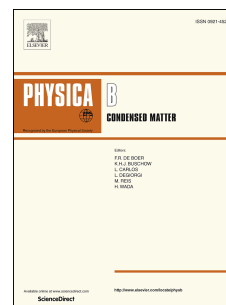


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Structural stability, elastic and thermodynamic properties of Au–Cu alloys from first-principles calculations

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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

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