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Structural evolution during crystallization of supercooled niobium: *ab initio* molecular dynamics simulations TEKALIGN T. DEBELA, H.Y. LU, X.D. WANG, P.Q. CAO, International Center for New-Structured Materials (ICNSM), Department of Materials Science and Engineering, Zhejiang University, D.X. ZHANG, State Key Laboratory of Modern Optical Instrumentation, Zhejiang University, J.Z. JIANG, International Center for New-Structured Materials (ICNSM), Department of Materials Science and Engineering, Zhejiang University
— We report on *ab initio* molecular dynamics simulations study of crystallization in metallic niobium supercooled liquid. Using various structural analysis methods including bond orientational order analysis, a scheme of crystallization process is revealed. Various locally favored clusters act as precursors for nucleation. Our findings reveal that crystallization is not primarily due to density fluctuations; rather it is caused by development of extended structured regions of high orientational order which gradually solidify. This crystallization behavior is consistent with that recently reported for hard sphere (colloidal) as well as soft sphere (Gaussian core model) systems.

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