Poster

Ni NANOCONTACTS RUPTURES: DEPENDENCE ON STRETCHING DIRECTIONS

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The comparison of experimental conductance histograms and results from computational simulations has allowed establishing 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 H(G). Furthermore, theoretical approaches to the study of the breaking mechanism of Ni nanowires do not shed light on the problem since different results appear in the literature [4,5]. With the aim of helping to the interpretation of the experimental results as well as previous computational studies, we have performed simulations of rupture of nickel nanocontacts 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 [6]. We start with a parallelepiped 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]). The exact knowledge of the set of atomic coordinates also allows monitoring 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. We analysed the histograms dependence on the stretching directions, temperature and original size of the samples. Six of these histograms are shown in Figure 1. All the histograms show marked peaks indicating the presence of favourable configurations during the last stages of the breaking process. However, the relative height of these peaks differs, indicating that preferred structures where atoms accommodate are different. The main conclusion of our study is that the expected conductance histogram strongly depends on the nanocontact stretching direction.

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 directly evolves from more complex structures, than monomers and dimmers, to the final rupture. Finally, we found that for all the stretching directions and temperatures the peaks around S_m = 0.5, 1.0 and 1.5 are mainly originated from dimmers, monomers + dimmers and complex structures respectively (See Figure 2.). Some anomalies are observed for the [100] stretching direction at 4K.

References.

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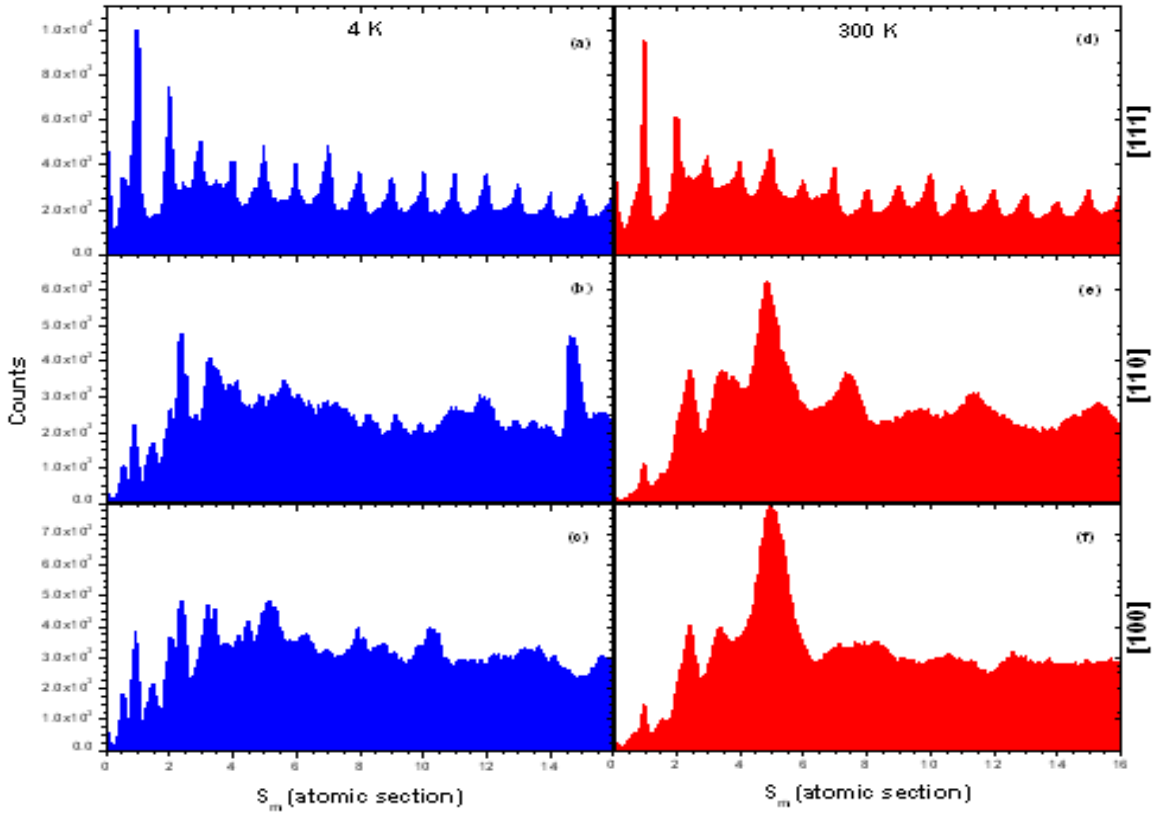

Figure 1: Minimum cross-section S_m histograms of Ni nanocontacts at T=4 K (a,b,c) and 300K (d,e,f) evolving under stretching along the [111] (a,d), [110] (b,e), and [111] (c,f) orientations. Histograms have been built with 300 independent ruptures from the initial released parallelepiped of 390 (a,d),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

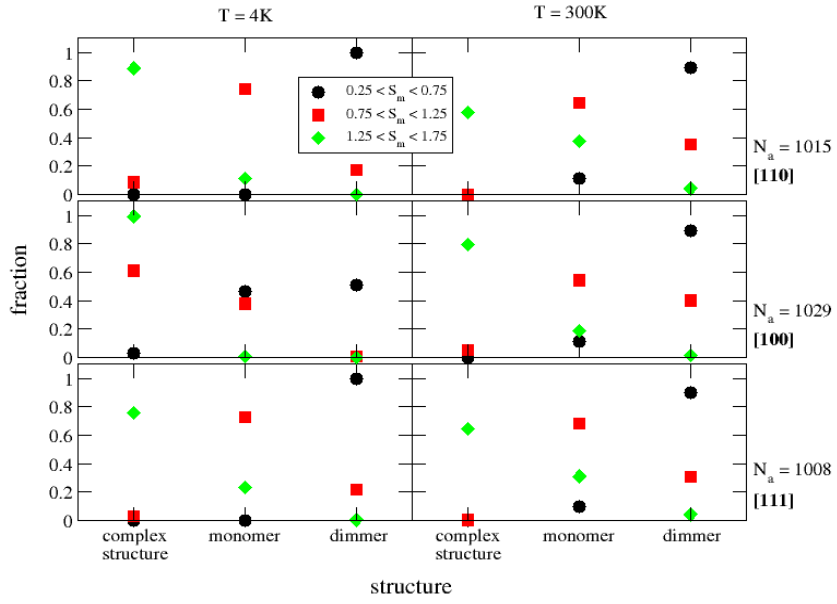

Figure 2: Fraction of monomers, dimmers and other complex structures for each one of the histograms peaks in the interval $0.25 < S_m < 1.75$ for different temperatures and stretching directions.