The preservation of C hexagons in the transformation of C allotropes

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The high pressure transformation of graphite to diamond [1] involves the preservation of C hexagons in going from a 2D van der Waals layering, with a topology of (6, 3) [2] and at a density of 2.27 g/cm^3, see Figure 1, to the densest possible sphere packing of C in 3D as the diamond lattice, with a topology of (6, 4) [2] and at a density of 3.56 g/cm^3, see Figure 2. The transformation of nanotubes with a topology of ($5^{(x/(x+y))}$, 3) [2, 3]; an example of which is shown in Figure 3, to the hexagonite lattice with a topology of (6, $3^{2/5}$) [2, 3], as shown in Figure 4, also involves the preservation of C hexagons, in going from a van der Waals cylinder packing of nanotubes, which then collapses into the densest possible C cylinder packing in the hexagonite lattice (see Figure 4).

One could thus picture the nanotube powder in the open gasket of a diamond anvil cell (DAC), at an ambient density of about 1.75 g/cm^3, and if the nanotubes are aligned with their cylinder axes normal to the pressure axis of the DAC, they form a van der Waals cylinder packing of nanotubes structurally comprised of component C hexagons. Pressure could be applied and the nanotubes would then eventually make physical contact with each other, and this would comprise a closest cylinder packing of nanotubes, but not the densest possible cylinder packing of C.

Evidently, at a pressure of about 1 Mbar [3], the densest possible nanotube cyclinder packing, collapses into the densest possible C cylinder packing, as the hexagonite lattice is created in the form of nanocrystals with a density of 2.45 g/cm^3, see Figure 4. Therefore, the transformation of powdered nanotubes to nanocrystalline hexagonite [3], is perfectly analogous to the transformation of graphite into diamond [1], as C hexagons are preserved in each respective transformation to the denser structure.

References

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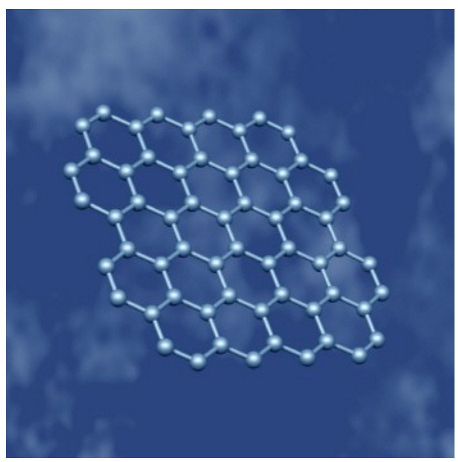

Figure 1: The graphene tessellation of trigonal planar C atoms arranged in hexagons in a 2-dimensional grid

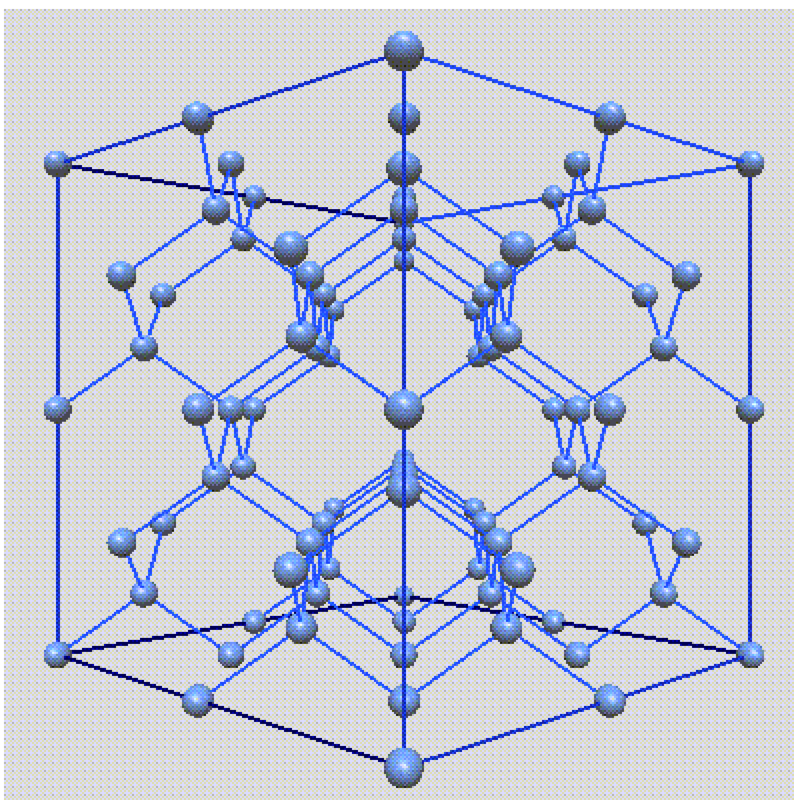

Figure 2: The diamond lattice as the densest possible sphere packing of tetrahedral C atoms arranged in hexagons

