A molecular dynamics study on intermediate structures during transition from amorphous to crystalline state

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Molecular dynamics (MD) simulations are carried out for model aluminium with 500, 864, 1372 and 2048 atoms interacting with Sutton-Chen version of embedded atom method (SCEAM) based on many body interactions. The systems equilibrated in an FCC structure have, first, been melted and then solidified with specifically selected single cooling rate which forms unstable amorphous state in the system. The local structures of the system have been analysed by bond orientational order parameters to distinguish the simple structures in the systems. The radial distribution functions (RDF) and atomic coordinates have also been analysed for determining the local structural properties. It has been observed that the phase sequences of the systems, except for those of the 2048 atoms, are FCC ! Liquid ! Amorphous ! Mixed Crystal. Types of the crystals in the mixed state depend on the number of the atoms in the system. The final phase of the system with 2048 atoms is amorphous state.

Keywords: Molecular dynamics; Embedded atom method; Solidification; Local order