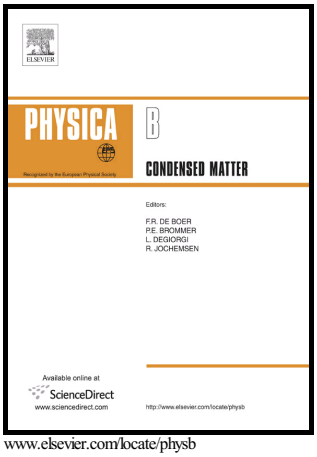
Mechanical Properties and Electronic Structures of Fe-Al Intermetallic

YaHui Liu, XiaoYu Chong, YeHua Jiang, Rong Zhou, Jing Feng



www.elsevier.com/locate/physb

PII: S0921-4526(16)30492-6
DOI: http://dx.doi.org/10.1016/j.physb.2016.10.032
Reference: PHYSB309692

To appear in: *Physica B: Physics of Condensed Matter*

Received date: 4 July 2016
Revised date: 15 October 2016
Accepted date: 20 October 2016

Cite this article as: YaHui Liu, XiaoYu Chong, YeHua Jiang, Rong Zhou and Jing Feng, Mechanical Properties and Electronic Structures of Fe-A Intermetallic, *Physica B: Physics of Condensed Matter* http://dx.doi.org/10.1016/j.physb.2016.10.032

Mechanical Properties and Electronic Structures of Fe-Al Intermetallic

YaHui Liu, XiaoYu Chong, YeHua Jiang, Rong Zhou, Jing Feng*

Faculty of Materials Science and Engineering, Kunming University of Science and Technology, Kunming 650093, P.R. China

*Corresponding author. Tel.: 15925200330; E-mail：jingfeng@kmust.edu.cn.

Abstract

Using the first-principles calculations, the elastic properties, anisotropy properties, electronic structures，Debye temperature and stability of Fe-Al (Fe_3Al, FeAl, $FeAl_2$, Fe_2Al_5 and $FeAl_3$) binary compounds were calculated. The formation enthalpy and cohesive energy of these Fe-Al compounds are negative, and show they are thermodynamically stable structures. Fe_2Al_5 has the lowest formation enthalpy, which shows the Fe_2Al_5 is the most stable of Fe-Al binary compounds. These Fe-Al compounds display disparate anisotropy due to the calculated different shape of the 3D curved surface of the Young's modulus and anisotropic index. Fe_3Al has the biggest bulk modulus with the value 233.2 GPa. FeAl has the biggest Yong's modulus and shear modulus with the value 296.2 GPa and 119.8 GPa, respectively. The partial density of states, total density of states and electron density distribution maps of the binary Fe-Al binary compounds are analyzed. The bonding characteristics of these Fe-Al binary compounds are mainly combination by covalent bond and metallic bonds. Meanwhile, also exist anti-bond effect. Moreover, the Debye temperatures and sound velocity of these Fe-Al compounds are explored.

Keywords