Once again about special properties of prenucleation clusters

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More or less coherent pattern of crystal formation, created over more than 100 years, has recently been revised in its fundamentals. Various recent models of nonclassical nucleation and growth of crystals [1–4] particularly suggested existence of stable prenucleation clusters. The phenomenon of formation of such clusters is easily explained even within the formalism of derivation of basic equations of the classical theory of nucleation, if we take into account the dependence of specific surface energy on size, characteristic of nanoscale particles. The obtained formulas imply possible formation and stable existence of prenucleation clusters absent in the classical theory. The size of such clusters is from δ to 4δ, where δ corresponds to the diameter of cluster-forming atoms. The lower boundary is related to the transition of the system through equilibrium, and the upper one is determined from the condition of their nonactivation formation.

The prenucleation clusters are not ordinary energy- and geometry-optimized particles. The dynamism of the structure, its fluctuating external form and surface, the oscillating nature of bonds between atoms, the relatively high proportion of surface atoms, and the impossibility of neglecting quantum effects in their behavior and a number of other unusual properties make the prenucleation clusters unique structures, a special form of structural organization of matter at the nanolevel. Such clusters retain for a long time the ability not to “fall” into the global energy minimum with fixed bonds. The arrangement of atoms is uncertain until the chemical bonds between them are completely built. After that, the characteristic structurelessness disappears, and they are transformed into other forms of nanoparticles, including crystalline nuclei.

Besides the prenucleation clusters are particularly main building units for crystal growth [4], not separate atoms (molecules, ions) and not crystalline particles, as is generally suggested.

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References

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