7. Dynamical and structural heterogeneities near liquid-liquid phase transitions: The case of gallium

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Recently, it was found through molecular dynamics simulations that liquid elemental gallium, described by a modified embedded-atom model, exhibits a liquid-liquid phase transition (LLPT) in the supercooled regime, between a high-density liquid (HDL) and a low-density liquid (LDL), about 60 K below the melting temperature [D. A. C. Jara, et al., J. Chem. Phys. 130, 221101 (2009)]. In this work, we studied the dynamics of supercooled liquid gallium near the LLPT. Our results show a large increase in the plateau of the self-intermediate scattering function (beta-relaxation process) and in the non-Gaussian parameter, indicating a pronounced dynamical heterogeneity upon the onset of the LLPT. The dynamical heterogeneity of the LDL is closely correlated to the structural one, since the fast diffusing atoms belong to high-density domains of predominantly 9-fold coordinated atoms, whereas the slow diffusing ones are mostly in low-density domains of 8-fold coordinated atoms. The energetics suggests that the reason for the sluggish dynamics of LDL is due to its larger cohesive energy as compared to that of the HDL. Work in collaboration with Samuel Cajahuaringa and Maurice de Koning. Published in J. Chem. Phys. 136, 064513 (2012).
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