Diamond and Lonsdaleite:
Beyond Defect Centers and Stishovite as Natural Seed

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Abstract

We address attention to the 3*D* lattice match between hexagonal lonsdaleite, a carbon allotrop denser and harder than diamond with a higher carrier mobility, and tetragonal stishovite (rutile structure). Both compounds are obtainable via shock wave synthesis route. Stishovite seeding may lower the high-pressure and low temperature synthesis conditions for lonsdaleite as a coming material for quantum computer chips better withstanding solar wind damage. The chips could be made of a forest of lonsdaleite nanorods with defect center based addressable high-fidelity and non-destructive qubits. Material science as well as geochemistry may gain profite from the remarkable three-dimensional lattice coincidence between stishovite and lonsdaleite as a groundbreaking suggestion. Interestingly, carbon dioxide can adopt the rutile structure at extreme conditions of pressure and temperature. This paws the way for new oxygen defect based research on lonsdaleite as chip material.

Keywords: Diamond, Lonsdaleite, Stishovite, Carbon Dioxide Rutile Phase, Defect Centers, Material Synthesis, Lattice Match, Quantum Computing.

Introduction

Today diamond is one of the most investigated materials with a virtually endless high-tech application potential. However, the denser and harder hexagonal carbon allotrope lonsdaleite is becoming an even more interesting material. Its carrier mobility is higher than that of diamond. Defect centers in diamond play a dominant role. We speak of color centers because they are responsible for different colors in natural diamonds. For instance, the blue color is caused by boron atoms that replace carbon ones. Nitrogen, the most common impurity in form of single atoms or clusters, is responsible for yellow, orange and even brown color nuances. One observes also Si replacement. Besides atomic impurities, diamonds show platelet clusters and mineral inclusions such as $CaSiO_3$ perovskite [1] or stishovite, the rutile variety of SiO_2, in superdeep diamonds of Earth's lower mantle [2]. Weak cubic $CaSiO_3$ perovskite is a major phase in the subduced oceanic crust [3]. Here we report of the three-dimensional lattice match between stishovite (rutile structure) and lonsdaleite and its recommended use for material synthesis. Finally, we combine the results with a non-molecular high-pressure phase of carbon dioxide adopting the rutile structure. The lattice parameter ratio of lonsdaleite approximates golden mean geometry and can adopt the exact ratio when moderate pressure is applied along

[001]. A maximum of hardness as well as carrier mobility may be reached under that condition.

Defect Centers and Mineral Seeds in Diamond and Lonsdaleite

Well-designed color center can be generated in synthetic diamond or lonsdaleite material by different sophisticated treatments for technical use [4]. Intrinsic self-interstitial defects can be created by radiation damage, electron irradiation and neutron or ion implantation followed by annealing. The nitrogen vacancy NV^- center in diamond as well as group IV element color centers (G4V, where G4 = Si, Ge, Sn, Pb) exhibit 4 spin orientations [5]. In contrast, the TR12 center possesses the maximum of 12 inequivalent spin orientations. If we choose the diamond <111> direction as *z*-axis, we get four orientations and then for each *z*-orientation three ones for the *x* and *y* axes. TR12 defects are optically addressable point defects and can be used as detector for full 3*D* magnetic fields [6]. This self-interstitial defect is known since 1956, but a structural characterization is still pending [7]. Also ST2 point defects discovered in natural and CVD grown diamond, again with 12 inequivalent spin orientations, can be used as magnetic field sensors, too [8]. Group-IV-vacancy color centers were recently comprehensively discussed by *Gu* [9], and about the generation of NV-centers in diamond was reported by *Popov et al.* [10].

