# FORMATION OF STABLE PENTAGONAL NANOWIRES UNDER STRETCHING ON FCC METALS

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Different works during the last decade have showed the formation of staggered pentagonal configurations on breaking nanowires [1-5]. These pentagonal nanowires are formed by subsequent staggered parallel pentagonal rings (with a relative rotation of $\pi/5$) connected with single atoms (Fig. 1). The atomic sequence -1-5-1-5- presents a fivefold symmetry with respect the nanowire axis. This symmetry does not correspond to any crystallographic FCC nor BCC structures. The -1-5-1-5- staggered nanowire configuration may be understood in terms of a sequence of interpenetrated icosahedra. This icosahedral symmetry is very common in very small systems [6].

The formation of staggered pentagonal configurations during the stretching process has been already reported for Cu [1] and Au [2] nanowires using different Molecular Dynamic (MD) approaches. In particular the high stability of the Cu nanowire was confirmed with ab-initio calculations [3]. Pentagonal motives also appear in infinite Al and Pb nanowires obtained from MD simulated annealing methods [4]. More recently such structures have been reported for stretched Ni nanowires with different crystallographic orientations [5]. These pentagonal structures are very stable, with lengths larger of 10 Å and presenting a high plastic deformation under strain.

The aim of the present work is to carry out a statistical study of the structural evolution of FCC nanowires under stretching for a broad range of temperatures and three crystallographic stretching directions. We have carried out hundreds of MD simulations of aluminium, copper and nickel nanowires breaking processes, within the EAM approximation, following the procedure used in previous works [5, 7]. This study will confirm the existence of pentagonal nanowires, and, more important, will present the optimal set of parameters (temperature, size, crystallographic orientation) required for maximizing their occurrence probability.

The formation of pentagonal nanowires is a very anisotropic process. In fact, long pentagonal structures are relatively common for [100] and [110] stretching directions, whereas rarely occur for the [111] case. These preferred configurations have a minimum cross-section of $S_m \sim 5$ and are unveil in computational minimum cross-section histograms $H(S_m)$ as a very large peak at $S_m=5$ (Fig. 2). The configurations that contribute to this peak are mainly staggered pentagonal nanowires. This type of arrangement is not seen at 4K because a larger temperature is required to explore and overcome those energy barriers leading to configurations able to develop these pentagonal chains. The probability of apparition of these structures and its stability it is reflected on the distribution function of time spent into the interval $4.5<S_m<5.5$ (Fig. 3): the long tail of the distribution corresponds to very long stable pentagonal nanowires. Depending on the material, the $S_m=5$ peak in $H(S_m)$ increases with temperature up to certain value ($\sim T_{melting}/3$), at the same time the tail of the pentagonal nanowire length distribution enlarges. At further temperatures there is a decreasing behaviour of both due to melting processes.

The present statistical study shows a protocol helpful to form these long pentagonal nanowires for different materials.

**References:**

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**Figures:**

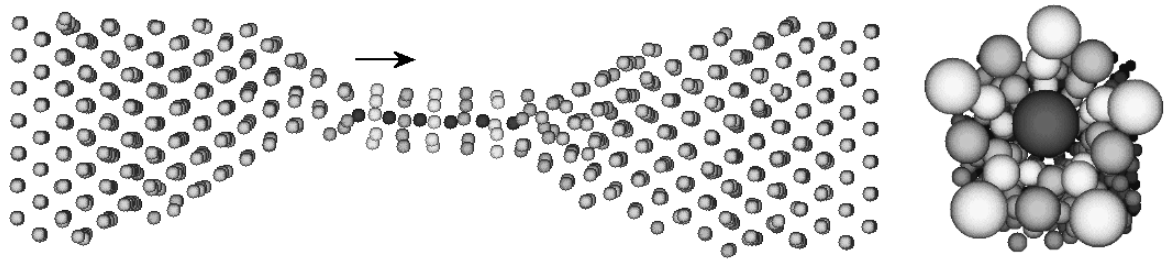

**Fig. 1:** Longitudinal (left) and cross-section (right) views of a Ni nanowire stretched along the [100] direction at 300K. The cross-section image shows a perspective view of the nanowire as seen from the position indicated on the longitudinal view. This image illustrates the appearance of staggered pentagonal structures -5-1-5-1-.

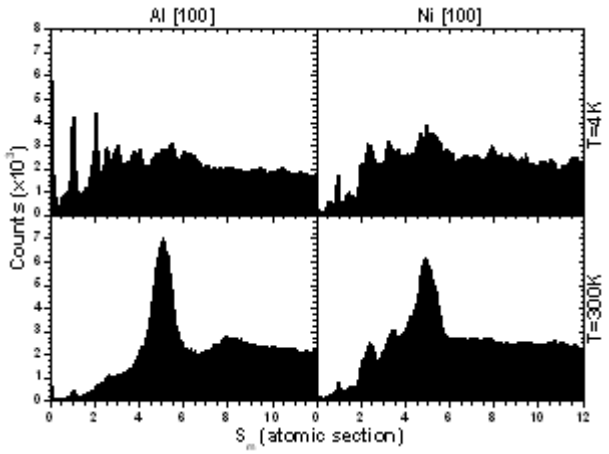


**Fig. 2:** Minimum cross section histograms $H(S_m)$ of Aluminium and Nickel breaking nanowires stretched along [100] direction at T=4 and 300K.

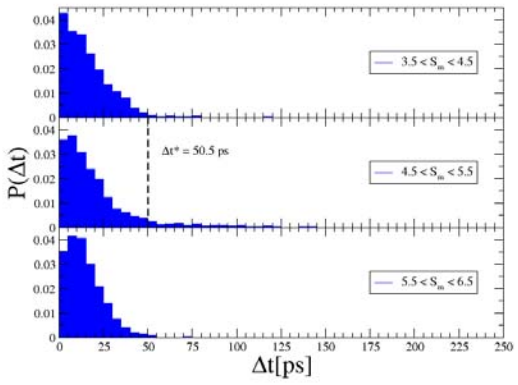


**Fig. 3:** Distribution function $P(\Delta t)$ of the time spent by Ni nanowires stretched at 300K along the [110] direction within the minimum cross section interval showed in the figure.