Molecular dynamics study of the glass transition temperature and elastic properties of the Zr–Nb amorphous alloy

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For the Zr–Nb alloy the crystalline phase has been well studied. For the amorphous phase, a detailed study of the structure and structural criteria of glass transition [1] was previously carried out, but the non-structural criteria and elastic properties remained unstudied.

The study was carried out using the molecular dynamics (MD) method with ADP-potential [2]. The calculations were carried out for Nb percentages ranging from 25 to 75 percent and a cooling rate of 11 K/ps. The glass transition temperature for different percentages of Nb was determined by varying the dependences of viscosity, heat capacity and diffusion coefficients on temperature. The data obtained are in good agreement with each other. The elastic properties of amorphous Zr–Nb were also investigated. Young's modulus for different percentages of Nb was determined. It is shown that the modulus of elasticity increases with decreasing free space in the structure, which is consistent with the assumed deformation mechanism of amorphous alloys. The presence of pressure hysteresis under compression and reverse tension, as well as its dependence on the percentage of Nb content is also consistent with the assumed deformation mechanism of amorphous alloys.

[1] Kliavinek S and Kolotova L 2020 *Journal of Experimental and Theoretical Physics* **131** 284–297

[2] Smirnova D and Starikov S 2017 *Computational Materials Science* **129** 259–272