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Relaxational Dynamics of a Model Glass-forming Metallic Liquid
ABHISHEK JAISWAL, Univ of Illinois - Urbana, STEPHANIE O'KEEFFE, Liquidmetal Technologies, ANDREY PODLESNYAK, GEORG EHLERS, REBECCA MILLS, Oak Ridge National Laboratory, KONSTANTIN LOKSHIN, WOJCIECH DMOWSKI, TAKESHI EGAMI, Univ of Tennessee - Knoxville, YANG ZHANG, Univ of Illinois - Urbana — Understanding the diffusional behavior of multicomponent glass-forming metallic liquids is of critical importance to the development of novel alloy systems such as bulk metallic glasses (BMG). However, such diffusions are highly activated and complicated because of structural disorder induced by quenching, and chemical disorders induced by size mismatch. Herein, we report temperature and wave-vector transfer (Q) dependence of two-step collective relaxations in the BMG (LM601: ZrCuNiAl) melt measured by quasi-elastic neutron scattering. Q-dependence of both fast and slow relaxation time, and the adiabatic sound speed are found to obey the principle of de Gennes narrowing. The measured spectra show a distinct vibrational mode at around 15 meV. Classical Molecular Dynamics (MD) simulation of CuZrAl system, using EAM potential shows that this acoustic mode arises from local vibrations of Al in the cage formed by Cu and Zr atoms. Furthermore, we observed a breakdown of Stokes-Einstein relation in the MD simulated system well above its melting temperature. Accompanied dynamical clustering was detected using unsupervised machine learning techniques. These mechanisms in tandem can be responsible for the excellent glass-forming ability of this material.

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