Why are detonation nanodiamonds small

Dolmatov V.Yu.[1]*, Yurjev G.S.[2], Myllymäki V.[3], Vehanen A.[3]

[1]FGUP «SCTB «Technolog», 192076 Saint-Petersburg, Russia
[2] Institution of RAS Nikolaev Institute of Inorganic Chemistry SB RAS, 630090, Novosibirsk, Russia
[3]Carbodeon Ltd. Oy, Bulevardi 2 A, 00120 Helsinki, Finland
**e-mail: DiamondCentre@mail.ru*

It is known that the synthesis of detonation nanodiamonds (DND) is accompanied by the creation of non-diamond forms of carbon such as onion carbon, graphite and so on.

The authors have calculated distribution of atoms in natural diamonds and DND of the various sizes (3D model of spherical nanodiamonds computed through the representation of coordination spheres (CS)). Experimental XRD patterns from DNDs were registered with use of synchrotron radiation.

The calculations showed that in DND_1 manufactured in FGUP "SCTB "Technolog" (explosive charge in an aqueous solution) and in natural diamond the similarity on number of carbon atoms in CS is observed up to the 32nd CS (R_{CS}=28,69 Å, N_{atoms}=1386). The distinction begins with 33d CS and further: in DND_1 R_{CS}=29,75 Å, N_{atoms}=1504, and in natural diamond R_{CS} =29,52 Å, N_{atoms}=1648. Thus, the structure of DND_1 with respect to distribution of atoms on CS differs from the structure of natural diamond, i.e. existence of the shell of different phase is detected and its structure is distinct from that of natural diamond at the size exceeding R_{CS}=28,97 Å (d~5,8 nm).

In DND_2 synthesized by SPA "Altai", Biysk (gaseous explosive charge) distribution of atoms up to 44th CS has the same parameters as in structure of natural diamond with parameters R_{CS}=38,48 Å, N_{atoms}=2748. Since 45th CS (R_{CS} = 39,28 Å, N_{atoms}=2428) the parameters of CS of DND_2 differ from those for CS of natural diamond (R_{CS} =39,18 Å, N_{atoms}=2680), i.e. the structure does not meet diamond.

Thus, the core of detonation nanoparticle has CS parameters of diamond structure up to R_{CS} =39,28 Å (d=7,6 nm), the shell of a diamond core has thickness ~4,7 Å with parameters ranging from R_{CS} =38,48 Å up to R_{CS} =42,19 Å and does not correspond to diamond structure.

It is shown that the factor limiting growth of a diamond core in DND (≤ 8 nm) is the accumulation of crystal structure defects during growth of carbon nanoparticle in post-detonation processes. The accumulated defects take away carbon surface layers from diamond structure (where density is lesser than in diamond). In further these carbon layers can be removed by chemical treatment.

[1] G.S. Yurjev, V.Yu. Dolmatov. *J. Superhard Materials* **32**, 29 (2010).