Cluster Mechanism of Homogeneous Crystallization (Computer Study)

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The molecular dynamics (MD) study of homogeneous crystallization of liquid rubidium is conducted with pair inter-particle potential (D. Price et al). The equilibrium crystallization temperature of the models was 313 K. Models consisted of 500, 998 and 1968 particles in basic cube. The main investigation method was as follows: to detect (along the MD run) the atoms with Voronoi polyhedra of 0608 type ("0608-atoms", as in BCC crystal) and to detect the bound groups of 0608-atoms ("0608-clusters") that could play the role of the seeds in crystallization. The full crystallization was observed only at the temperatures lower than 185 K with the creation of predominant BCC crystal.

The crystallization mechanism of Rb models differs drastically from the mechanism adopted in the classical nucleation theory. It consists of the growing of the total number of 0608-atoms at cooling and in forming the 0608-clusters analogously to the case of coagulation of solute from supersaturated two-component solution [1]. At the first stage of the process the clusters have very loose structure (something like medusa or octopus with many tentacles) and include inside atoms with other Voronoi polyhedron types. Linear size of clusters quickly enhances and approaches the size of basic cube. 0608-atoms play the leading role in the crystallization process and activate the transition of included atoms in 0608-coordination. The fast growth of maximum cluster begins after its mounting to critical size (about 150 0608-atoms). The fluctuations of cluster sizes are very important in the creation of 0608-cluster of critical (threshold) size. These fluctuations are especially great in the interval 180-185 K.

[1] D.K. Belashchenko and E.S. Lobanov, *Russ. J. Phys. Chem.* (2005).