

## ABSTRACT

### **Ab initio calculations of theoretical strength of copper under uniaxial tension**

Miroslav Černý<sup>1,2</sup>, Mojmír Šob<sup>2</sup>, Pavel Šandera<sup>1</sup>, Jaroslav Pokluda<sup>1</sup>

<sup>1)</sup> Institute of Engineering Physics, Faculty of Mechanical Engineering, Brno University of Technology, Technická 2, CZ-616 69 Brno, Czech Republic

<sup>2)</sup> Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Žitkova 22, CZ-616 62 Brno, Czech Republic

Ideal strength of copper based on simulation of tensile test along [001] direction is performed using ab-initio pseudo-potential linear plane waves method. The generalized gradient approximation (GGA) was used to evaluate exchange-correlation contribution to the total energy. Equilibrium lattice parameter, Young modulus and shear modulus are computed to assess reliability of our results by comparing them with experiment. Stability conditions for uniaxially loaded system are presented and analyzed.