

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

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Today diamond is one of the most investigated materials with a virtually endless high-tech application potential. However, the densest hexagonal carbon allotrope lonsdaleite is becoming an even more interesting material. 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 subducted oceanic crust [3].

Well-designed color center can be generated in synthetic diamond or lonsdaleite material by different sophisticated treatments for technical use. Intrinsic self-interstitial defects can be created by radiation damage, electron irradiation and neutron or ion implantation followed by annealing.

The nitrogen NV center in diamond as well as group IV element color centers exhibits 4 spin orientations [4]. In contrast, the TR12 center possesses the maximum of 12 inequivalent spin orientations. This self-interstitial defect is known since 1956, but a structural characterization is still pending [5]. If we choose the diamond $\langle 111 \rangle$ 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 3D magnetic fields [5]. 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 [6].

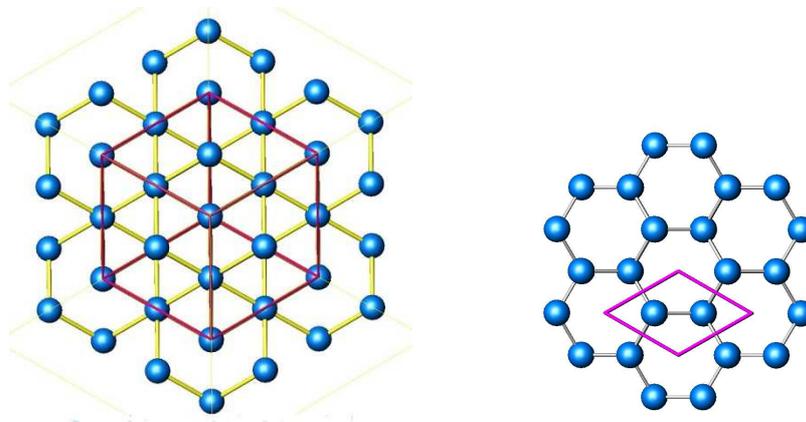


Figure 1. Crystal structure projection of diamond down $[111]$ (left) and lonsdaleite down $[001]$ (right). Puckering of the hexagonal rings can not be seen in the projection. The projected unit-cells are isplayed in magenta.

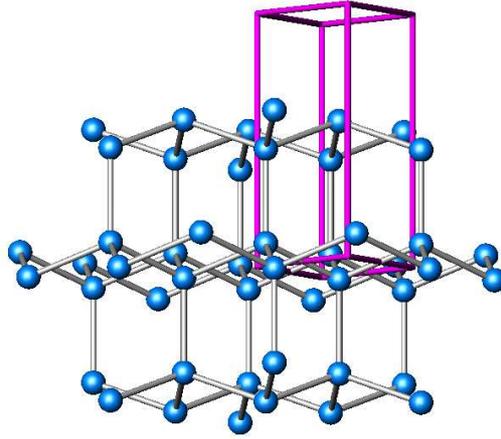


Figure 2. Puckered hexagonal rings of lonsdaleite. Unit-cell in magenta.

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

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

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

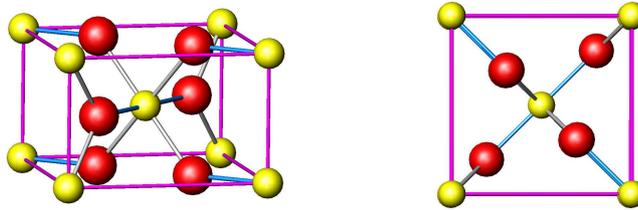


Figure 3. Crystal structure of stishovite and its projection down [001].

Nearly lattice match conditions are a prerequisite for epitaxial growth of two phases and coexisting 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.

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

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

The lattice match between lonsdaleite and stishovite is not only a two-dimensional match, but a three-dimensional one. Stishovite seeding may remarkably 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 2D lonsdaleite, named lonsdaleane, or the synthesis of nano-rods from that material. 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. Some reflections and suggestion of the present author about the diamond synthesis and diamane have been written down recently [7] [8].

Conclusion

Besides addressable color centers in diamond and lonsdaleite, operating as qubits for quantum computation or magnet field sensors, we address attention to the 3D 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.

References

- [1] Kopylova, M. et al. (2018) CaSiO₃ perovskite indicates the recycling of oceanic crust into the lower mantle. *Nature* **555**, 237-241.
- [2] Litvin, Y. A., Spivak, A. V., and Dubrovinsky, L. S. (201) Magnetic evolution of the material of the Earth's lower mantle: Stishovite paradox and origin of the superdeep diamonds. *Geochemistry International* **54**, 936-947.
- [3] Yang, L. et al. (2021) Lonsdaleite: The diamond with optimized bond length and enhanced hardness. *arXiv:2111.09176v1*.
- [4] Bradac, C. et al. (2019) Quantum nanophotonics with group IV defects in diamond. *Nature Communications* **10**, 5625.
- [4] Foglzing, J. et al (2022) TR12 centers in diamond as room temperature atomic scale vector magnetometer. *Quantum Information* **8**:65
- [5] Clarke, C. D., Ditchburn, R. N., and Dyer, H. B. (1956) The Absorption Spectra of Natural and Irradiated Diamonds. *Proceedings of the Royal Society of London, Series A* **234**, 363-381.
- [6] Foglzing, J. et al. (2024) Discovery of ST2 centers in natural and CVD diamond. *arXiv:2501.00570v1*.
- [7] Otto, H. H. (2025) Diamond Synthesis: Reflections and Suggestions. *viXra:2509.0061*
- [8] Otto, H. H. (206) Diamane Fibonacci Nanotubules for Quantum Computing *viXra:2602.0088*.