Formation of carbon clusters in detonation products of high explosives

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Detonation products of a number of high explosives (TNT, RDX in composiotion with TNT, and others) contain a large amount of free carbon that releases in amorphous (soot) or crystal (graphite, diamond) phases. The process of carbon condensation behind the detonation front of carbon-rich high explosives is studied in the present work.

The molecular dynamics (MD) method was used for the numerical simulation of the free carbon aggregation in the detonation products (DP). The ensemble consisting of the two sorts of the particles (atoms) was studied. The particles of a sort C represented the atoms of the free carbon whereas the P-sort particles were the detonation products. The Lennard-Jones potentials (LJP) were used for describing the interactions between the atoms. The phase composition of the condensed carbon was not taken into account in the model.

Starting from the initial state with approximately homogeneous distribution of the carbon atoms in DP, the formation of carbon nanoparticles of the linear sizes from 10 to 50 atoms occurs in the substance. Then, the clusters of the nanoparticles are formed with the characteristic linear size about 10 particles. The subsequent dynamics depends on the initial concentration of the free carbon in the detonation products. If the carbon volume fraction is about 8 percents and higher then the clusters form the net spatial structures of mesoscopic sizes bridging the opposite sides of the simulation region. The aggregation is done with the formation of separated clusters if the carbon concentration is small.

Thus, condensation of carbon in the detonation products to clusters and spatial nets was simulated using molecular dynamics method. The result obtained is in satisfactory agreement with experimental measurements of electrical conductivities in the zone of the detonation of the DP of carbon-rich high explosives.