Effects of Temperature and Grain Size on the Properties of Copper Nanotwinned Structures

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Introduction of twin boundaries within nanocrystalline grains has given scientists an opportunity to enhance mechanical properties that are usually mutually exclusive: strength and ductility. Present research is focused on developing a complete understanding of the deformation characteristics of copper nanotwinned structures by large-scale Molecular Dynamics simulations. Moreover, the influences that grain size, twin width, and temperature have on the properties of Cu nanotwinned structures have been investigated. Simulation results have shown that materials' properties (e.g. strength, toughness) can be enhanced by introducing nanotwins, however, this enhancement is more pronounced at the higher temperatures. At the lower temperatures, some unique deformation characteristics may lead to the unusual behaviors of materials. The existence of the 'inverse Hall-Petch' behavior for Cu nanotwinned structures has also been investigated. This research will, therefore, contribute towards further development of the theory of plasticity of nanomaterials and advancement of nanostructures with enhanced and unique mechanical properties.