Features of interface formation in crystallites under mechanically activated diffusion. A molecular dynamics study.

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ABSTRACT

Mechanical acceleration technology is widely used in modern science and industry to improve the efficiency of chemical reactions and physical and mechanical processes under conditions of combining of normal pressure and shear strain. An example of practical application of the acceleration effect of diffusion processes due to mechanical activation is the technology of friction stir welding (FSW). FSW is a relatively new method of obtaining permanent joint of material due to the acceleration of diffusion and mechanical mixing of materials in the weld area. Note that since mechanoactivated processes are inseparably linked with the intensive formation of discontinuities, generation of structural defects, mass transfer, the most preferred is the use of the method of discrete description of the simulated environment. The aim of paper is to analize of atomic mechanisms that occur as the result of mechanoactivated diffusion processes using of molecular dynamics simulation.

In this paper we carried out investigation of behavior of the material under loading condition identical those used in FSW. The loading was modelled by a rigid rotating "tool" that movies along boundary between two grains. Additionally an oscillation of the tool was modeled. We analyze the influence of speed and shape of the tool and direction of the additional vibration impact on the structure of the weld. We considered pairing of two crystallites of copper, crystallites of copper and iron, and two crystallites of aluminum 2024. Analysis of the structure of the sample showed the intermixing and stirring of dissimilar atoms as a result the FSW tool pass at the inter-crystallite boundary. It was shown, that under certain condition of loading when tool passes there a region where atoms can occupying the original position of the crystal lattice. We also show influence of an additional oscillating impact applied to the moving tool on the structure of the resulting weld.

In spite of the fundamental differences in characteristic spatial and temporal parameters, computer simulation results are in good qualitative agreement with those of experimental studies. Computer model may be a test bed serving for better understanding the basic laws of structural inhomogeneitiy origin in FSW. The simulation results obtained can be those of practical importance. They allow discovering new ways and mechanisms to obtain non-equilibrium states in the crystal lattice due to the initiation of the mechanically activated metal interdiffusion at the atomic level.