Ni NANOCONTACTS RUPTURES: STATISTICAL STUDY OF LAST CONFIGURATIONS BEFORE BREAKING

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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 [1-3]. 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 along different directions 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). In our simulations we use state of the art EAM inter-atomic potentials able to fit bulk and surface properties [4]. 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 full determination of the atomic positions in the simulation allows us to study the evolution of the nanocontact geometry during its breakage and to determine the existence of preferred atomic configurations (as in previous Au and Al works [1-3]).

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 300 ruptures. Six different histograms are shown in Figure 1 depending on the stretching direction and temperature. 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.

Additionally we performed a statistical analysis of the presence of monomers and dimmers during last steps of the rupture. When the stretching direction is the [111] the system mainly evolves trough a sequence monomer-dimmer towards the rupture. On the other hand, for the [100] and [110] stretching directions, the system mainly evolves from more complex structures, than monomers and dimmers, to the final rupture.

References.

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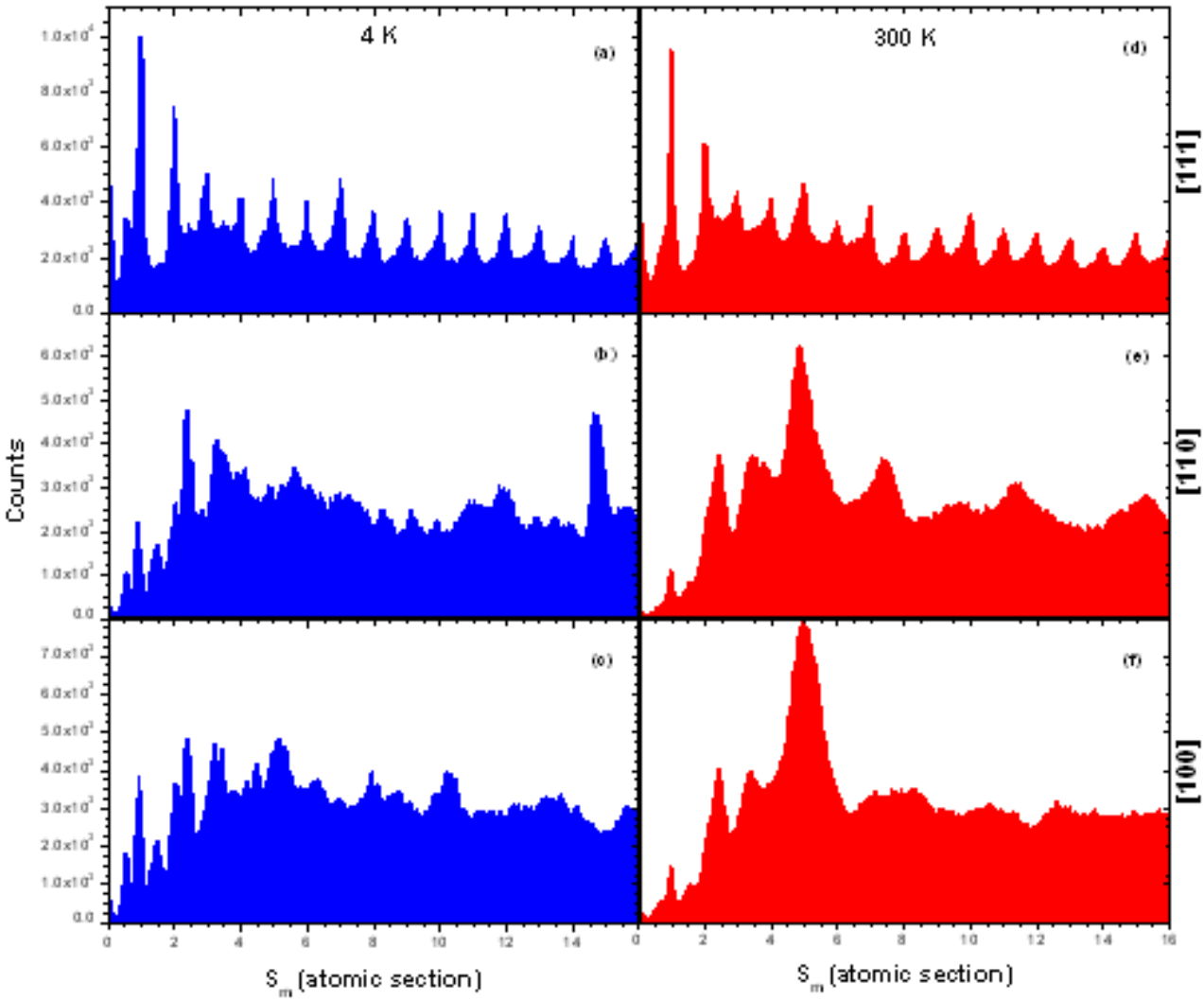

Figure 1: Minimum cross-section S_m histograms of Ni nanocontacts at T=4 K (a,c,e) and 300K (b,d,f) evolving under stretching along the [111] (a,b), [110] (c,d) and [111] (e,f) orientation. Histograms have been built with 300 independent ruptures from the initial released parallelepiped of 390 (a,b), 420 (c,d) and 375 atoms (e,f). Different initial orientations have similar aspect ratio.