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# A comparison between EAM interatomic potentials for Al and Ni: from high to low coordination systems

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## Abstract

Two different kinds of interatomic potentials within the Embedded Atom Method (EAM) have been used to study several properties of selected crystalline structures and nanowire configurations (ordered and helical) for Al and Ni based systems. Results clearly indicate the existence of increasing differences in the calculated quantities (cohesive energy and geometrical parameters) as the atomic coordination number decreases. This implies that EAM potentials must be cautiously used when analyzing low coordination systems such as metallic nanowires.

**Key words:** Interatomic potentials, EAM, nanowires.

# Comparación entre potenciales interatómicos EAM para Al y Ni: de sistemas de alta a sistemas de baja coordinación

## Resumen

Se han utilizado dos diferentes potenciales interatómicos de tipo EAM (Método de Átomo Embebido) para estudiar tanto estructuras cristalinas como configuraciones de tipo nanohilo (ordenadas o helicoidales) en Al y Ni. Los resultados muestran la existencia de notables diferencias entre ambos potenciales para las cantidades calculadas a medida que la coordinación disminuye. Esto implica que los potenciales EAM deben ser usados con ciertas precauciones cuando se estudian situaciones de baja coordinación, como nanohilos metálicos.

**Palabras clave:** EAM; nanohilos; potenciales atómicos.

## Introduction

Nanotechnology is based on the combination of methodologies for synthesis, fabrication and characterization of materials to fabricate systems or devices with particular properties derived from their nanometric dimensions (1). The computational determination of nanometric systems with favorable configurations is of capital interest in Nanotechnology to predict their intrinsic proper-

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ties as well as their evolution under modification of external parameters. Ab-initio based computational techniques constitute a reliable and standard approach (2) to determine the electronic structure and chemical bonding features of matter. Nevertheless, ab-initio calculations are restricted to systems containing few hundreds of atoms. The computational description of systems formed by many atoms requires alternative routes. The Embedded Atom Method (EAM) (3) represents an effective approach to efficiently describe interatomic potentials and, thus, optimize large atomic systems.

EAM interatomic potentials (3-6) are usually designed to describe bulk systems, characterized by large coordination numbers, $N_c$. Therefore, it is not clear whether these potentials are able to describe low coordination situations (clusters, nanowires, etc) of interest in emerging Nanotechnology. In this work we present a comparative study between two EAM interatomic potentials, for Al and Ni, in a range of systems with high and low atomic coordination.

## Computational methods

EAM describes the structural energy $E$ of a metallic system through the expression $E = \frac{1}{2}\sum_i \sum_{j\neq i} \phi(R_{ij}) + \sum_i F_i(\rho_i)$ where, $\phi(R_{ij})$ is a pair repulsive term and $F_i(\rho_i)$ is the embedding function (the required energy to embed an atom of type $i$ into the background electron density $\rho_i$). The density generated by the neighboring atoms is expressed as $\rho_i = \sum_{j\neq i} k_j(R_{ij})$, where $k_j(r)$ is the electron density of atom $j$. In the present study we have used two different parameterizations of the embedding function. On one hand, we have considered the approach proposed by Mishin et al. (5) (denoted as MFMP in this work). On the other hand, we have used the Sutton-Chen (SC) (4) approach, suitably designed to reproduce ab-initio results for the most stable bulk configurations (6). This approximation has been used to describe the geometry of ultra-narrow metallic nanowires (7).

We have determined the optimized structure of several 1, 2 or 3-dimensional (1D, 2D, 3D) crystalline systems with different coordination number, as well as the favourable configurations of Al and Ni ultra-narrow nanowires. This set of calculations constitutes an exigent benchmark of the EAM predictive power. The studied structures are represented by a supercell containing several atoms (ranging from 1 to 96), taking into account periodic boundary conditions (PBC) when needed. The optimized minimum energy atomic configurations are calculated using conjugate gradients optimization methods.

