Structural properties of liquid carbon: Atomistic modeling

Dereka S A[1,2,@] **and Orekhov N D**[1,2,3]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[3] Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia

[@] st.dereka@gmail.com

Experimental data on the melting curve of graphite and thermodynamic properties of liquid carbon remain controversial despite the long history of investigation [1]. The results of several dozen experimental works cover the wide span from 3800 to 5000 K for the graphite melting temperature that is essentially larger uncertainty than the errors of individual experiments. Liquid carbon remains the source of several unsolved questions related to its structure, pressure–temperature regions of stability, and the possibility of the existence of liquid–liquid phase transitions. Extending our previous results on the melting kinetics and parameters of graphite melting line [2], we study properties of liquid carbon on the basis of molecular dynamics with machine learning-based Gaussian approximation potential (GAP) for carbon [3] and density functional theory (DFT). The properties (such as density and atom hybridization proportions) modeled with GAP-20 are in excellent agreement with DFT data. The structural properties and atom hybridization for liquid carbon at $T = 5000$–6000 K and $P = 1$–3 GPa are calculated. We demonstrate that in the given range of temperature and pressure the majority of atoms are sp-hybridized and form one-dimensional chains.

[1] Savvatimskiy A 2005 *Carbon* **43** 1115–1142
[2] Orekhov N and Stegailov V 2015 *Carbon* **87** 358–364
[3] Deringer V L and Csányi G 2017 *Phys. Rev. B* **95** 094203