Tensile strength of Ni grain-boundary with segregated sp-impurities

M. Černý[1,2*], P. Šesták[1,2], P. Řehák[1,2], M. Šob[3,1,4], M. Všianská[3,1]

[1]*Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Žižkova 22, 616 62 Brno, Czech Republic*
[2] *Faculty of Mechanical Engineering, Brno University of Technology, Technická 2896/2, 616 69 Brno, Czech Republic*
[3]*Central European Institute of Technology, CEITEC MU, Masaryk University, Kamenice 5, 625 00 Brno, Czech Republic*
[4]*Department of Chemistry, Faculty of Science, Masaryk University, Kotlářská 2, 611 37 Brno, Czech Republic*

Grain boundaries (GB) represent extended planar defects with a crucial effect on macroscopic strength of polycrystalline materials. In this first principles study, we calculate the ideal tensile strength of ∑5(210) tilt GB in nickel crystal under uniaxial loading applied perpendicularly to the GB plane. A computational supercell containing 64 atoms is subjected to three different modes of simulated deformation comprising rigid grain shift, uniaxial deformation with optimized atomic coordinates and fully optimized uniaxial loading (ionic positions in the supercell as well as the cell shape are optimized at each step of deformation).

Results for these models are compared and tensile strength of clean GB is compared with that of GB with segregated impurities (S and Al) and with the results of previous studies. Differences in computed values show not only the effect of the impurities on the ideal strength but also an importance of full lattice optimization during the simulation of tensile test.

**corresponding author: Tel.: +420 54114 2709 Fax:+420 54114 2842 e-mail:cerny.m@fme.vutbr.cz*