## Results and Discussion

In a first set of calculations we have determined for several optimized configurations of Al and Ni (Table 1), the cohesive energy per atom $E_c$, the nearest neighbor distance $\lambda$, and the quantity $\beta_\lambda = d^2E_c / d\lambda^2$ evaluated at the minimum of the total energy potential well. Results corresponding to MFMP and SC approaches are compared with ab-initio or experimental results where available.

Optimized 3D geometries were: face-centered-cubic (FCC) and body-centered-cubic (BCC). In addition, 2D (hexagonal and square) and 1D (linear chain) geometries have been included to test low coordination situations. As expected, both parameterizations accurately describe the FCC geometry. In general, those situations with $N_c > 6$ are reasonably described by both EAM approximations. However the results are very different for decreasing $N_c$ values. It seems that MFMP approach shows better agreement with experimental or theoretical values of $\lambda$, even for the lowest coordination situations. On the contrary, it seems that the SC approach provides better cohesive energies for both Al and Ni in low coordination situa-

Table 1
MFMP and SC values of cohesive energy per atom $E_c$, nearest-neighbours distance , and the quantity (see text) for different Al and Ni structures. Column labelled as "T/E" refers to ab-inito or experimental values (a: Ref. (8), b: Ref. (9), c: Ref. (10), d: Ref. (5), e: Ref. (11)).

| | *Nc* | $E_c$ (eV/atom)) | | | $\lambda$ (Å) | | | $\beta_\lambda$ (eV/Å$^2$) | |
|---|---|---|---|---|---|---|---|---|---|
| | | MFMP | SC | T/E | MFMP | SC | T/E | MFMP | SC |
| *Geometry* | | | | Aluminum | | | | | |
| 3D-FCC | 12 | 3.36 | 3.36 | 3.36[a] | 2.86 | 2.86 | 2.86[a] | 8.80 | 8.53 |
| 3D-BCC | 8 | 3.25 | 3.35 | 3.40[b] | 2.81 | 2.79 | 2.81[b] | 5.51 | 8.56 |
| 2D-HEX | 6 | 2.43 | 2.90 | | 2.80 | 2.62 | | 5.18 | 8.52 |
| 2D-SQ | 4 | 2.19 | 2.84 | | 2.80 | 2.5 | | 3.20 | 9.83 |
| 1D-chain | 2 | 1.48 | 2.48 | 1.87[c] | 2.73 | 2.28 | 2.41[c] | 3.48 | 10.09 |
| | | | | Nickel | | | | | |
| 3D-FCC | 12 | 4.45 | 4.45 | 4.45[a] | 2.49 | 2.49 | 2.49[a] | 19.59 | 20.31 |
| 3D-BCC | 8 | 4.34 | 4.41 | 4.34[d] | 2.42 | 2.42 | | 13.95 | 20.14 |
| 2D-HEX | 6 | 3.07 | 3.50 | | 2.47 | 2.36 | | 12.54 | 17.24 |
| 2D-SQ | 4 | 2.59 | 3.32 | | 2.37 | 2.28 | | 13.48 | 17.69 |
| 1D-chain | 2 | 1.08 | 2.59 | | 2.45 | 2.16 | 2.11[e] | 6.83 | 14.84 |

tions. Finally, the curvature at the minimum of the total energy curve (i.e. $\beta_\lambda$) strongly depends on the kind of EAM parameterization. In particular we have found for $\beta_\lambda$ that SC values are 3-4 times larger than those obtained from MFMP when $N_c < 4$.

It is very important to see that EAM approaches have less predictive capacity for low coordination systems. This possible lack of efficiency is very important in order to study low coordinated nanometric systems. For instance, the geometry as well as the cohesive energy of simulated metallic nanowires could strongly depend on the particular choice of the interatomic potential. Furthermore, these systems are of fundamental interest since it has been found both theoretically (7, 12) and experimentally (13) that, in some situations, free standing narrow metallic nanowires lose their bulk crystalline ordering by forming weird or helical structures, and, therefore, predictive and reliable tools are required to explain this phenomenon.

