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Abstract

Structural Transformation in Liquid Tellurium from Stillinger–Weber Potential †

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Abstract: Structural evolutions in liquid tellurium (Te) are observed by employing molecular dynamics simulations at various temperatures ranging from 1500 K to 300 K. Local structural variations are noticed in radial correlation functions, structure factors, bond angle distribution functions, Honeycutt–Anderson index, Voronoi tessellation, and coordination numbers. Upon quenching, we found that icosahedral short-range motifs dominated in a stable and supercooled liquid state. The first peak of the radial distribution function at 970 K and 722 K is in excellent agreement with the findings of neutron diffraction. The transformation to a supercooled liquid state with distorted icosahedral patterns is observed at 600 K and to a body-centered cubic cluster after 600 K. Finally, we also show that near the melting point diffusion coefficient of liquid tellurium is fairly consistent with the tight-binding and experimental models. We assume that our findings not only replicate all the remarkable characteristics but also predict useful transition mechanisms through the use of the well-known Stillinger–Weber potential.

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