ICSMA19 Metz, France, June 26 - July 1, 2022
International Conference on Strength of Materials

Effects of mechanical stresses on grain growth of nanocrystalline FCC metals

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Molecular dynamics simulations of nanocrystalline Al and Cu were performed to determine the effects of mechanical stresses on grain growth. For this purpose, microstructures consisting of 100 randomly oriented grains were synthesized and simulated at different thermomechanical conditions. To simulate the effect of the stress, unstressed systems were compared to systems where a hydrostatic stress of 50 MPa for Al and 75 MPa for Cu was applied. We utilized in-house developed algorithms to reconstruct the grains and geometrically characterize the grain boundaries and interfaces of the microstructure throughout the grain growth process. The features of the boundary's surfaces and the distribution of other interfaces were then correlated with grain growth rate. The corresponding driving force was then estimated and compared with existing models of grain growth. Mechanical stresses were found to affect primarily the onset of events at the grain scale, but the general kinetics were not substantially influenced. This is attributed to the random texture of the specimen.

Keywords: Molecular Dynamics Simulation, Grain reconstruction, Grain growth, Grain Boundary, Interfaces

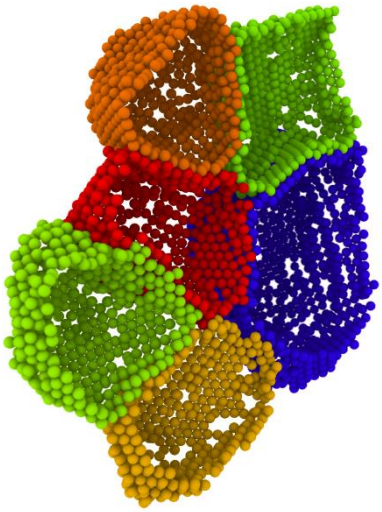

Fig.1 Atoms representing parts of the grain boundaries of six neighboring grains

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