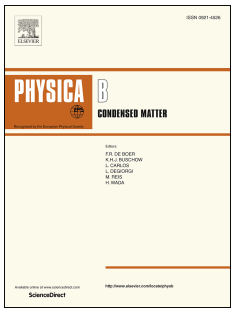
Accepted Manuscript



Structural stability, elastic and thermodynamic properties of Au–Cu alloys from first-principles calculations

Ge-Xing Kong, Xiao-Juan Ma, Qi-Jun Liu, Yong Li, Zheng-Tang Liu

PII: S0921-4526(18)30004-8

DOI: 10.1016/j.physb.2018.01.003

Reference: PHYSB 310650

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

Received Date: 1 November 2017

Revised Date: 31 December 2017

Accepted Date: 2 January 2018

Please cite this article as: G.-X. Kong, X.-J. Ma, Q.-J. Liu, Y. Li, Z.-T. Liu, Structural stability, elastic and thermodynamic properties of Au–Cu alloys from first-principles calculations, *Physica B: Physics of Condensed Matter* (2018), doi: 10.1016/j.physb.2018.01.003.

Structural stability, elastic and thermodynamic properties of Au–Cu alloys from first-principles calculations

Ge-Xing Kong[1], Xiao-Juan Ma[1*], Qi-Jun Liu[1], Yong Li[1], Zheng-Tang Liu[2]

[1]*Key Laboratory of Advanced Technologies of Materials of Ministry of Education of China, School of Physical Science and Technology, Southwest Jiaotong University, Chengdu 610031, China*

[2]*State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, Xi'an 710072, China*

Abstract

Using first-principles calculations method based on density functional theory (DFT) with the Perdew–Burke–Ernzerhof (PBE) implementation of the generalized gradient approximation (GGA), we investigate the structural, elastic and thermodynamic properties of gold-copper intermetallic compounds (Au–Cu ICs). The calculated lattice parameters are in excellent agreement with experimental data. The elastic constants show that all the investigated Au–Cu alloys are mechanically stable. Elastic properties, including the shear modulus, Young's modulus, Poisson's ratio and Pugh's indicator, of the intermetallic compounds are evaluated and discussed, with special attention to the remarkable anisotropy displayed by Au–Cu ICs. Thermodynamic and transport properties including the Debye temperature, thermal conductivity and melting point are predicted from the averaged sound velocity and elastic moduli, using semi-empirical formulas.

Keywords: A. Intermetallics

B. Anisotropy

* Corresponding author at: School of Physical Science and Technology, Southwest Jiaotong University, Key Laboratory of Advanced Technologies of Materials, Ministry of Education of China, Chengdu 610031, People's Republic of China. Tel.: +86 02887601758

E-mail address: mxj_swjtu@126.com (X.-J. Ma)