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Tensile strength of Ni grain-boundary with segregated sp-impurities — •Miroslav Černý[1,2,3], Petr Šesták[1,2], Petr Řehák[1,2,3], Monika Všianská[1,3], and Mojmír Šob[1,3,4] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [3]Central European Institute of Technology, Brno, Czech Republic — [4]Faculty of Science, Masaryk University, 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 $\Sigma5(210)$ tilt GB in nickel crystal under uniaxial loading applied perpendicularly to the GB plane. A repeat cell 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 the importance of full lattice optimization during the simulation of tensile test.

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