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Graphite melting: atomistic kinetics bridges theory and experiment NIKITA OREKHOV, Moscow Institute of Physics and Technology, VLADIMIR STEGAILOV, Joint Institute for High Temperatures of the Russian Academy of Sciences (JIHT RAS) — Unique thermophysical properties of graphite result in its important role in science and engineering. However, the experimental data on graphite melting temperature (T_m) still remain controversial despite the long history of investigation. The experimental results of several works cover the wide span from 3800 to 5000 K that is an essentially larger uncertainty than the errors of individual experiments. In this work we deploy the molecular dynamics (MD) method and study the kinetics of graphite melting, concerning the aspects of defect formation, single graphene layer melting and the rates of spontaneous liquid nuclei formation. Our MD calculations show an unexpectedly weak kinetics of the melting front propagation in graphite that is several orders slower than that in metals. We demonstrate that at sufficiently high heating rates (higher than $10^5 - 10^6$ K/s) the temperatures 500-1000 K above the graphite melting temperature can be reached before the crystal decay. It allows us to explain long-standing problem of the discrepancy in the experimental data making a hypothesis that there is a strong dependence between experimentally measured graphite melting temperatures and corresponding rates of heating.

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