Bol. Mus. Nac. Hist. Nat. Parag. Vol. 29, Art. e2025004: 15 pp.

Lower mantle lonsdaleite

Lonsdaleita del manto inferior

Jaime L.B. Presser*

*JP Exploration, Asunción, Paraguay. Email: presserjaime@gmail.com.

Abstract.- This brief document offers a review of the concept of hexagonal diamond, also known as H-diamond or lonsdaleite, a mixture of C (cubic) diamond and H (hexagonal) diamond. The text addresses the methods for detecting this form of diamond, its presence in the Earth's mantle, and the formation pressure based on experimental data. Raman spectroscopy and X-ray diffraction (XRD) are used to characterize diamonds (C-type diamonds) and the mixture of C-diamonds and hexagonal diamonds (C/H-type diamonds) or lonsdaleite diamonds. Upper mantle diamonds show XRD patterns characteristic of C-diamond, while lonsdaleite diamonds exhibit patterns reflecting C/H stacking disorder. Raman spectroscopy is fundamental to the study of lonsdaleite diamonds, as it allows the identification of the presence of hexagonal stacking in diamond and provides information on the degree of stacking disorder. Measuring the full width at half maximum (FWHM) in Raman spectra is crucial to determine the degree of crystallinity and infer the eventual lonsdaleite content in diamonds. The analysis of experimental data from C-type and C/H-type diamonds reveals a direct linear relationship between the formation pressure and the FWHM value of the D peak in Raman spectroscopy. Analyses that have allowed the derivation of the equation that relates the formation pressure of diamonds to the FWHM value in Raman spectra, opening new possibilities for the research of impact diamonds, cratonic (C-type) and ultra-deep (C- and C/H-types) diamonds: P (GPa) = (0.3416xFWHM) + 3.2044.

***Keywords**: Lonsdaleite, Hexagonal diamond, C/H-type diamonds, Raman spectroscopy, X-ray diffraction (XRD), Full width at half maximum (FWHM), Formation pressure.*

Resumen.- Este breve documento ofrece una revisión del concepto de diamante hexagonal, también conocido como diamante H o lonsdaleita, una mezcla de diamante C (cúbico) y diamante H (hexagonal). El texto aborda los métodos de detección de esta forma de diamante, su presencia en el manto terrestre y la presión de formación basada en datos experimentales. Se utiliza la espectroscopia Raman y la difracción de rayos X (XRD) para caracterizar los diamantes (diamantes de tipo C) y a la mezcla de diamantes C y diamantes hexagonales (diamantes tipo C/H) o diamantes lonsdaleíticos. Los diamantes del manto superior muestran patrones XRD característicos del diamante c, mientras que los diamantes lonsdaleíticos exhiben patrones que reflejan el desorden de apilamiento C/H. La espectroscopia Raman es fundamental para el estudio de los diamantes lonsdaleíticos, ya que permite identificar la presencia de apilamiento hexagonal en el diamante y proporciona información sobre el grado de desorden del apilamiento. La medición del Ancho a media altura (FWHM) en los espectros Raman es crucial para determinar el grado de cristalinidad e inferir el eventual contenido de lonsdaleita en los diamantes. El análisis de datos experimentales de diamantes de tipo C y tipo C/H revela una relación lineal directa entre la presión de formación y el valor de FWHM del pico D en la espectroscopia de Raman. Análisis que han permitido derivar la ecuación que relaciona la presión de formación de diamantes con el valor de FWHM en espectros Raman, abriendo nuevas posibilidades para la investigación de diamantes cratónicos (tipo C) y ultraprofundos (tipos C y C/H): P (GPa) = (0,3416xFWHM) + 3,2044.

***Palabras clave**: Lonsdaleita, Diamante hexagonal, Diamantes tipo C/H, Espectroscopía Raman, Difracción de rayos X (DRX), Ancho total a la mitad del máximo (FWHM), Presión de formación.*

Lonsdaleite, also known as hexagonal diamond, is a nanocomposite that was discovered in the Canyon Diablo iron meteorite. This nanocomposite is formed by diamonds with disordered stacking of cubic (C) and hexagonal (H) layers and crystallographically intergrown diaphite (Salzmann, *et al.*, 2015; Garvie, & Németh, 2009; Németh, *et al.*, 2020; Németh *et al.*, 2022a; 2022b; 2022c; Németh, *et al.*, 2023). Disordered C/H stacking means that the layers of

