Nanocomposites and nanomaterials

The effect of crystallographic orientation and surface tension forces on the bcc nanocrystals size effect

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The serial processing molecular dynamics computer simulations of the tensile strain dynamics of Mo cylindrical shaped nanosamples of the orientation along the deformation axes [100], [110], [111] was carried out in order to establish the influence of the bcc nanocrystals size on their level of strength.

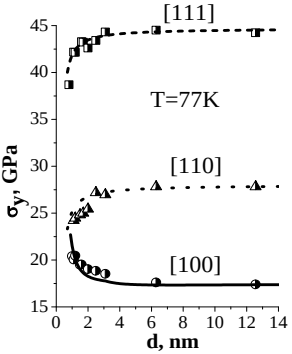

Fig. 1. Mo nanocrystals strength as a function of its diameter under the uniaxial tension with [100], [110] and [111] orientations at T = 77 K.

It is established (Fig. 1) that for all three crystallographic orientations with diameters <5 there is a sharp change in strength, namely the size effect is manifested. However, for Mo samples oriented along [110], [111] the change in strength is found to be a reduction, when for samples with the [100] orientation the strength is increasing with decreasing of the crystal diameter.

When stretching the Mo nanocrystals in the [110] and [111] direction, the achievement of instability at the local area is associated to the dislocations formation at the surface layer, where tensile stresses are acting. It facilitates the stretching process and leads to the global voltage reduction and to the loss of Mo nanowires stability. In this case, the decrease in the nanosample diameter leads to reduction of its strength. The distinguishable tendency is observed during the stretching along the [100] direction, where the strength level of the Mo nanowire is controlled by the formation of the twin. Nucleation of this defect is associated with the loss of stability of the crystal at the larger volume. It means that the instability region of the crystal structure that is required for the twin formation has high length. As a result, one area of the crystallographic plane where the twin is formed is under the action of tensile stress and the second area is under contraction, which leads to an increase in applied voltage required for twin formation.

The analytical relation of the effect of nanocrystal size and values of surface tension forces on the level of its strength is proposed.