals using ab-initio technique. Furthermore an influence of atomic ordering on electronic structure is studied thoroughly. Decreasing of ordering degree in Fe<sub>3</sub>Al alloy augments variety of local surroundings of atoms. It leads to more complicated densities of states and causes an increase of total magnetic moment. Doping Fe<sub>3</sub>Al with small amount of chromium does not change ordering of alloy. However, total energies of totally ordered and partially disordered alloys are nearly the same. According to the total energy calculations, manganese entering into (A,C) position can introduce B-D type of disorder in the parent compound.

9.7 cm

13.4 cm

**Subject category :**

3. Magnetic Structure and Dynamics

**Presentation mode :**

poster

**Corresponding author :**

A. Go

**Address for correspondence :**

Faculty of Physics, University of Białystok  
Lipowa 41, 15-424 Białystok  
Poland

**Email address :**

annago@alpha.uwb.edu.pl