Editor responsable: Bolívar R. Garcete-Barrett* / Recibido: 19.xii.2024 / Aceptado: 7.iv.2025 / Publicado online: 6.v.2025
*Museo Nacional de Historia Natural del Paraguay, San Lorenzo, Paraguay.

carbon atoms do not follow a regular and repetitive pattern (Németh, *et al.*, 2023; Salzmann *et al.*, 2015; and Németh *et al.*, 2022a, 2022b and 2022c). Diaphite, on the other hand, is a form of carbon with a structure similar to graphite, but with curved and irregular layers (Németh *et al.*, 2020; Németh *et al.*, 2022b). The first definitions of lonsdaleite were based mainly on X-ray diffraction (XRD) data; however, these studies had limitations. Often, only tables of observed d-spacings were shown, obscuring the true complexity of the diffraction patterns (Németh & Garvie, 2009). In addition, the broad diffraction features in the XRD data, along with the overlap of cubic (c) diamond reflections with the putative H-diamond reflections, complicated the analysis and led to misinterpretations (Németh *et al.*, 2022a).

Modern analytical techniques, such as Raman spectroscopy and high-resolution transmission electron microscopy (HRTEM), have enabled a more accurate characterization of lonsdaleite (Németh *et al.*, 2020; Németh *et al.*, 2022a and 2022b; and Németh, *et al.*, 2023). HRTEM studies reveal that Canyon Diablo lonsdaleite is composed of highly disordered C/H stacking of diamond, intergrown with diaphite (Németh, *et al.*, 2023; Németh *et al.*, 2022a and 2022b). This structural complexity explains the intricate HRTEM images and the continuous streaking of reflections in the diffraction patterns, indicating the absence of three-dimensional repeats at the nanoscale (Németh, *et al.*, 2023). The work of Németh et al. challenges the traditional definition of lonsdaleite as a discrete hexagonal (H) diamond phase (Németh, *et al.*, 2023; and Németh *et al.*, 2022a and 2022b). They argue that Canyon Diablo lonsdaleite is not a pure phase but a complex nanocomposite. They propose that Canyon Diablo lonsdaleite is not a discrete mineral phase but a nanocomposite of disordered C/H stacked diamond and diaphite. They suggest reserving the term "H-diamond" for the fully hexagonal diamond polytype.

Regarding the Canyon Diablo meteorite impact diamonds, Németh's works, while not being statistically representative, could be considered as an argument to be taken into account, at least in relation to impact diamonds.

This work briefly reviews the concept of hexagonal diamond or h diamond or lonsdaleite diamond, its detection methods, its presence in the Earth's mantle, and formation pressure based on experimental data (among others).

Methods

Standardizing the treatment of Raman spectra as the first task, each raw spectrum was baseline fitted in the CrystalSleuth software (https://rruff.info/about/about_download.php). Noisy spectra refinement was smoothed in the RCH software (https://www.fabrizionestola.com/rch). FWHM calculations were performed in Spectragryph (https://www.effemm2.de/spectragryph/about.html); ArDI (https://ardi.fmm.ru/), RCH and Fityk (https://fityk.nieto.pl/) softwares. The X-ray diffraction (XRD) spectra were observed in the Fityk software. Spectra that are best interpreted by avoiding peak and valley fitting. Some spectra were scanned to produce txt tables in the RCH software. The text presented is written with the assistance of three different AIs, where one of them is specialized in assisting with the refinement of texts to be published: 1- https://notebooklm.google.com/ 2- https://openai.com/index/chatgpt/ 3- https://gemini.google.com/app.

