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Molecular Dynamics Simulations of Ti Crystallization with Solid–Liquid Configuration Method

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The computation models were created with the solid–liquid configuration method. The molecular dynamics simulations were performed to exhibit the crystallization process of liquid pure Ti to hexagonal close packed (HCP) and face-centered cubic (FCC) structure crystals. The results showed that both HCP and FCC crystallizations start from the solid-liquid interfaces and develop toward the middle. The system energy sharply falls at the beginning of crystallization, then is reduced slowly, and finally has a sudden down jump at the end of crystallization. The first peak of RDF is increased significantly with time and some new secondary peaks occur, which is consistent with configuration evolution. The HCP crystal has a longer crystallization process but lower stable energy than the FCC crystal.

Keywords: Ti crystallization, solid?liquid configuration method, molecular dynamics simulation.