Features of Nucleation and Evolution of Defect Structure in Vanadium under Constrained Deformation

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ABSTRACT

The onset and evolution of plastic deformation on a microscopic level determines the deformation behavior of materials at higher scale levels. In view of the smallness of the spatial and temporal scales of the processes computer simulation is a powerful tool for studying the dynamics of structural transformations at the micro level. It should be noted that some of the grains in the bulk can be in the constrained conditions during the deformation of polycrystalline materials that affect their mechanical response under load. In this connection this work is devoted to the study of the vanadium crystallite behavior under constrained deformation. The calculations were based on the molecular dynamics method. The interatomic interaction was described in the Finnis-Sinclair approximation. The initial vanadium crystallite had a parallelepiped shape and was heated to the room temperature. To simulate the constrained deformation the crystallite was uniformly stretched in one direction and compressed in other two directions without changing its volume. The crystallite was stretched along one of following crystallographic directions: $[11\bar{2}]$, [111] and $[1\bar{1}0]$. It has been found that the threshold deformation at which the plastic deformation occurs is different for these directions. Loading of the crystallite leads to nucleation and growth of twins, which is accompanied by the generation of 1/2<111> dislocations and considerably lower number of <100> dislocations. The formation of twins leads to the fragmentation of the crystallite. When the crystallite is stretched along the $[11\bar{2}]$ direction a large twin is formed, while stretching along the [111] and $[1\bar{1}0]$ directions leads to the formation of a large number of grains.

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