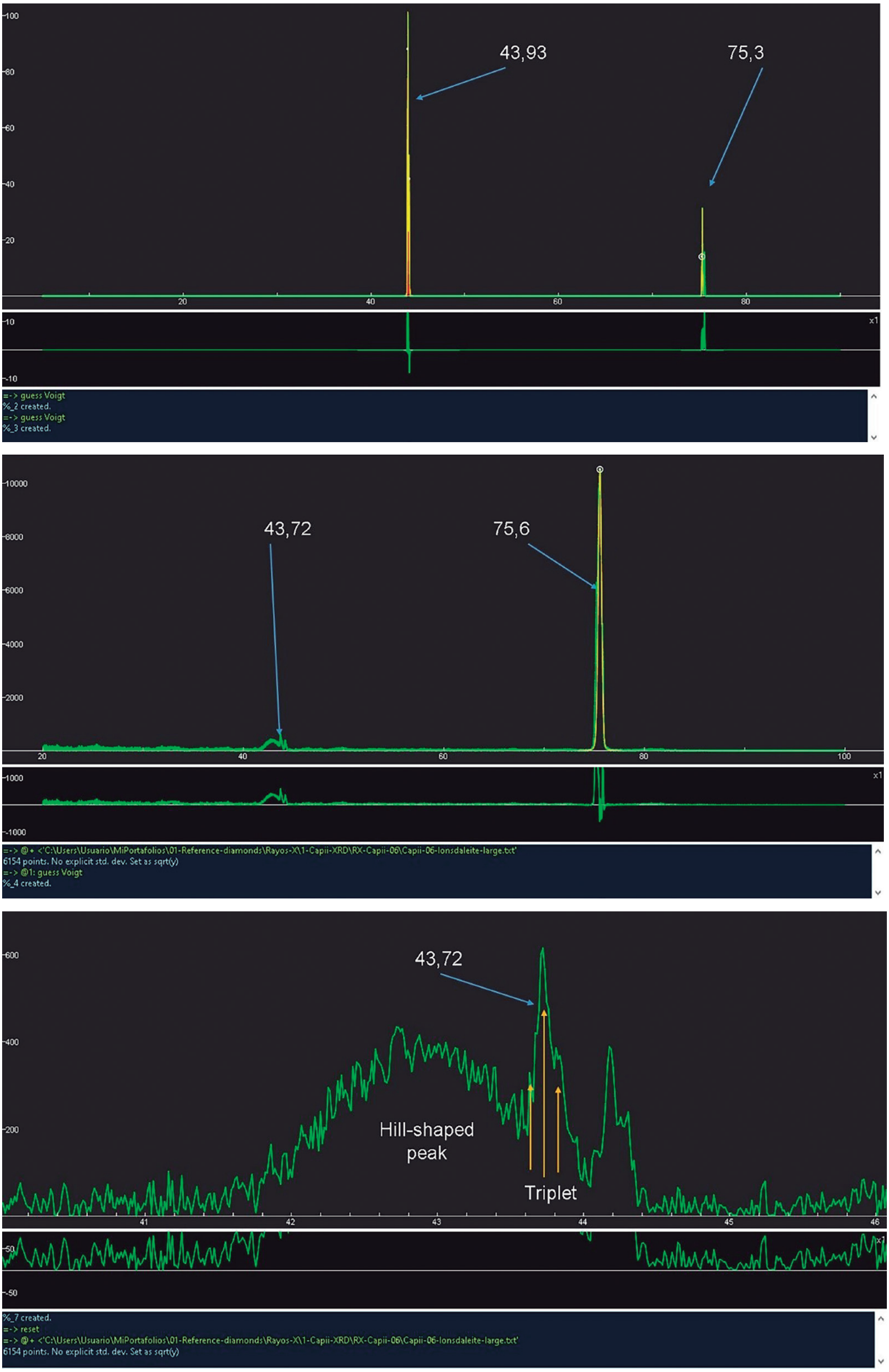
Vision of two basic analytical processes: XRD and Raman Spectroscopy

In **X-ray diffraction analysis**, upper mantle diamonds show XRD patterns with characteristic peaks of cubic diamond, with pronounced peaks at 43.9° (111) and 75° (220) 2θ degrees (e.g., Yelisseyev *et al.*, 2015; Ohfuji *et al.*, 2017); Figure 1. Presser's (2024 and references therein) lonsdaleite diamonds, on the other hand, exhibit XRD patterns that reflect cubic/hexagonal stacking disorder, including a pronounced peak at 75° (110-220) 2θ degrees, a "triplet" or "doublet" of

