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Concept of a Bond in Metallic Glasses. Bond's Lifetime in a Supercooled Liquid. MD Modeling. VALENTIN A. LEVASHOV, TAKESHI EGAMI, University of Tennessee, Knoxville, TN 37996, RACHEL S. AGA, JAMES R. MORRIS, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6115 — We have done constant volume MD simulations of a one component system of particles interacting via modified Johnson pair potential previously developed for iron. Negative curvature of the potential at the distances beyond potential minimum leads to the clear differentiation between the first and second nearest neighbors observed in the pair distribution function. Therefore a concept of a bond could be introduced. We studied the distribution of bond lifetimes in a liquid state. At high temperatures probability to find a long living bond is very small. As temperature decreases there appear bonds whose lifetime is very long. At the same time, the number of bonds whose lifetime is relatively small remains significant. This could be considered as an indication of the separation of the system into solid-like and liquid-like regions. Obtained bond lifetime distributions will be analyzed from this point of view of the presence in supercooled liquids different kinetic regimes at different temperatures.

Valentin A. Levashov
University of Tennessee, Knoxville, TN 37996

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