Quasi-stable structures in liquid antimony: DFT analysis

A.A. Tsygankov[1,2], B.N. Galimzyanov[1,2], A.V. Mokshin[1,2]

[1] Kazan Federal University, Institute of Physics, Kazan, Russia
[2] Udmurt Federal Research Center of the Ural Branch of the RAS, Izhevsk, Russia

Nuclear magnetic resonance method is frequently used for local structure analysis of liquids [1]. Liquids are often characterized by the presence of a homogeneous distribution of atoms at large distances and short-range order at small distances. However, liquid antimony is an unusual system due to its structure, which exhibits anomalies in the form of shoulders in the radial distribution function and static structure factor [2–4]. The reason for the existence of this anomaly is not yet fully understood [4, 5]. The precence of bonded structures was confirmed by various methods, in particular, with nuclear magnetic resonance. The radial distribution function is a characteristic of the probability of finding a particle at a certain distance from another particle. Therefore, we can conclude that this feature can only occur if atoms form at least quasi-stable structures [5–7]. To reproduce the structural features of liquid antimony, ab-initio molecular dynamics simulations were performed in the VASP package [8] using density functional theory (DFT) methods at temperature T = 923 K and pressure P = 1.0 atm.

To determine the possibility of the existence of stable structures in liquid antimony, the distribution of particles by neighbourhood times was calculated from the obtained results of ab-initio molecular dynamics simulations. In the framework of the Williams-Landel-Ferry model, it was shown that in the regions bounded by a sphere of radius 5 Å there are stable formations with a lifetime greater than 1.6 ps [9]. In order to identify such structures, the order parameters q_4 and q_6 were estimated and the structures were characterized. The results demonstrated the formation of triangular structures with lengths a = 3.07 Å, b = 4.7 Å and angles α = 45° and β = 90° in liquid antimony (Fig. 1). Furthermore, the quasi-stable formations were observed to exert a

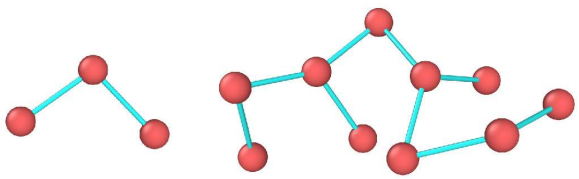

Fig. 1. Example of triangular structure and chain formed by antimony atoms.

direct influence on the presence of a shoulder in the radial distribution function and the static structure factor.

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