1

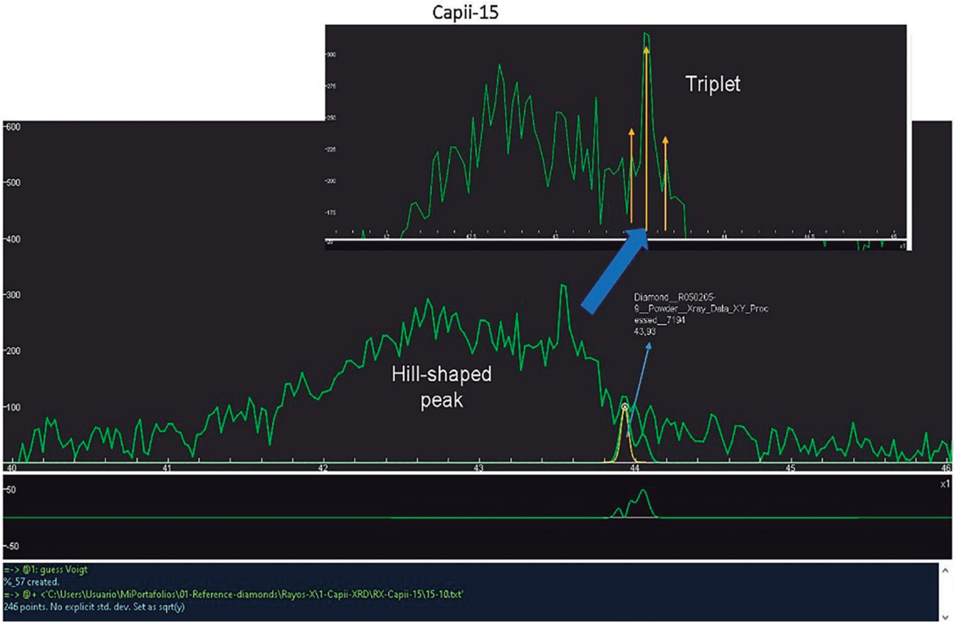
2

3

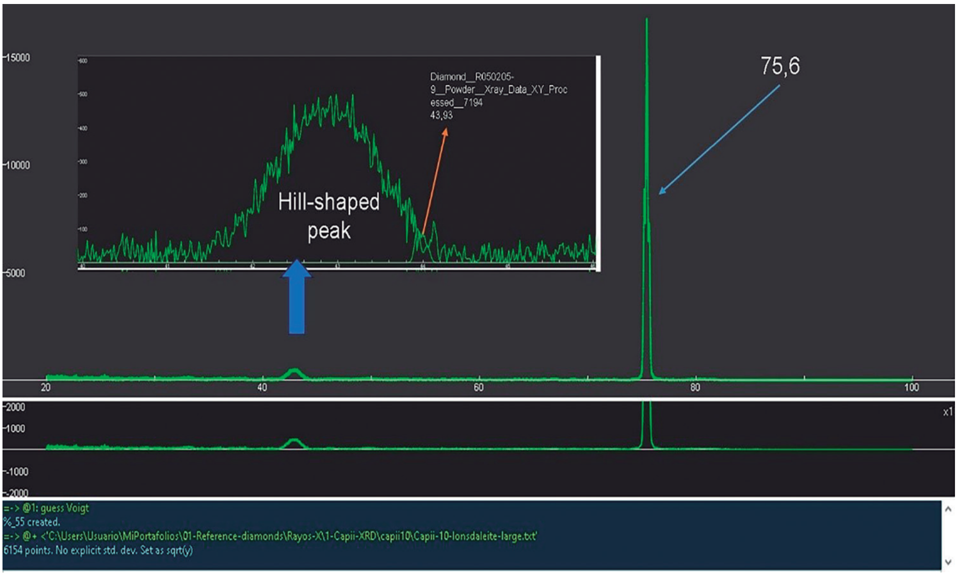


Lower mantle lonsdaleite

4



5



Previous and current page: Figures 1-5. XRD spectrum of mantle diamonds and londsdaleite diamonds. **1)** Upper mantle diamond. **2-5)** lower mantle lonsdaleite diamonds. **2-5)** Data from Presser *et al.*, 2024b and 2024c. **1)** Pronounced and well-defined peaks at 43.9° (111) and much less intense 75° (220) 2θ degrees. Diamond__R050205-9__Powder__Xray_Data_XY_Processed__7194 (RRuFF). **2)** A pronounced peak at 75° (110-220) and a less intense one at 43.72° (111) 2θ degrees. The peak at 75°, which may be more intense due to overlap with cubic diamond. Capii-6 lonsdaleite diamond. **3)**. Spectrum where the presence of the characteristic "triplet" of diffraction peaks is observed between 40° and 50° (100-111-101) together with 43.72 (=111) 2θ degrees. Capii-6. **4)** Here also, the presence of the characteristic "triplet" of diffraction peaks is observed between 40° and 50° (100-111-101) 2θ degrees; although with a somewhat less pronounced peak in relation to that of Figure 3. It presents a peak at 43.42 (=111) 2θ degrees. Capii-15. **5)** Presence of a "hill-shaped peak" between 40° and 50° 2θ degrees, which would be due to interferences of the peaks of C-diamond, H-diamond, and mineral inclusions such as bridgmanite (or its derived phases such as corundum and enstatite), ferropericlase. Capii-10. However, it was possible to read that it presents a peak at 43.52 (=111) 2θ degrees.