In the present study we have restricted ourselves to the analysis of a particular example for two specific nanowire-like configurations for both Al and Ni. Firstly, we have considered an ordered metallic nanowire formed by subsequent equilateral triangles with atoms located at the vertex positions. Two subsequent triangles are rotated 60° between them (Figure 1a). The second kind of metallic nanowire we have studied is a helical system formed by a sequence of equilateral triangles having a relative rotation angle different from 60° (Figure 1b). During the computational procedure the nanowire atomic positions as well as the supercell length $L_z$ have been simultaneously optimized. After the optimization procedure we have determined three quatities: cohesive energy per atom $E_c$, optimized linear density $\rho_L = N_a / L_{opt}$ (where $N_a$ is the number of

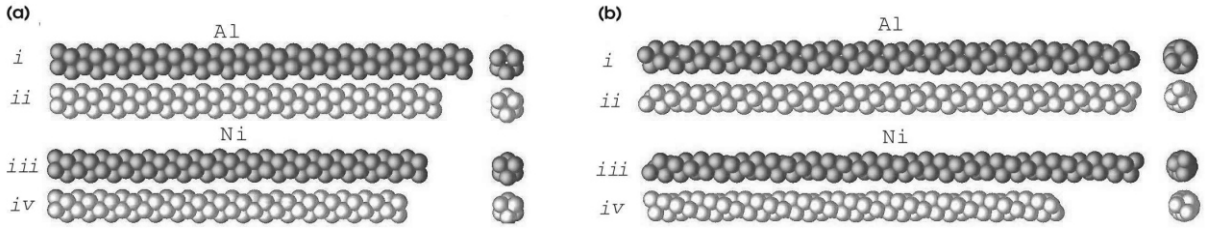


Figure 1. Configurations of ordered (a) and helical (b) nanowires of Al (i,ii) and Ni (iii,iv) optimized using MFMP (dark) and SC (clear) EAM interatomic potentials.

Table 2
Cohesion energy per atom $E_c$, linear density $_L$ and the quantity (see text) for ordered and helical Al and Ni nanowires. Two different interatomic EAM potentials (MFMP and SC) have been considered.

| | | $E_c$ (eV/atom) | | $_L$(atoms/Å) | | (eV/Å) | |
|---|---|---|---|---|---|---|---|
| | Structure | MFMP | SC | MFMP | SC | MFMP | |
| Al | Ordered | 2.48 | 2.91 | 1.34 | 1.45 | 5.25 | 4.41 |
| | Helical | 2.43 | 2.85 | 1.15 | 1.15 | 5.63 | 4.43 |
| Ni | Ordered | 3.14 | 3.53 | 1.51 | 1.59 | 11.85 | 10.08 |
| | Helical | 2.97 | 3.46 | 1.15 | 1.38 | 12.89 | 9.53 |

atoms in the supercell and $L_{opt}$ is the optimized supercell length), and $\eta = L_{opt}$ (defined as the product of the Young's modulus by the nanowire surface). Results for these quantities are summarized in Table 2.

Both EAM potentials determine that the ordered nanowire is energetically favourable with respect the helical nanowire (with an energy difference of approx. 0.05 eV/atom), in agreement with previous results for Al (21). We have found a similar trend for Ni nanowires. In general, the SC approximation provides larger cohesive energies and linear densities than the MFMP one, being the differences of the order of 12%-17% for $E_c$ and 5%-20% for $\rho_L$ (excluding the Al helical nanowire case). Regarding the elastic behaviour, the MFMP approach provides optimized nanowires with larger $\eta$ values (15%-30%) with respect the SC values. It is important to notice that, for Al, $\eta$ is in larger in the helical case when compared to the ordered wire, independently on the EAM approach. This is not true for Ni, were the two EAM approximations give rise to a different ordering of $\eta$ values.

## Conclusions

Different EAM interatomic potentials parameterizations provide different values of important physical properties (cohesive energy, nearest neighbor distance) as the coordination number decreases (especially in very low coordination situations). This fact has important implications when modeling the behavior of nanometric systems, where a non-negligible amount of atoms present low coordination situations. In particular, we have shown that ordered and helical narrow nanowires present different cohesive energy, linear density and elastic constant depending on the kind of EAM parameterization. Therefore it is clear that some uncertainty

emerges when considering EAM to describe the properties of nanometric systems.

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