Modeling breakage properties of metallic nanowires with random orientations

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During the last two decades, the study of the properties of nanowires has been one of the keystones of the development of nanotechnology since these nanoobjects exhibit electrical and mechanical properties of interest in fundamental knowledge as well as technological applications [1]. In particular, many experimental studies of electrical and mechanical properties of metallic nanowires have been addressed in order to describe the quantum features appearing due to electron transversal confinement. The standard approximation for the experimental study of such metallic nanowires includes the formation, elongation and breakage of ultranarrow nanocontacts, as for instance, those formed between an STM tip and a metallic surface. With the use of powerful computational resources and accurate description of the atomic interactions, many of the formation-breaking experiments can be reproduced "in silicon" [2], being possible even to analyse situations and structures that experimentally are difficult to address [3].

It has been stressed the importance of statistical studies of these phenomena [3, 4] because, given a particular initial geometrical configuration and temperature, each breakage event evolves differently, that is the standard approximation for the experimental study of metallic nanowires, where statistical data is accumulated during many indentation-retraction cycles.

However, the comparison between experimental results and the usual numerical simulations requires an additional element. Experimental data usually correspond to the statistical average of nanowire breaking events involving random stretching directions. In a standard experiment there is no reason that indicates that any particular orientation would be preferred during the nanowire formation and breakage. Therefore, to accomplish a complete statistical analysis equivalent to the experimental one, computational calculations must simulate breaking events on random stretching directions. This could be a potential problem since it is not easy to perform simulations with arbitrary (random) initial stretching directions. Fortunately, it is not necessary to compute "every" stretching orientation to get the statistical behaviour of the breaking nanowires.

In an experiment, the final stages and behaviour of a nanowire during its breakage are leaded by the type of crystalline structure closest to its elongation direction. So it should be in simulations. Therefore, it is needed only to analyse main crystalline orientations, those that show different structural type, and average their results according to their occurrences. I.e., to achieve orientation statistics in computational simulations, results from the main crystalline directions have to be merged with the appropriate weights. These weights will be proportional to the zone axis multiplicity [5]. Of course, each main direction must have an accurate

statistics to guarantee the correctness of the global results, but this is easily achieved performing many simulations with the same initial structure at a given temperature [3,4].

In this work we will present the method used to merge the statistical results corresponding to the three different stretching directions ([100], [110] and [111] for a *fcc* structure) in order to reproduce results from random orientations and compare with experimental findings. We will show the results on some properties of this weighted average for three metallic species (Ni, Al, Cu). As an example of these results, figure 1 shows for Ni nanowires the probability of obtain of a monomer, dimer or other structure as final configuration before the breakage.

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Figures:

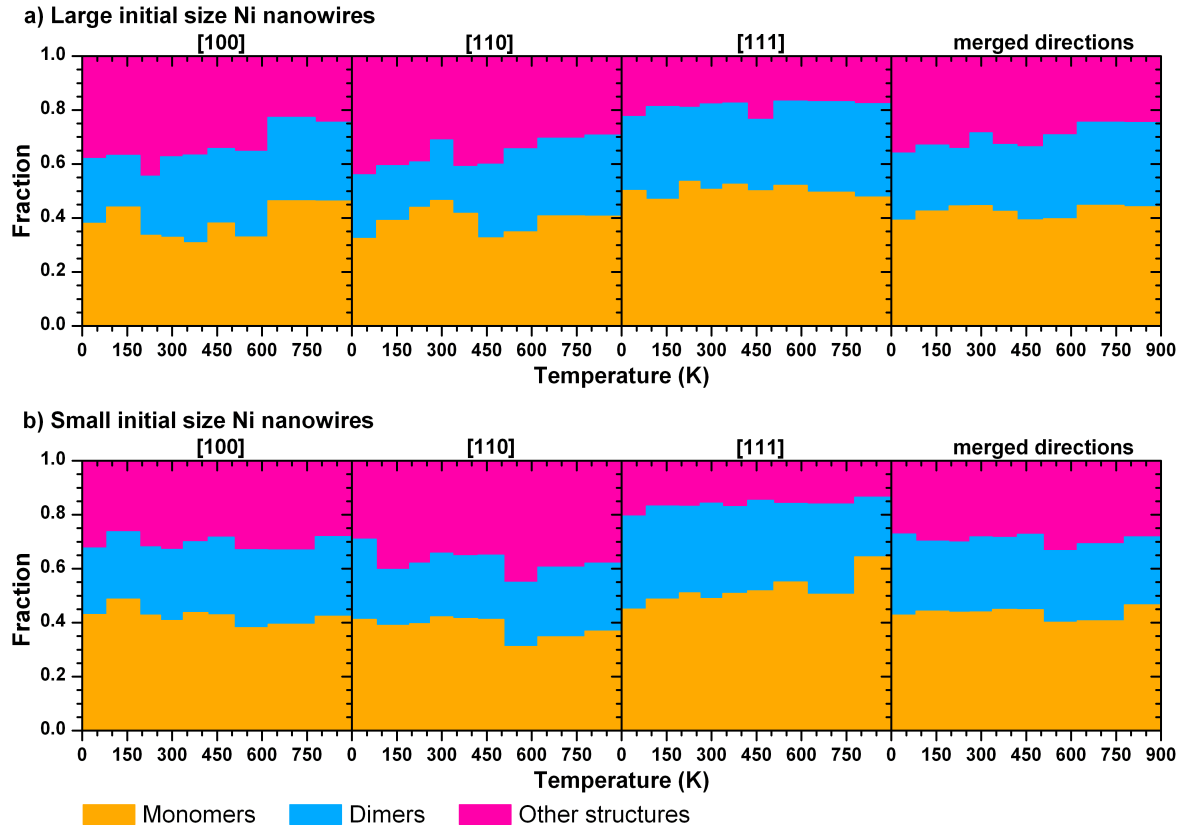

Figure 1: Fraction of monomers, dimers and more complex structures appearing during the Ni nanowire breaking process as functions of the temperature for Ni nanowires of large (~1000 atoms) **(a)** and small (~180 atoms) **(b)** initial size. Different columns correspond to nanowires stretched along [100], [110], [111] and random (merged) crystallographic directions.