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A Molecular Dynamics Approach for Predicting the Glass Transition in pores

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Molecular dynamics study of the glass transition process in metallic glasses is performed. As an example, the liquid aluminum film is taken. The embedded atom method potential is used at the simulation of isobaric cooling [1]. There is a number of glass transition criteria: the decrease of the specific heat of material (calorimetric criterion) [2], the splitting of the second peak of the pair correlation function and the icosahedral short-range order (structural glass transition criteria) [3], the change of diffusivity behavior (dynamic criterion). However, the difference between the calorimetric glass transition temperature and the temperature, obtained using the structural and dynamic criteria might reach several hundred kelvins [4]. In the current work we obtain the glass transition temperature using two methods based on the shear stress correlations behavior. The first method is based on the stress correlations in the plane of the film and the steep change of the kinematic viscosity, obtained using Green-Kubo formula. The second method is based on the transverse oscillations in the film. The glass transition temperature is estimated from the temperature dependence of the oscillation damping of the stress correlation functions. The increasing in the kinematic viscosity correlates with the decrease of transverse oscillations damping in the film [5]. The obtained glass transition temperature agrees with the calorimetric temperature. Also, the temperature when the system becomes non-equilibrium is estimated, which is also in a good agreement with the obtained results.
The new methods of obtaining the glass transition temperature are validated on a metallic melt which is in contact with the walls. As an example, the Al-Fe alloy between titanium walls is taken. The embedded atom method potential is used to simulate titanium-aluminum systems, the Finnis-Sinclair embedded atom method potential is used for describing the interaction between Al and Fe. The interaction between Ti atoms is described by the Modified Embedded Atom Method potential. The alloy is cooled by changing the walls temperature. The glass transition temperature is obtained using the glass transition criterion based on the transversal sound propagation. Also, the viscosity behavior is considered. The dependence of the glass transition temperature on the pore size is obtained.
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