A PROBABLE MECHANISM OF FORMATION OF DETONATION NANODIAMONDS

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Abstract – In the given work we suggest a new mechanism of formation of nanodiamond crystallites during detonation synthesis. The basis of process is formation of nanodiamond nuclei – ionized adamantane molecules from a radical-like dimer C_2 in the plasma of a chemical reaction zone and further growth of the crystallites due to multiple attack of a growing nanodiamond particle by the dimer C_2.

A theory of the resulting in formation of detonation diamond particles (DND) has a discussion type up to now. Analysis of own and other authors' results on blasting of hydrogen-free benzotrifuroxane (BTF) and alloy of TNT/RDX composition (~50/50) allows to approach an understanding the mechanism of formation of DND step-by-step.

Decomposition of explosive molecules provides rather high concentration of «free» carbon in the time limited ($0{,}5 \cdot 10^{-6}$ sec) and volume limited chemical reaction zone (its extension – tens of micron). Density of the medium («plasma») is ~2,3 g/cm^3.

Bond breakage in TNT-molecule is accompanied by separation of a methyl-group to give an active methyl radical and, partially, nitro-group; by fragmentation of a benzene ring in the «plasma» of chemical peak to form radicals C_2, C, C_3, CN, CH_x, respective ions and hydrogen (Fig.1). Bond breakage in RDX-molecule goes along C-N-bonds to give also C_2, C, CN. Formation of C_2 is possible from C-radical as in RDX there are no C-C-bonds.

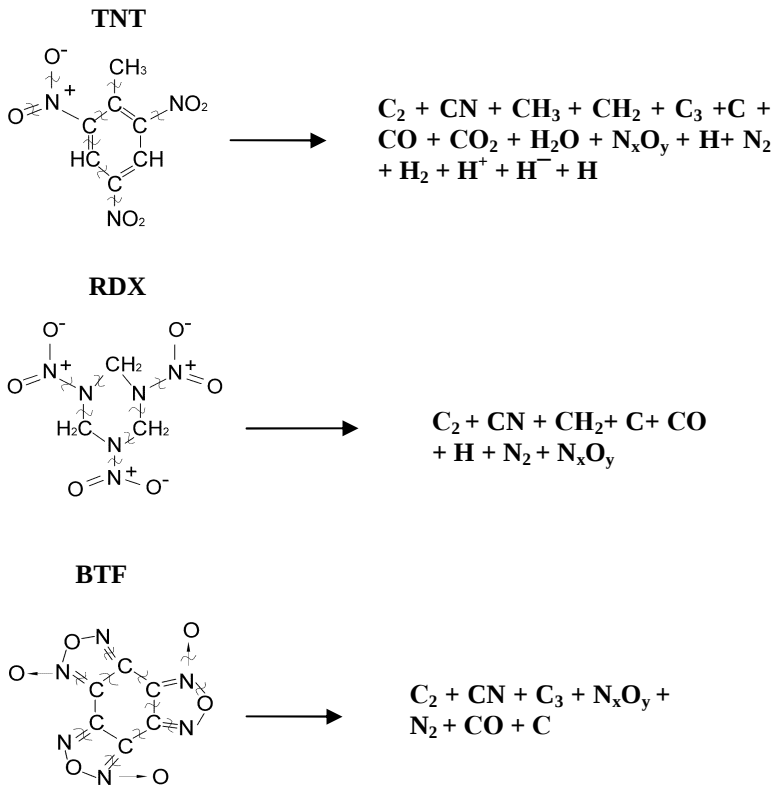

Figure 1 – A supposed disintegration of explosive molecules in the chemical reaction zone. DND are formed from ~95 wt.% carbon of TNT and ~5 wt.% carbon of RDX at detonation of TNT-RDX mixture

Decomposition of hydrogen-free BTF proceeds to yield C_2, C_3, CN, N_xO_y, CO.
Formation of primary fragments of the future nanodiamonds begins from the middle to the end of chemical reaction zone (to the Chapman-Jouguet plane) from carbon radicals. At that cyclohexane (more energy-profitable), not benzene ring is formed. Some drops of liquid carbon formed by liquid-

drop coalescence mechanism are amorphized at the first stage of expansion of gaseous detonation products.

A primary «block» is most likely a radical C_2 interring into chemical interaction with the same particles to form cyclohexane or at once adamantane molecules. Possible formation of adamantine in the chemical peak zone was first noted in [1]. Nitrogen gets to a DND-crystallite in the result of C-N-radical bonding.

An adamantane molecule consists of three cyclohexane fragments being in conformation «armchair». Spatial arrangement of carbon atoms in the adamantane molecule replicates arrangement of atoms in the diamond crystal lattice. An adamantane molecule has high symmetry and thermostability.

Growth of a DND-particle goes on the diffusion mechanism through chemical reactions proceedings on their surface at adsorption of free carbon and/or hydrocarbon radicals. During of diamond particle growing its surface is constantly covered with these radicals.

Growth of a DND-particle is stopped because of action of two factors: 1) defect accumulation of the structure when growing the particle and discontinuation of transition of sp^2–hybridized carbon into sp^3– hybridized «diamond» carbon; 2) depletion of carbon radicals.

So, in authors' opinion, one of the probable mechanisms of formation of detonation nanodiamond is possible enough: decomposition of explosives in the chemical reaction zone into radicals $C_2^{\bullet}$, formation of cyclohexane from $C_2^{\bullet}$ which is then isomerized into adamantane as a result of catalytic action of ionized aluminium; adamantane is a diamond-like nucleus of the future DND-particle. Further growth of nanodiamond arises from interaction with carbon radicals.

REFERENCES

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