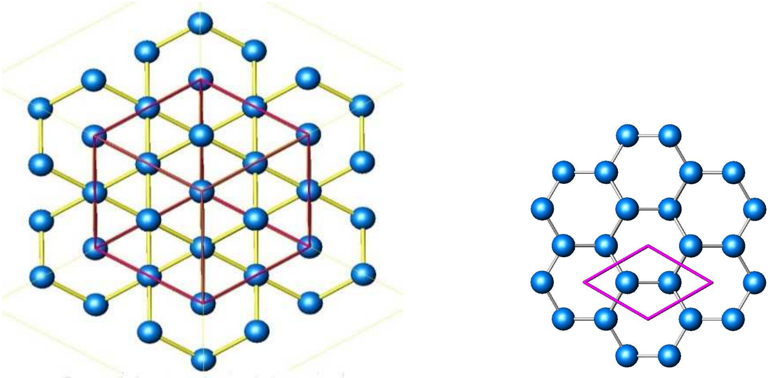

Figure 1. Crystal structure projection of diamond down [111] (left) and lonsdaleite down [001] (right). Puckering of the hexagonal rings can not be seen in the projection. The projected unit-cells are displayed in magenta.

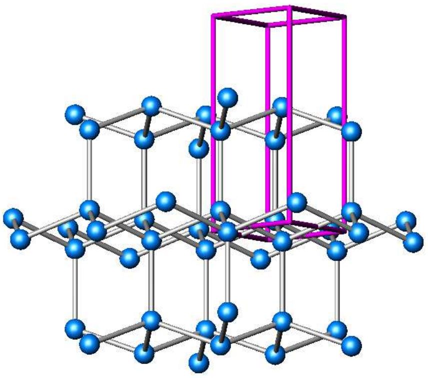

Figure 2. Puckered hexagonal rings of lonsdaleite. Unit-cell in magenta.

The lattice parameter for diamond is a = 3.567(Å) and the cubic unit-cell volume V_d = 45.385(Å^3). The lattice parameters of the hexagonal carbon modification lonsdaleite are related to that of dimond by the following equations

$$a_l \approx \frac{\sqrt{2}}{2} a_d = 2.5221\ \text{Å} \qquad c_l \approx \frac{2}{\sqrt{3}} a_d = 4.1186\ \text{Å}$$

For tetragonal stishovite (rutile structure depicted in **Figure 3**) we have lattice parameters a = 4.177(Å) and c = 2.665(Å) and a comparable unit-cell volume of V_{st} = 46.497(Å^3).

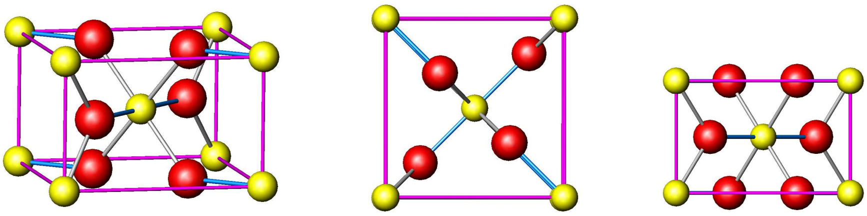

Figure 3. Crystal structure of stishovite and its projection down [001] respectively down [010] onto (101). Space group $P4_2$/mnm, No 136. Silicon atoms yellow, oxygen atoms red.

Due to the small lattice parameter of c = 2.665(Å) stishovite forms mainly needle-like crystals down [001]. Nearly lattice match conditions are a prerequisite for epitaxial growth of two phases and ceeding during crystal growth. The parameters of the orthogonal setting of the lonsdaleite crystal structure are surprisingly similar to the lattice parameters of stishovite (see the data below). Both minerals originate from shock wave treatment in nature. We propose to use stishovite as seed for lonsdaleite synthesis even if it is a high-pressure phase and today not available for large-scale synthesis use.

Lonsdaleite: $c = 4.119\ (\text{Å})$ $a\sqrt{3} = 4.369\ (\text{Å})$ $a = 2.522\ (\text{Å})$ $V_l = 45.385(\text{Å}^3)$

Stishovite: $a = 4.177\ (\text{Å})$ $a = 4.177\ (\text{Å})$ $c = 2.665\ (\text{Å})$ $V_{st} = 46.497(\text{Å}^3)$

