Structural properties and heat capacity of liquid carbon: Molecular dynamics with machine learning

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The list of unresolved issues related to the structural properties and the thermodynamic stability limits of the liquid phase of carbon still remains quite extensive. In particular, the nature of the sharp, almost twofold, drop in density at pressures $P < 3$ GPa is not completely clear [1]. In addition, the value of the heat capacity of liquid carbon, which systematically exceeds $3R$, has not found an unambiguous interpretation [2]. In this work, using the classical molecular dynamics with the machine-learning potential of GAP-20 [3], we study the behavior of carbon in the range of temperatures $T = 5$ to 6.5 kK and pressures $P = 0.5$ to 4 GPa. We show that a decrease in density in the region of lower pressures, in addition to the known change in hybridization from sp^2 to sp, is accompanied by the appearance of nanosized pores. The low-density liquid phase resembles a three-dimensional network consisting of linear sp-hybridized chains and is highly compressible. The energy spent on the rearrangement of covalent bonds and the change in hybridization during expansion can explain the magnitude of the experimentally observed heat capacity values.

[1] Savvatimskiy A I 2008 *J. Phys.: Condens. Matter* **20** 114112
[2] Kondratyev A M and Rakhel A D 2019 *Phys. Rev. Lett.* **122** 175702
[3] Orekhov N and Logunov M 2022 *Carbon* **192** 179–186