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Topological Properties of Microstructures in Nanocrystalline Materials. TAO XU, MO LI, Georgia Institute of Technology — Recent experiments show that the topological properties of microstructures in nanocrystalline materials play an important role in the mechanical properties of nanocrystalline materials. However, the fundamental structure-property relationship has not been fully understood due to the difficulties in determining and controlling the microscopic properties of nanocrystalline materials experimentally. In this study, we investigate how different topological properties affect the thermal and mechanical responses of nanocrystalline materials, including grain size distribution, surface area distribution, triple junction length distribution, grain boundary misorientation, etc. Digital microstructures with desired topological properties are generated using Inverse Monte Carlo method and are then relaxed and deformed by large-scale molecular dynamic simulation. In order to characterize the relaxed and deformed digital samples, we use a new grain boundary characterization method to accurately determine the position and thickness of each grain boundary during both relaxation and deformation. Finally, this newly developed algorithm enables us to study the correlation between topological and mechanical properties of nanocrystalline materials.

Tao Xu
Georgia Institute of Technology

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