Abstract Submitted
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First-principles calculation of dislocation properties of ductile rare-earth intermetallic compounds MIN JI, CAI-ZHUANG WANG, Ames Laboratory, US DOE, Ames, IA 50011, USA, KAI-MING HO, Ames Laboratory, US DOE, Ames, IA 50011, USA and Department of Physics, Iowa State University,Ames,IA,50011, QIAN CHEN, XIANG-YANG LIU, BULENT BINER, Ames Laboratory, US DOE, Ames, IA 50011, USA — We have used first-principles calculations to study the mechanical properpies of rare-earth intermetallic B2 compounds which exhibit significant ductility. According to Peierls-Nabarro model and slip plane observed in tensile experimens, we have calculated and compared the 110 gamma surface energy for both brittle NiAl and ductile YCu. We also compared unstable stacking fault and twinning energy for a series of B2 compounds with different ductilily. Correlation between these energetics and the ductilily are discussed.

Min Ji
Ames Laboratory, US DOE, Ames, IA 50011, USA

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