Abstract Submitted
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Super-localization of atomic dynamics in liquid Iron[1] MADHUSUDAN OJHA, DAVID J. KEFFER, The University of Tennessee, DON M. NICHOLSON, Oak Ridge National Laboratory, TAKESHI EGAMI, The University of Tennessee and Oak Ridge National Laboratory — Lattice dynamics in crystals is well described in terms of phonons. However, phonons cannot give precise description of the atomic dynamics in liquids because they are highly damped. We carried out MD simulations of liquid iron at high temperatures. The results are presented in terms of the dynamic pair-density function (DPDF), which describes the atomic correlation, or the distribution of atomic distances over time, at the angular frequency ω. Our analysis shows that the atomic dynamics in liquid iron above the boson mode (BM) is confined to only the nearest neighbors, resulting in super-localization of atomic dynamics. The dynamics of nearest neighbor shells is well described in terms of atomic level stresses. This super-localization of atomic dynamics in liquid iron implies that the dynamics of the local atomic level stresses represents the normal modes in liquids at high temperatures, and justifies the equipartition law observed for the atomic level stresses [1].

[1] V. Levashov, et al. Phys. Rev. B 78,064205 (2008)

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