Topological description of mechanical behavior of Cu, Ag and Au: A first-principle study

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Abstract
Mechanical properties and stress-strain curves of Cu, Ag and Au single crystals are calculated using ab initio methods. Elastic and Plastic regions are scrutinized. Yield stress and slope of these curves can shed light on brittleness and ductility of these metals that prove Cu, despite its high ultimate tensile strength, is less ductile than Au and Ag. Analysis of topology of charge density along with stress-strain curves shows that the elastic-plastic transition accompanies topological transition and for these metals, both transitions occur in the same strain. Some characteristics of critical point, especially bond points, are inspected.

Keywords: mechanical properties, quantum stress, stress-strain curve, topology of charge density

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