Evaluation of the glass-forming ability of alloys by molecular dynamics simulations

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In this work the molecular dynamics simulation was used in order to evaluate the glass-forming ability of alloys. There is a very well known correlation between the fragility index of a liquid, m, and its glass-forming ability upon cooling. The fragility index indicates the viscosity behaviour as a function of the temperature around the glass transition, i.e, when the viscosity of different liquids converges to 10^{12} Pa.s. The same convergence is observed at high temperatures when the viscosity approaches 10^{-5} Pa.s, which makes possible the definition of a second fragility index, n, directly correlated with the previous one, m. Since the molecular dynamics can be applied only to simulate materials in very short periods of time the viscosity can be calculated at high temperatures where the relaxation time is also very short. It makes possible the calculation of the fragility index, n, and the comparison of different alloys in order to score their glass-forming ability. For such an attempt the classical molecular dynamics was adopted with the LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) software. The EAM (Embedded Atom Model) was used to describe the interatomic energy potentials. An orthogonal simulation box was used with around 250,000 atoms and different alloy compositions. The initial temperature was far above the melting temperature in the NVT ensemble and the system was stabilized for 10 ps. After that the system was stabilized with the NPT ensemble, pressure around zero and the desired temperature for 10 ps. The final stabilization was performed with the NVE ensemble for 10 ps. The viscosity calculation followed a reverse non-equilibrium approach according to the Müller-Plathe algorithm which was applied for 150 ps. The resulting fragility index was thus compared with the experimental glass-forming ability of the alloys reported by the literature.