## Nanocomposites and nanomaterials

# Size effect at deformation and fracture of bcc metal nanowires

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Simulation of uniaxial strain of a number of nanowires of bcc metals (Mo, W, Fe) is performed by molecular dynamics method. Tension of cylindrical nano-specimens of diameter 1-10 nm and orientation [100], [110], [111] was simulated at the temperature 77K. The dependence of change in strength of nanowires of bcc metals on their size (size effect) is established. It is shown that for all orientations this effect manifests itself for sizes less than 5 nm. However, for nanowires with orientations [110] and [111] size reduction gives rise to decrease in strength, and for the nanowire of orientation [100], vice versa, size reduction results in strength growth. (Fig. 1). Mechanism that governs the level of nanowire strength lies in the formation of defects (dislocations or twins) in the surface layer as a result of the local lattice instability. The defect type depends on crystallographic orientation of tension of the specimen. It is exhibited that size effect is due to surface tension. The analytical dependence is offered to describe the effect of both nanowire size and surface tension on the level of nanowire strength.

**Fig. 1**. Dependence of nanowire strength (Mo (a), W (b), Fe (c)) on it diameter under the uniaxial tension in directions [100], [110], [111] at T=77K.