Structural Transformation in Liquid Tellurium from Stillinger-Weber Potential

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Structural evolutions in liquid tellurium (Te) are observed employing molecular dynamics simulations at various temperatures ranging from 1500 K to 300 K. Local structural variations are noticed in radial correlation functions, structure factor, bond angle distribution functions, Honeycutt-Anderson index, Voronoi tessellation, and coordination number. Upon quenching, we find that icosahedral short-range motifs dominate in a stable and supercooled liquid state. The first peak of the radial distribution function at 970 K and 722 K shows excellent agreement with the findings of neutron diffraction. The transformation to a super-cooled liquid state with distorted icosahedral patterns is observed at 600 K and to a body-centred 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 purposed models. We assume that our findings not only replicate all the remarkable characteristic but also predict useful transition mechanisms through the use of the well-known Stillinger-Weber potential.

Introduction

Crystallization is the approach of phase transition from liquid or gas to the solid, which consist of an arrangement of atoms. Frank was the first to conjecture in a supercooled state local structure of pure melt elements contains icosahedral short-range order (ISRO), which is conflicting with a long-range order of periodicity. In current years, considerable development has been completed theoretically and experimentally to apprehend the atomic shape of metallic melts. The metallic melt elements solidification may support the emergence of a metastable crystal structure in the non-equilibrium state of thermodynamics. Neutron and X-ray diffraction, various emission and absorption spectroscopies and scattering measurements were used to examine the deformed or disordered phases of Te. In addition, experimentally it has been argued that presence of short range and long range distance responsible for the phase transition in a liquid Te near the melting point (722 K), although, the accurate measurements at high temperature would be needed to explore the temperature dependence on structural evolution. Also, the experimental technique only provides a qualitative picture beyond the pair correlation function. For the first time, we investigated structural evolution by using the pair-correlation function, coordination number, bond angle distribution function, structure factor, Honeycutt-Anderson index, and Voronoi tessellation analysis of liquid Tellurium.

Results

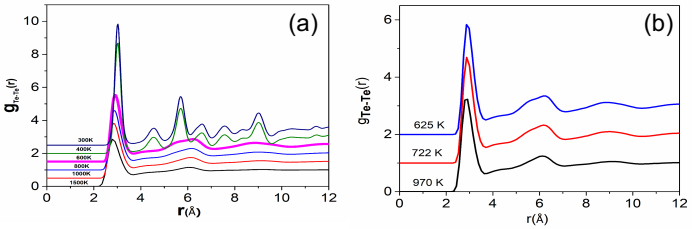

Fig.1 (a,b)Radial distribution function of liquid tellurium (Te) during solidification process.

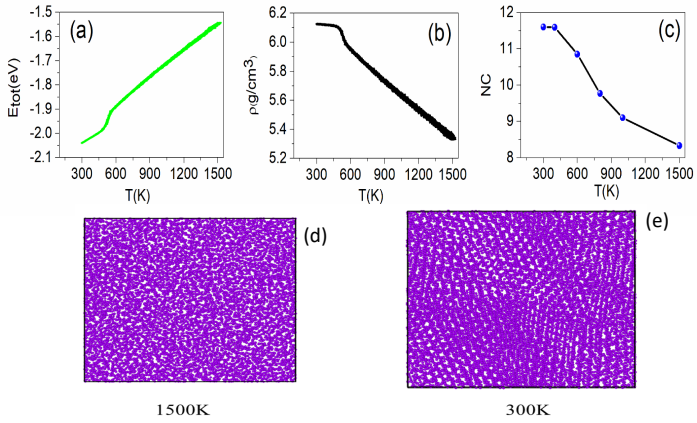

Fig.2 (a) Total energy per atom, (b) density, (c) coordination number (N_C), (d) structure of liquid tellurium (Te) at 1500 K, and (e) 300 K during solidification process at distinct temperatures

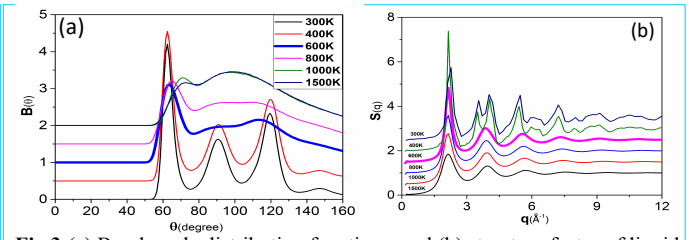

Fig.3 (a) Bond-angle distribution functions, and (b) structure factor of liquid tellurium (Te) at distinct temperatures.

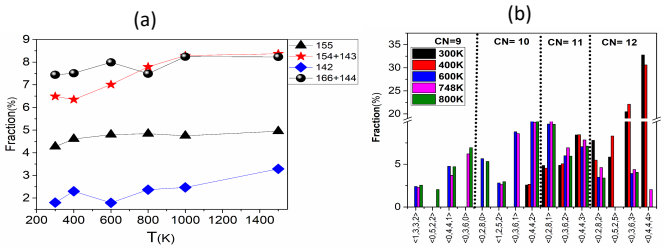

Fig.4 (a) Fractions percent of pair analysis, and (b) top voronoi-index clusters of liquid tellurium (Te) at distinct temperatures during the solidification process.

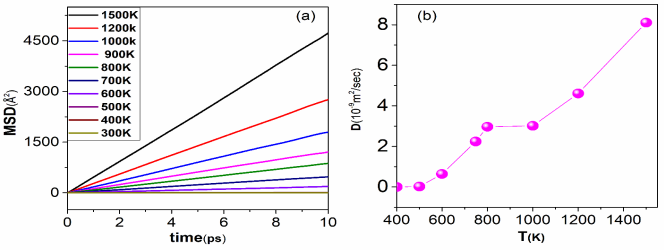

Fig.5 (a) The mean square displacement (MSD) with time dependence, and (b) variation of the self-diffusion coefficient at distinct temperatures during the cooling process.

Conclusions

By using well known Stillinger-Weber potential we investigated the structural and dynamic evolution of Te during the solidification process. The pair correlation functions, coordination number, structure factor, bond angle distribution function, HA analysis, and Voronoi tessellation were used to explore the structural properties of liquid tellurium at various temperatures. It is observed that the fivefold icosahedral symmetry influence the local atomic structure of stable liquid and super-cooled liquid tellurium. The liquid-crystal phase transition observes after 600 K, and super-cooled liquid tellurium transformed into icosahedral, distorted icosahedral and body-centered cubic like clusters. The calculated self-diffusion coefficient also shows good agreement at 743 K with the experimental and empirical tight-binding Hamiltonian model. In our conjecture whole evaluation presents a fairly and illuminating perspective of the behavior of the liquid tellurium.