Structural nanoheterogeneity of melts and their surface tension

ASKHABOV, A. M.

Institute of Geology of Komi SC UB RAS, Syktyvkar, Russia
xmin@geo.komisc.ru

Many experimental and theoretical data testifying of ultramicroheterogeneous structure (nanohenerogeneity) of crystal-forming media has been accumulated by this time [1] [2]. 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. This problem is discussed in presented work. 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 formations consisting of a 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 icosahedron (n=60). It is also obvious that these areas of structural nanoheterogeneity in melt can be considered as an area of short-range order.

The work is done with support of Scientific School-4795.2014.5 and RFBR № 14-05-90403.

[1] D. Gebauer, H. Cöffen. Nano Today, 2011, N 6, pp. 564–584. [2] Askhabov A.M. Zapiski Russian Mineralogical Society, 2004. № 4, pp. 108–123. (in Russian). [3] Askhabov A.M. Doklady Earth Sciences, 2011. Vol. 436. P.1. pp. 73-75.