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Supplementary information

Roughening transition as a driving factor in the formation of self-ordered one-dimensional nanostructures

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Supplementary text

As a result of surface diffusion of atoms at elevated temperatures, the roughly-cylindrical wire at the initial stage of its transformation takes on a shape bounded by planes with minimal surface energy densities. Fig. S1 demonstrates such a configuration for a nanowire with a radius $r_{nw} = 30$ achieved at moderate temperature: $\alpha = 1.5$ and $p = 0.65$. The lateral surface of the nanowire at a given time is mainly formed by bands of (110)-type faces, onto which there is a stream of atoms from intermediate zones (narrower bands of (100)-type faces).

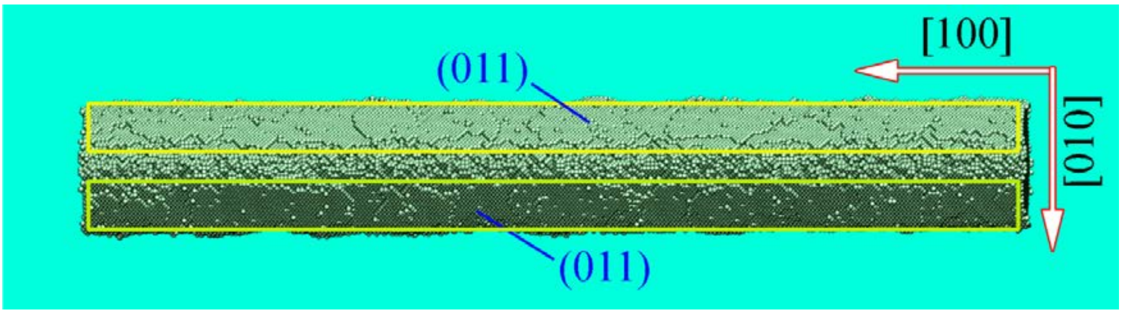

Fig. S1. Configuration of a nanowire with a body-centered lattice oriented along the [100]-direction at the initial stage of its evolution: $\alpha = 1.5$ and $p = 0.65$; $r_{nw} = 30$.

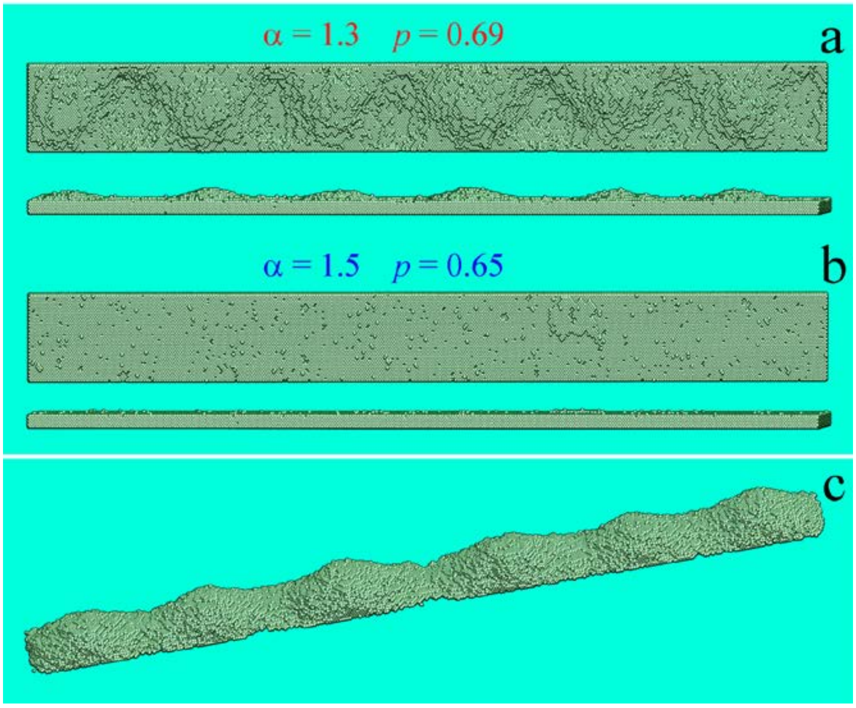

Fig. S2. Morphology of a slab with the upper (110) face after time $t = 10^7$ MC steps. $L = 630$, $w = 70$, and $h = 10$. Sub-images (a) and (b) show a modification of the slab that is "immersed" in a substrate of "frozen"/moveless atoms. Configuration (c) shows the shape of the plate, which is placed on the substrate: $\alpha = 1.5$ and $p = 0.65$.

This "external" stream of atoms can stimulate the formation of stepped hillocks on (110) faces. In the absence of external atomic flows, a pronounced modification of the (110)-type face (roughening transition) is possible only at a temperature exceeding the threshold. The threshold character of development of the roughening transition is shown in Fig. S2. Sub-images (a) and (b) represent the modification of the surface of a thin slab after time $t = 10^7$ MC steps. In this case, it is assumed that the slab is a part of a substrate with a (110) outer face. However, only the atoms that make up the plate are movable. The boundary condition for the movable atoms is reflective boundaries installed along the outer perimeter of the slab.

Data presented in Fig. S2 indicate that there is some intermediate value $1.5 > \alpha_R > 1.3$, which corresponds to the critical temperature, T_R, necessary for the occurrence of roughening transition. If the slab is not immersed in the substrate, but lies on it, then with a sufficiently small thickness it can break up into single fragments with a stepped structure. With a thicker slab, periodic perturbations of its surface occur in a two-mode regime.

At the initial stage of evolution, intense atomic fluxes from the side edges to the central part excite short-wavelength modulations of the slab height. As the edges are rounded and fast streams relax, longer wavelength modulations begin to play a dominant role (see video file Slab_on-Substrate.avi).

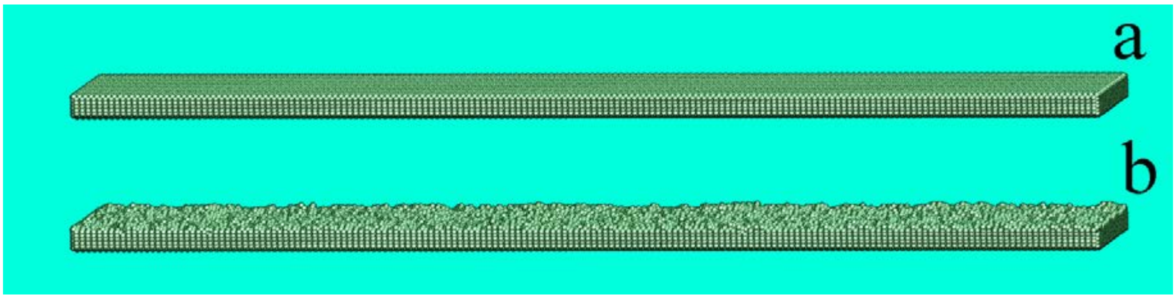

Fig. S3. Modification of the surface of the slab, the upper face of which is a (111)-facet; $\alpha = 1.3$ and $p = 0.69$. The geometrical dimensions of the plate are the same as in Fig. S1.

The roughening transition effect occurs only on faces of a certain type. Fig. S3 shows that only short-scale perturbations of a small-amplitude surface are observed on the (111) face — strictly ordered long-wavelength surface modulations do not develop.