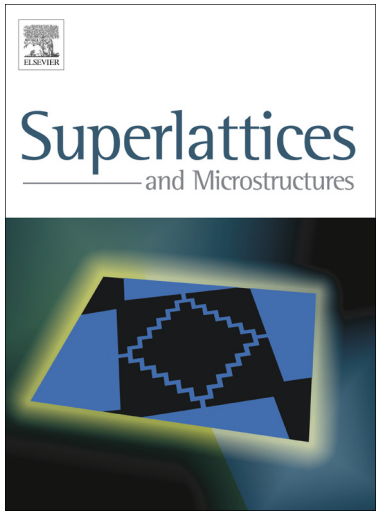

First-principles investigation of the elastic, Vickers hardness and thermodynamic properties of Al-Cu intermetallic compounds

Haichuan Chen, Lijun Yang, Jianping Long

PII: S0749-6036(14)00411-X
DOI: http://dx.doi.org/10.1016/j.spmi.2014.11.005
Reference: YSPMI 3480

To appear in: *Superlattices and Microstructures*

Received Date: 10 October 2014
Accepted Date: 6 November 2014

Please cite this article as: H. Chen, L. Yang, J. Long, First-principles investigation of the elastic, Vickers hardness and thermodynamic properties of Al-Cu intermetallic compounds, *Superlattices and Microstructures* (2014), doi: http://dx.doi.org/10.1016/j.spmi.2014.11.005

First-principles investigation of the elastic, Vickers hardness and thermodynamic properties of Al-Cu intermetallic compounds

Haichuan Chen*,[1] Lijun Yang[2] and Jianping Long[2]

* Corresponding author: e-mail haichuanchenxhedu@163.com

1. College of Electrical Engineering and Information Technology, Xihua University, Chengdu 610039, P.R.China

2. College of Materials and Chemistry & Chemical Engineering, Chengdu University of Technology, Chengdu 610059, P.R. China

Tel.: +86 13981720115

Fax: +86 28 84077930

Abstract: The elastic and thermodynamic properties of Al-Cu intermetallic compounds have been investigated by using the first-principles density functional theory (DFT) within the generalized gradient approximation (GGA). The computed lattice constants of Al-Cu are in good agreements with the experimental data. The calculated elastic constants reveal that all of Al-Cu intermetallic compounds are mechanically stable. The shear modulus, Young's modulus, Poisson's ratio σ, the ratio *B/G*, shear anisotropy and elastic anisotropy are also calculated. Finally, the Vicker hardness, Debye temperature, melting point and thermal conductivity have been predicted.

Keywords: Intermetallic compounds; Crystal structure; Elastic properties;