MERGING NANOWIRES BREAKAGE RESULTS FOR DIFFERENT STRETCHING DIRECTIONS TO COMPARE WITH EXPERIMENTAL ONES

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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 advent of powerful computational resources and realistic descriptions of the atomic interactions, it has been possible to reproduce many of such formation-breaking experiments “in silicon” [2]. An important part of these simulation studies have been done using Molecular Dynamics (MD) algorithms, allowing to elucidate how this formation-elongation-breakage occurs. Furthermore MD simulations allow us to determine the kind of structures that appear during the final stages of the breaking process. Getting insight of such structures is a crucial matter since they control the electron transport of the nanowire, allowing a comparison with the experimental data.

However, the comparison between experimental results and MD computational simulations requires an extra ingredient: statistics. It is necessary to statistically address the study of many nanowire breaking events, mimicking the experimental indentation-retraction cycles used to accumulate data. Statistic in this context implies take into account two facts: a) breaking events involving random stretching directions; b) given a particular initial geometrical configuration, each breakage event evolves differently. The last condition is easily achieved performing many simulations with the same initial structure at a given temperature [3]. Obtain an accurate statistic that take into account the first condition is tricky because it is not easy to perform simulations with arbitrary initial stretching directions. There is no reason that indicates that any particular orientation would be preferred, but the final stages and behaviour of the experimental nanowire break must be determined by the structure type closest to its elongation direction. Then, to achieve orientation statistic, results for the three main fcc directions [100], [110] and [111]) (with a good samples statistic) have to be merged with weights proportional to their zone axis multiplicity (6, 12 and 8 respectively) [4].

References:

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Figures:

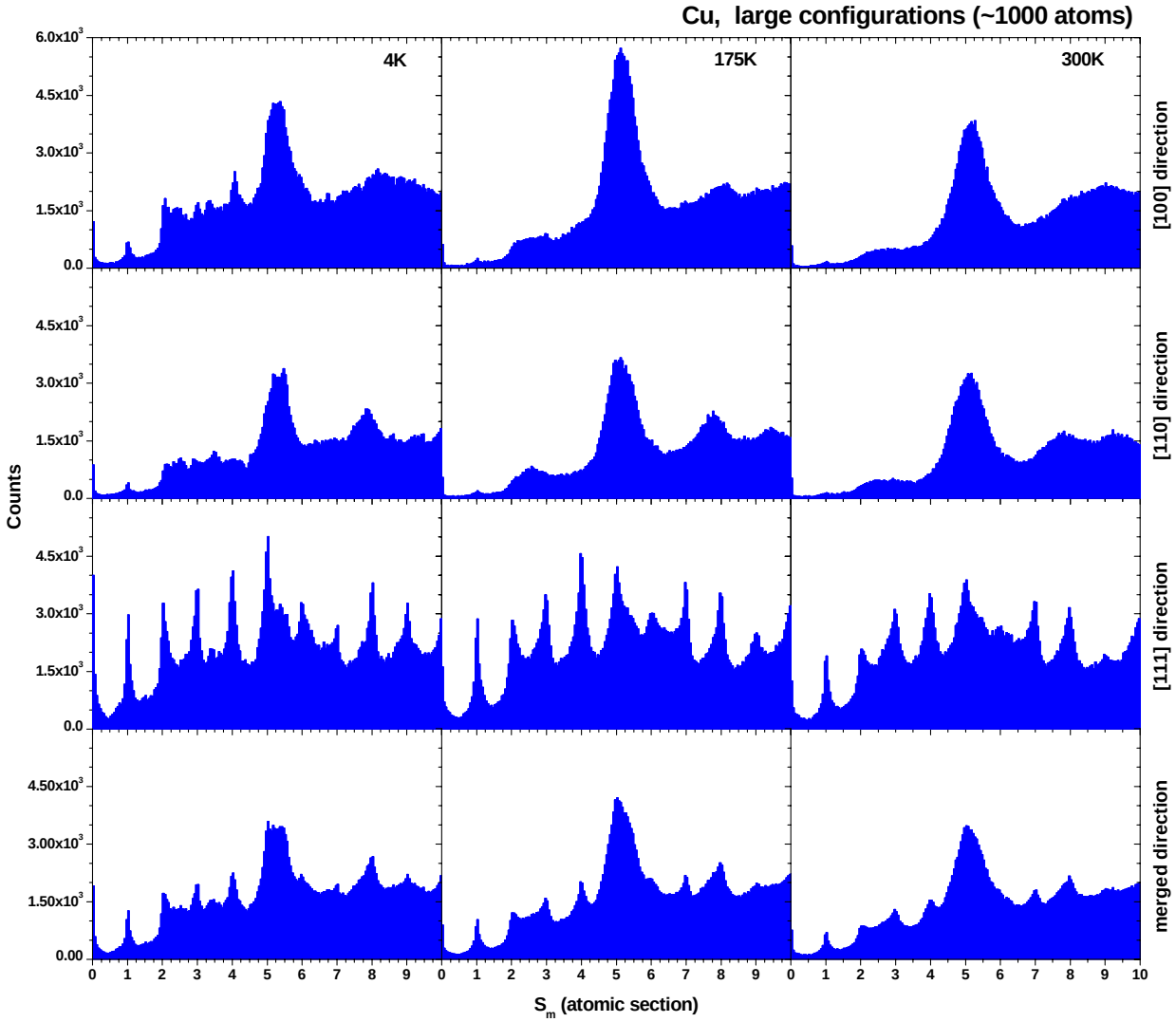

Figure 1: Minimum cross-section S_m histograms of Cu nanocontacts evolving under stretching at T= 4, 175 and 300 K. Histograms correspond to [100], [110] and [111] orientation (built each with 300 independent ruptures), and a normalised average of the three orientation taking into account their axis multiplicity (6, 12 and 8 respectively) [4].