AB INITIO STUDY OF SURFACE OF NANOPARTICLES AG AND NI

Svatava POLSTEROVÁ[1*], Martin FRIÁK[2,3,5], Monika VŠIANSKÁ[3,2], and Mojmír Šob[4,2]

[1] *Department of Advanced Materials and Nanosciences, Faculty of Science, Masaryk University, Kamenice 753/5, 625 00 Brno, Czech Republic*

[2] *Institute of Physics of Materials, Academy of Sciences of the Czech Republic, v.v.i., Žižkova 22, 616 62 Brno, Czech Republic*

[3] *Central European Institute of Technology, CEITEC MU, Masaryk University, Kamenice 753/5, 625 00 Brno, Czech Republic*

[4] *Department of Chemistry, Faculty of Science, Masaryk University, Kamenice 753/5, 625 00 Brno, Czech Republic*

[5] *Department of Condensed Matter Physics, Faculty of Science, Masaryk University, Kotlářská 2, Brno, Czech Republic*

**svatava.zup@gmail.com*

We present results of quantum-mechanical study of structural, energetic and elastic properties of extended defects related to pentamerous-symmetry decahedron nanoparticles formed by nonmagnetic Ag and ferromagnetic Ni. Despite the complexity of decahedral shape, these nanoparticles are often observed in fcc metal particles under 50 nm. We determine surface energies of both metals for different crystallographic orientations together with the grain-boundary/quadruple-junction energies in case of the Σ3(111){110} grain boundary and a quadruple junction of Σ5(210) boundaries. These thermodynamic properties as well as structural and anisotropic-elastic properties are predicted by means of state-of-the-art density functional theory (DFT) ab initio calculations. Complementarily to studying individual extended defects separately, we also simulated decahedron nanoparticles containing a number of mutually interacting extended defects. These simulations have been performed for a number of nanoparticles with different sizes.