The lattice match between lonsdaleite and stishovite is not only a two-dimensional match, but a three-dimensional one. Stishovite seeding may remarkedly reduce the shock wave conditions to produce lonsdaleite at room temperature and is emphasized as a synthesis tool. A sophisticated use may open the way for the production of 2*D* lonsdaleite, named lonsdaleane, or the synthesis of nano-rods supported by needle-like stishovite crystals and the manufactoring of forests of such rods. The coupled occurrence of lonsdaleite and stishovite in nature can be well explained by the given crystallographic facts. Young researchers should be encouraged to do some work in this scientific field, equally relevant for materials science and geochemistry. If stishovite is not available, why not try to start an experiment with some rutile: TiO_2 : a = 4.5937(Å), c = 2.9587(Å) or a solid solution of SiO_2 in rutile with reduced and more adapted lattice parameters, using a monocrystal cut perpendicular to [010] that deliveres the pseudohexagonal crystal plan (101) as substrate (see the right picture in **Figure 3**)?

Interestingly, carbon dioxide as a non-molecular solid can obviously adopt the ruile structure, space group $P4_2$/mnm (No 136), a = 3.516(Å) and $c´$ = 2.052(Å), under extreme pressure of 40(GPa) at 1500(K) [11] [12]. So it seems possible to discover such structure hosting in diamond respectively lonsdaleite or even implant some oxygen to generate corresponding defects in lonsdaleite for a detailed characterization and applicability research. Sharing the results, a solid solution between stishovite and the rutil phase of CO_2 even at high pressure seems to be possible. The small lattice mismatch between lonsdaleite and such an solid solution could be further reduced especially in the (101) crystal plane as substrate by about 10 at-% silicon replacing carbon in the rutile structure. Tentatively we also can conceive the stoichiometric composition $SiCO_4$ within a rutile-based unit-cell with reduced symmetry, where for instance the origin is occupied by Si and the center by C or vice versa.

If we go from micro-scale mineral inclusions within diamond and lonsdaleite towards nano-scale defects, we may ask what charge and spin state oxygen could adopt in stishovite-based defect centers that have only unit-cell dimension [13].

The synthesis of diamond and lonsdaleite, when we aim for ambient conditions of temperature and pressure, can be catalytically mediated by liquid gallium with its unique diatomic molecular structure and the tendency not to react with carbon [14] [15]. Some reflections and suggestion of the present author about the diamond synthesis and diamane have been written down recently [14] [15]. The seminal contribution of *Ruoff* and coworkers about a novel ambient pressure route of diamond synthesis using liquid gallium metal is highly recommended [16] as well as the contribution to the diamond synthesis, written by *Kaplunenko and Kosinov*, renowned experts in catalysis science [17].

Recently it has been reported about an exceptionally high carrier mobility even in lonsdaleite that underlines efforts towards optimal syntheses of this high-tech material [18].

Number theoretical and philosophical addendum:

The lattice parameter ratio of lonsdaleite approximates well the golden ratio of $\varphi = \frac{\sqrt{5}-1}{2} = 0.61803398\ldots$ as fundamental number of nature

$$\frac{c}{a} = \frac{2.5221}{4.1186} = \frac{\sqrt{6}}{4} = 0.61237$$

Strained lonsdaleite crystals can adapt exact golden ratio condition by excerting medium pressure along [001]. I wouldn’t wonder, when hardness as well as carrier mobility of such crystals could reach a maximum. In philosophical parlance lonsdaleite can be considered as golden material. In technological terms it may become a golden material, too. The lattice parameter ratio of stishovite can exactly adjust the golden ration by uptake of CO_2 in the rutile-phase solid solution [19].

Conclusion

Besides addressable color centers in diamond and lonsdaleite, operating as qubits for quantum computation or magnet field sensors, we address attention to the 3*D* lattice match between hexagonal lonsdaleite and tetragonal stishovite, both obtainable via shock wave synthesis route, where stishovite seeding may lower the high-pressure and low temperature synthesis conditions for lonsdaleite. Material science as well as geochemistry may gain profite from the remarkable three-dimensional lattice coincidence between stishovite and lonsdaleite. The next generation of non-destructive chips for quantum computers better withstanding solar wind damage could be made of a forest of lonsdaleite rods with defect center based qubits showing exceptionally high carier mobility.

Conflicts of Interest

The author declares no conflict of interests regarding the publication of this paper. No artificial intelligence was used.

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