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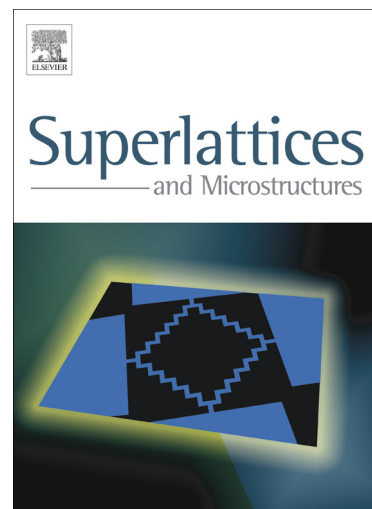
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First-principles investigation of the elastic, Vickers hardness and  
thermodynamic properties of Al-Cu intermetallic compounds

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**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  $\sigma$ , 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;

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