OPTIMAL STRUCTURES FOR Al AND Ni NANOWIRES. NEIGHBORHOOD AND POTENTIAL EFFECT.

S. Peláez[(a)], P. García-Mochales[(b)] and P. A. Serena[(a)]
[(a)] Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC)
[(b)] Universidad Autónoma de Madrid. Dpto. Física Mat. Condensada
spelaez@icmm.csic.es

Over the last years there has been an increasing interest in the study of noncrystalline structures formed in very narrow metallic nanowires. Ab initio calculations -though very reliable- are too expensive for treating metallic systems of thousands of atoms. On the other hand, Molecular Dynamics (MD) simulations within the framework of many-body empirical and semiempirical interatomic potentials has allowed a comprehensive study of these structures. Both theoretical[1,2] and experimental[3] 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 hellical 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[4], Votter and Chen (VC)[5], Sutton and Chen (SC)[6] and Mishin et al.[7] 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 high coordination systems. However it is not clear what are the advantages of using one potential insted of another when lower coordination systems are studied.

In this work a comparison is made between two different potentials: Sutton-Chen and Mishin. We analyse their performance in describing the equilibrium configurations of Al and Ni systems in various coordination situations: bulk *fcc* and *bcc* crystal, surfaces reconstruction, monolayers, monatomic linear chain and dimer. From these results a "relative error" between the potentials can be defined to describe their discrepancies. It was found that as the coordination number of the system decreases, discrepancies between the two potentials increase enormously.

Finally the helical structure of the 3-strand Ni and Al nanowires have also been studied. We have performed a comparison between the structures obtained by the former two potentials. We found that besides the potential effect on the equilibrium configuration of these nanowires, the use of periodic boundary conditions (PBC) in

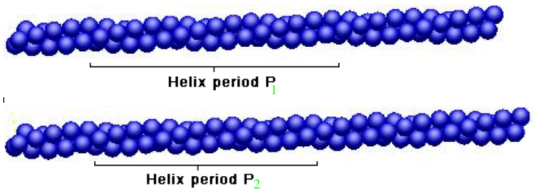

Figure 1: The size of the simulation box and the number of atoms N alter the period of the helix.

the simulations restraints the wire to a certain helicity wich depends on the length of the unit cell and the number of atoms N (see figure 1). By means of large scale conjugate gradients calculations, the optimal structure of the "real" nanowires (as N tends to infinity) was extrapolated. These results are shown in table 1.

	Al	Ni	Ni
	Mishin	Mishin	Sutton-Chen
Cohesive energy per atom Ec(eV/atm)	-2.42	-3.07	-3.44
Linear density ρ(1/Å)	1.11	1.27	1.33
Helix period P(Å)	34.76	30.39	29.14
Mean distance to wire axis R(Å)	1.49	1.28	1.23
dZ(Å)	0.90	0.79	0.75
θ(deg)	129.27	129.33	129.23

Table 1. Geometrical parameters of the "real" 3-strand nanowires

References:

[1] B. Wang, X. Chen, G. Chen, G. Wang, J. Zhao, Solid State Commun. **129**, 25 (2004).

[2] O. Gülseren, F. Ercolessi and E. Tosatti, Phys. Rev. Lett. **80**, 3775 (1998).

[3] Y. Kondo, K. Takayanagi, Science **289**, 606 (2000).

[4] M. S. Daw, M. I. Baskes, Phys. Rev. Lett. **50**, 1285 (1983).

[5] A. F. Voter and S. P. Chen, in High temperature ordered intermetallic alloys, edited by R. Siegel, J. Weertman and R. Sundan, MRS Symposia Proceedings No. 82 (Materials Research Society, Pittsburgh, 1987), p. 175.

[6] A. P. Sutton and J. Chen, Philos. Mag. Lett. **61**, 139 (1990).

[7] Y. Mishin, D. Farkas, M. J. Mehl, D.A. Papaconstantopoulos. Phys. Rev. B **59**, 3393 (1999).