Thermo-mechanical coupling model for metallic crystalline materials at micro-nano scale

†*Jieqiong Zhang [1] , Junzhi Cui [2,1], †Zihao Yang [1], Meizhen Xiang[3]

1 Department of Applied Mathematics, Northwestern Polytechnical University, Xi'an, 710072,CHINA.
2 LSEC, ICMSEC, Academy of Mathematics and Systems Science, CAS, Beijing, 100090, CHINA.
3 Institution of Applied Physics and Computational Mathematics, Beijing 100088, China

*Presenting author: jieqiongzhang@mail.nwpu.edu.cn
†Corresponding author: jieqiongzhang@mail.nwpu.edu.cn, yangzihao@nwpu.edu.cn

Abstract

A thermo-mechanical coupled model at micro-nano scale is proposed to studied the thermoelastic deformation and thermodynamic properties for metal crystalline materials. Firstly, the motion of metallic atoms is decomposed into the structural deformation and thermal vibration. Further, the structural deformation is divided into the thermal deformation influenced by temperature and mechanical deformation influenced by stress. While thermal vibration equations are established on the structural deformation positions and dynamically change with the stress and temperature. Then the free energy that depended on the structural deformation and thermal vibration frequencies is obtained. Finally, the thermoelastic constitutive relations and thermodynamic properties like heat capacity, thermal expansion, internal energy and entropy are derived from the free energy. The numerical results of heat capacity and TEC for metals Cu, Al, Au, Ag, Ni, Pd, Pt and Pb show a temperature dependence and agree well with the experimental data. This work suggests an efficient approach to calculate thermodynamic properties of metal materials based on the thermo-mechanical coupling behaviours.

Keywords: metal crystalline materials, thermo-mechanical coupling, thermoelastic constitutive, thermodynamic properties, micro-nano scale