Two-phase molecular dynamic modeling of graphite melting

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For many years the graphite melting curve has been the object of essential debates due to large discrepancies in experimental data. We report here the two-phase molecular dynamic simulations of graphite melting with the semiempirical bond-order potential AIREBO. In the pressure range up to 14 GPa the graphite melting line is obtained and properties of liquid carbon are investigated. For the superheated graphite the melting front velocity dependencies on temperature are calculated to verify the melting temperatures values. The influence of the defect formation in superheated crystal on melting process is considered. Different melting regimes are revealed. The results provide a possible way to resolve the long-standing question for the reasons of large discrepancies in experimental data.