Molecular Dynamics Simulation of Microstructural Change in a Polycrystalline FCC Metal under Compression

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ABSTRACT

Microstructure strongly affects the mechanical propertied of material, and various methods have been developed to improve the microstructure. Especially, a large compressive deformation is effective to refine the crystal grains, and some of the schemes such as ARB and ECAP have been applied to industrial processes. In this study, change in microstructure during large deformation is simulated using molecular dynamics method. A polycrystalline fcc metal is assumed and compressive external force is imposed on the model. The plastic deformation behaviour, such as change in grain shape, motion of grain boundary, generation of dislocation and slip, are investigated. Initial orientation of each grain and the combination of the adjacent grains are varied, and the dependency of the crystallographic conditions on the change in microstructure is discussed.

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