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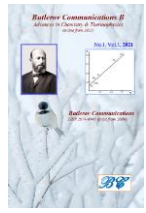

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Molecular dynamic modeling of mechanical deformation of iron upon application of an external magnetic field

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Abstract

Despite the fact that for several decades the processes of artificial aging under the influence of an external magnetic field have been carefully studied by many researchers, the interest in studying these processes does not weaken both among practitioners and theorists, specialists in the field of phase transformations. The influence of an external magnetic field on the aging processes of diamagnetic metal alloys, called a magnetoplastic effect, has been experimentally established. However, there is still no complete theoretical model for this phenomenon. In this regard, it is important to simulate aging processes when a magnetic field is applied. Interest in this topic does not fade, firstly, due to the lack of a general physical theory explaining these processes and due to the complexity of the nature of this phenomenon, and secondly, due to the large number of alloys in which the magnetoplastic effect is detected. However, there is still no theoretical model for this phenomenon. In this regard, it is important to simulate the aging process when a magnetic field is applied. The magnetoplastic effect is most fully studied in copper alloys. The method of molecular dynamics used in this work, the potentials of interatomic interaction, and the consideration of the magnetic field as an expression for the Hamiltonian of N interacting spins on a fixed lattice are described. Due to the fact that at present, when modeling by molecular dynamics methods, it is possible to take into account the influence of the magnetic field only for ferromagnets, the copper-iron system was chosen for modeling, which is characteristic of a large number of experimentally studied alloys. The magnetoplastic effect has been studied most extensively in copper alloys. Since the influence of the magnetic field can be taken into account only for ferromagnets by modeling using current molecular dynamics methods, the copper-iron system, which is characteristic for a number of experimentally studied alloys, was chosen. A numerical experiment of tensile deformation under application of an external magnetic field has been carried out. The results revealed that

an increase of the magnetic field induction leads to a decrease of the dislocation density under certain conditions.

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