Structure of amorphous carbon experimentally quenched from the liquid state: Multiscale simulations

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The structure of amorphous carbon (a-C) experimentally quenched from the liquid state on a cold diamond substrate is numerically reproduced using a multiscale approach. At the macroscopic level, we solve the time-dependent heat conduction equation for experimental samples of actual size. As a result, we determine the distribution of the quenching rate, which varies with the distance from the substrate within 10^{14}–10^{12} K/s. At the microscopic level, we perform molecular dynamic simulation of the liquid carbon quenching using the obtained quenching rates. The density of the model a-C samples increases from 1.5 to 1.93 g/cm^3 with the decreasing of quenching rate from 10^{14} to 10^{12} K/s.

The main structural characteristics of the model a-C samples are studied in detail: the relative number of carbon atoms with different hybridization (sp^1, sp^2, sp^3), radial distribution function, angular distribution function, and the statistical analysis of rings. The structure of model a-C samples, depending on the quenching rate, varies from that of amorphous graphene to a highly porous material with a large number of sp^1 chains. We discuss the mechanisms underlying the strong effect of the quenching rate on the structure of a-C.

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