ULTRATHIN METALLIC NANOWIRES: STRUCTURE DEPENDENCE WITH THE SIMULATION POTENTIAL

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Over the last years there has been an increasing interest in the study of noncrystalline structures formed in very narrow metallic nanowires. Molecular Dynamics (MD) simulations within the framework of many-body empirical and semiempirical interatomic pontentials has allowed a comprehensive study of these structures. Both theoretical and experimental groups have found structural reconstructions in ultra-thin metallic nanowires. When heated up and annealed, Au, Ti, Zr, Rh, Pb and Al nanowires abandon their bulk-like structure to form helical noncrystalline wires.

In spite of the amount of theoretical studies that use MD simulations to reproduce these helical structures, no efforts have been made in order to account for the dependency of this results with the potentials used in the simulations. The most widely used potentials in metallic nanowires simulations are those proposed by Daw *et al*, Votter and Chen, Sutton and Chen and Mishin *et al*. All of these potentials belong to the family of the embedded atom method (EAM) potentials. These potentials have been designed as to account for some properties (e.g. cohesive energy, lattice parameter, phonon frequencies, vacancy energy, etc) in bulk systems. However it is not clear how good these potentials are at describing lower coordination situations, such as metallic surfaces and nanowires.

In this work we have implemented a Conjugate Gradients (CG) algorithm to find the minimal energy structure of Al and Ni nanowires using two diferent EAM potentials: Sutton-Chen's (SC) and Mishin *et al*.(MFMP) Starting from cylinder-shaped atomic arrangements keeping their original bulk-like interatomic distances, the CG method finds the new atomic coordinates that minimize the total potential energy of the system. A comparison is made between the results from each potential regarding cohesive energy, linear atomic density, nanowire radius and Young's modulus.

References:

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