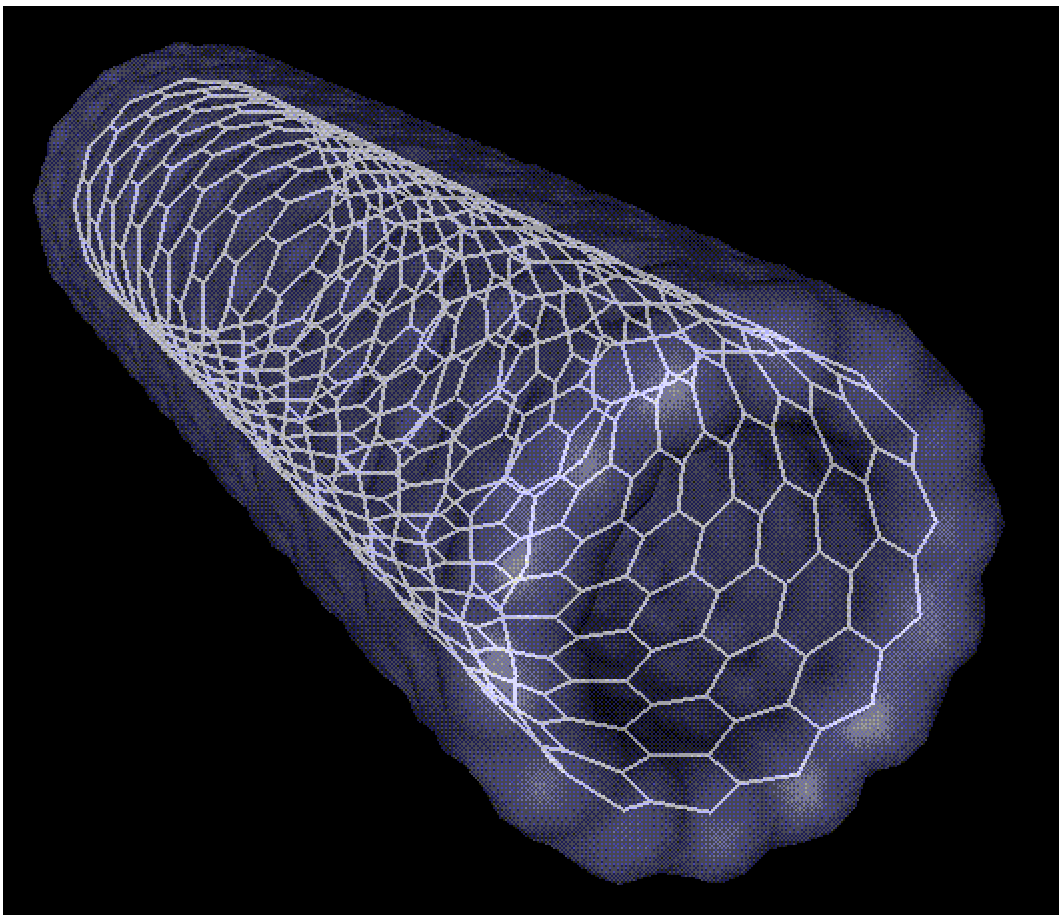

Figure 3: A carbon nanotube cylinder which can be bundled into a closest packing arrangement of nanotubes under pressure

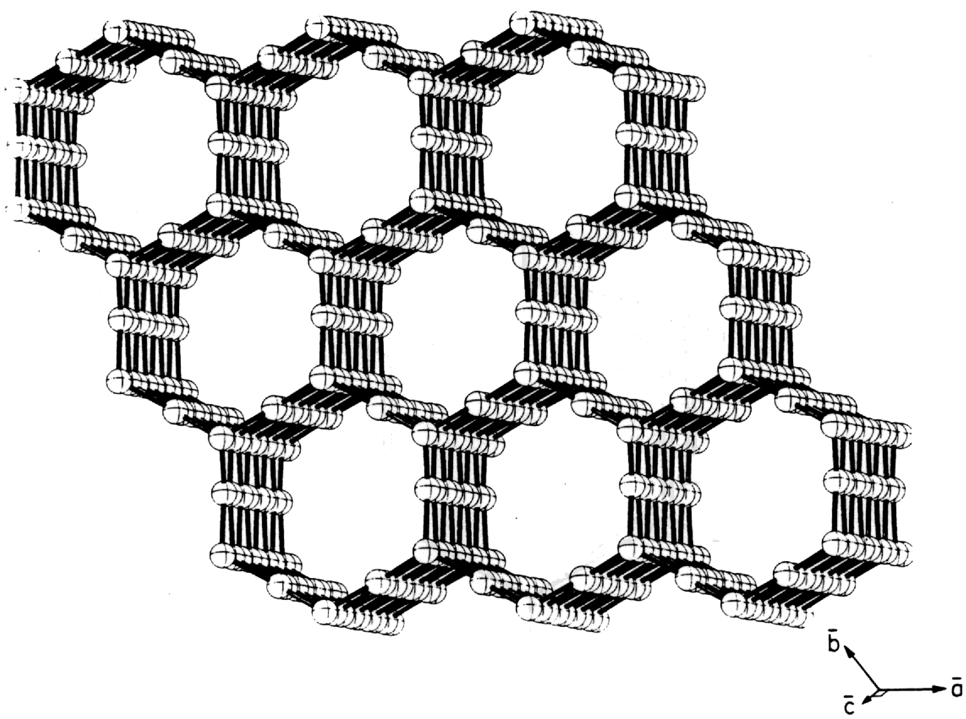

Figure 4: The hexagonite lattice as the densest cylinder packing that C can attain in hexagons