EDGE ENERGIES AND ELASTIC PROPERTIES OF ORDERED METALLIC NANOWIRES. AN EMBEDDED ATOM METHOD STUDY.

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Equilibrium configurations of aluminum and nickel ordered nanowires are studied by means of a conjugate gradients minimization of the cohesive energy. This cohesive energy is computed using Embedded Atom Method (EAM) semi-empirical potentials. Two different parameterizations of these potentials have been used, the one proposed by Mishin et al.(Phys. Rev. B (59) 3393, (1999)) (MFMP) and that of Sutton and Chen (Philos. Mag. Lett. (66) 139 (1990)) (SC) to allow the identification of potential-dependent nanowire properties. We have determined the equation of state (Tosatti et al. Phys. Rev. Lett. (80) 3775 (1998)) which describes the nanowire cohesive energy as a function of its effective radius (R). This equation of state depends directly on the surface energies and the fraction of the different exposed facets of the wire, as well as on its edge energies. From the dependence of the equation of state on the nanowire orientation we are able to determine the edge energies for different edge geometries. Our results show remarkable differences for these edge energies between both EAM approaches, as expected from our previous work on the applicability of EAM approach to low atomic coordination systems (Peláez et al. Phys. Stat. Sol. (in press)). Furthermore, elastic properties of these systems are also of interest, due to their anisotropy, and will determine the phonon properties in such systems. Thus, elastic constants for these nanowires have been calculated. Again, for decreasing radius, large discrepancies arise between MFMP and SC EAM approximations. These disagreements between different EAM parameterizations implies that EAM potentials must be used very cautiously when analyzing low atomic coordination systems as ultra thin nanowires (Zhang et al. Phys. Lett. A (331) 332 (2004)).

Fig.1: x-y view of the nanowire families under study. Families have been labeled according to their cross sectional shape and the crystallographic orientation of their axis (perpendicular to this plane view). For the thickest nanowire of each family the corresponding exposed surfaces are labeled.