



## **Indirect estimation of structural nanoheterogeneity of crystal-forming media (melts)**

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Many experimental data testifying of ultramicroheterogeneous structure (nanoheterogeneity) of crystal-forming media has been accumulated by this time [1]. Numerous attempts of theoretical substantiation of existence in supersaturated (overcooled) medium of differently structured atomic-molecular formations named differently-associates, clusters etc. are also widely known. In particular, formation in crystal-forming media of specific nanoclusters of “hidden phase” (quatarons) is the key idea of the concept of cluster self-organization of matter at nanolevel in nonequilibrium conditions, developed by us [2]. However the question on whether there is any connection between structured of medium and such a fundamental its characteristic as surface tension (specific surface energy) was not discussed yet.

In this work we propose a simple way of determination of the first correction to surface energy (tension) on curvature of interphase boundary, on this basis an attempt on the solution of the problem of connection of the crystal – forming media structure with values of their surface energy is undertaken. The question theory is given in our earlier published work [3].

As a result we obtained the data that evidence of nanoheterogeneity of crystal-forming media even near to equilibrium. According to the calculations made under the obtained formulas with use of known values of surface tension of melts, the quataron structures characterizing structural nanoheterogeneity of crystal-forming media, close to melting temperature represent cluster formation consisting of small number of atoms. In geometrical interpretation, despite the non – rigid structure and oscillating character of bonds between atoms, the quatarons in most cases can be characterized in terms of simple polyhedrons – from an octahedron with number of surface atoms  $n=6$  to truncated icosahedrons ( $n=60$ ).

It is also obvious that these areas of structural nanoheterogeneity in melt can be considered as an area of short-range order.

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1. D. Gebauer, H. Coffen. *Nano Today*, 2011. 6. P. 564-584.

2. A.M. Askhabov. Cluster (quataron) self-organization of matter at nanolevel and formation of crystalline and non-crystalline materials // *Zapiski Russian Mineralogical Society*, 2004. 4. P. 108-123 (in Russian).

3. A.M. Askhabov. Surface Energy and Structural Heterogeneity of Crystal-Forming Media // *Doklady Earth Sciences*, 2011. 436.1. P. 73-75.