

Ni NANOCONTACTS: STUDY OF ATOMIC CONFIGURATIONS DURING FORMATION AND RUPTURE

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The comparison of experimental conductance histograms and results from computational simulations has allowed to establish a relation between the electronic and structural properties of Au and Al nanocontacts [1]. In the Ni case, there is in the literature a great variety of experimental results showing a noticeable diversity of behaviours of the conductance histogram. With the aim of helping to the interpretation of the experimental results, we have performed simulations of the formation and rupture of nickel nanocontact to analyse their structural evolution as well as the minimum cross section histograms.

Nanowires are simulated using Molecular Dynamics (MD) where the interatomic interactions are described within the framework of the embedded atom method (EAM). The full determination of the atomic positions in the simulation allows us to study the evolution of the nanocontact geometry during its formation/breakage and to determine the existence of preferred atomic configurations. The studied configurations are analysed in two different cases: i) starting from an initial ordered structure, the nanowire is stretched till its breakage (as in previous Au and Al works [1,2]); ii) the nanocontact is created and broken several times within the same simulation. Figure 1 shows some snapshots obtained from the simulation of one of these formation-rupture cycles.

Equally we can evaluate the evolution of the minimum cross-section S_m of the nanocontact. Minimum cross-section histograms $H(S_m)$ have been built accumulating S_m traces during hundreds of indentation/ruptures. Three different histograms are shown in Figure 2 depending on how S_m has been obtained: i) during the nanowire creation period (Fig. 2a); ii) during its breakage (Fig. 2b); or iii) from the rupture of the initial parallelepiped configuration (Fig. 2c). The three histograms show marked peaks at all the integer values of S_m . But the relative height of these peaks differs, indicating that preferred structures where atoms accommodate are different.

In our simulations we use state of the art EAM inter-atomic potentials able to fit bulk and surface properties [3]. We start with a parallelepiped of hundred of atoms ordered according to a fcc structure. After a relaxation process, two bilayers slabs at the top and bottom of the parallelepiped are frozen and separated at constant velocity of 2 m/s till the nanocontact breaks. The histogram of Figure 3c has been built repeating this rupture 300 times. Whereas to obtain Figure 3a and 3b histograms, the last stage of the previous simulation is used to start a new (single) simulation where the nanowire is put repeatedly (150 times) in and out of contact. Simulations have been performed at different (constant) temperatures and from different initial crystalline orientations.

References.

- [1] E. Medina *et al.*, Phys. Rev. Lett. **91**, 026802 (2003).
 [2] A. Hasmy, E. Medina, and P. Serena, Phys. Rev. Lett. **86**, 5574 (2001).
 [3] Y. Mishin *et al.* Phys. Rev. B **59**, 3393 (1999).

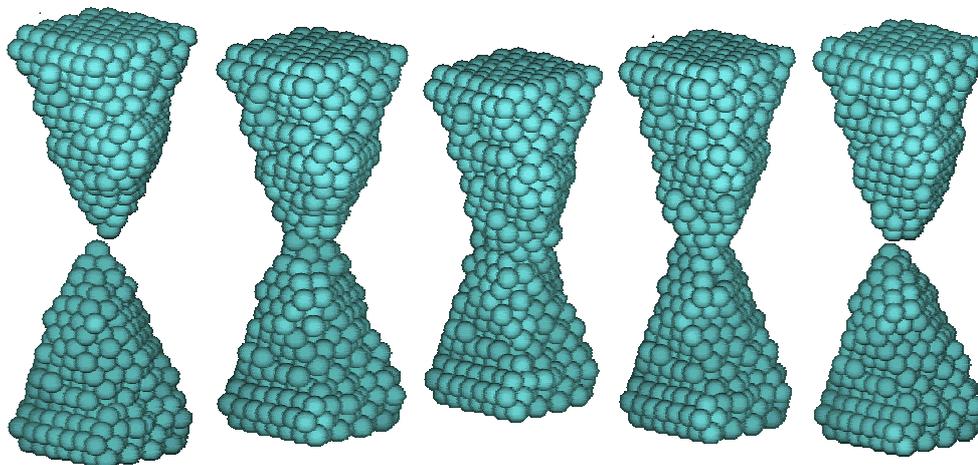


Figure 1: Snapshots of a Ni nanowire structure during its formation and breakage (a pushing/pulling loop) at $T=300$ K. The stretching direction is parallel to the (111) direction.

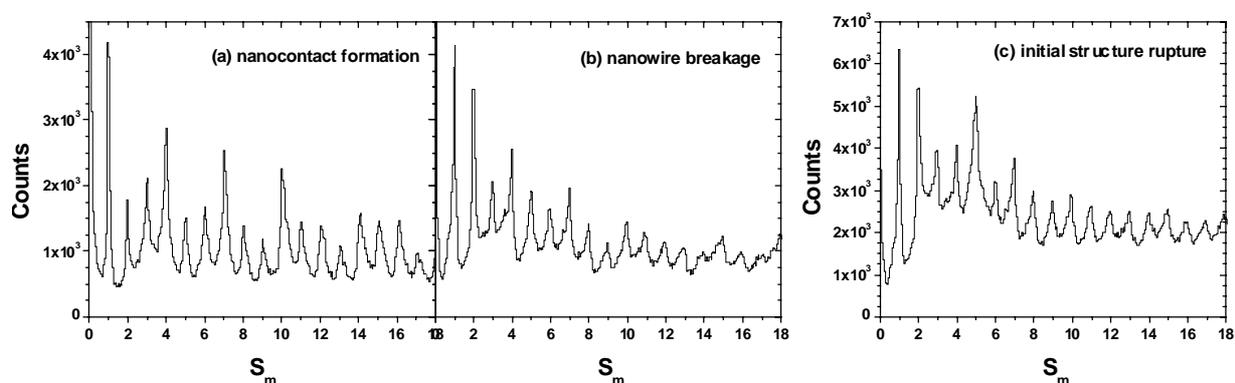


Figure 2: Minimum cross-section S_m histograms of Ni nanocontacts at $T=300$ K stretching along the (111) orientation. Histogram (a) and (b) have been obtained during 150 consecutive pushing/pulling loops. Histogram (a) corresponds to the accumulation of data from nanowire formations whereas (b) corresponds to the nanowire ruptures. Histogram (c) has been built with 300 independent ruptures.