peaks between 40° and 50° (100-111-101) 2θ degrees, Figure 3 and Figure 4. Shifted peaks of 43.9° (111) as those in Figures 2 to 5 are indicative of the presence of lonsdaleite (in this regard see Ovsyuk *et al.* (2019); Yelisseyev *et al.* (2019); Afanasiev *et al.* (2019); Afanasiev *et al*. (2022); Chepurov *et al.* (2023); Shames *et al.* (2015); Jones *et al.* (2016); Murri *et al.* (2019); Denisov *et al.* (2011); Németh *et al.* (2023 and their references); Chen *et al.*, 2019; among others). A "hill-shaped peak" was also characterized in lonsdaleite diamonds between 40° and 50° 2θ degrees (Presser *et al.*, 2024a and 2024b found in Presser, 2024); Figures 2, 3, 4, and 5. This last peak is attributed to interferences of the peaks of cubic (C) diamond, hexagonal (H) diamond and mineral inclusions in the analyzed crystals, such as bridgmanite (or its retrograde minerals such as corundum and enstatite) and ferropericlase (Presser *et al.*, 2024a and 2024b found in Presser, 2024).

Raman spectroscopy is another essential technique for the study of diamonds (Raman vibration mode for cubic diamond corresponds to the first-order scattering of F2g symmetry at 1332 cm-1) (El Mendili *et al.*, 2022; Saitoh *et al.*, 1999) and lonsdaleite diamonds (Jones *et al.*, 2016; Murri *et al.*, 2019; Baek *et al.*, 2019; Goryainov *et al.*, 2018; Ovsyuk *et al.*, 2019; Presser *et al.*, 2020; Presser & Sikder, 2022; Presser & Sikder 2024; Presser *et al.*, 2024; Ohfuji *et al.*, 2015; among others). The presence of hexagonal stacking in diamond can be identified by the ab initio calculations predict three fundamental vibrational modes: 1207 cm−1 (E2g), 1307 cm−1 (A1g), and 1330 cm−1 (E1g) (e.g., El Mendili *et al.*, 2022); however, as commented in (Presser 2024 and references; see also Yelisseyev *et al.*, 2019) the peak of greatest intensity (A1g) in this D band could be shifted to higher or lower values by virtue, for example, of the size of the nanocrystals in stacking. Raman spectroscopy can also provide information on the degree of stacking disorder in lonsdaleite diamonds (Ovsyuk *et al.*, 2019) and would (apparently) allow the estimation of the lonsdaleite content in diamonds (Ovsyuk *et al.*, 2019; Presser 2024 and references; Presser & Sikder 2023; Presser *et al.*, 2024). Measuring the full width at half maximum (FWHM) in Raman spectra of impact diamonds and lower mantle diamonds (Presser, 2024 and references; Presser *et al.*, 2024) is crucial to determine their greater or lesser degree of crystallinity or also to infer the lonsdaleite content, but it is a complex process (Ovsyuk *et al.*, 2019; Presser 2024 and references; Presser & Sikder 2023; Presser *et al.*, 2024); Table 1 and Figures 6 to 10. Raw spectra often exhibit distortions that must be corrected to obtain accurate FWHM measurements. The choice of smoothing method can also influence the final FWHM value, which can make it difficult to compare results obtained by different researchers (*cf.*, Ovsyuk *et al.*, 2019; Presser 2024 and references; Presser & Sikder 2023; Presser *et al.*, 2024). A larger FWHM would generally be associated with a greater presence of lonsdaleite (Ovsyuk *et al.*, 2019); properly more than 58.1 cm^{-1} (this work).

In summary, lonsdaleite is not a simple hexagonal polytype of diamond but a much more complex material. This redefinition, based on XRD studies and modern analytical techniques such as HRTEM and Raman spectroscopy, has significant implications for understanding the properties and formation of this material.

Conceptual development and analysis

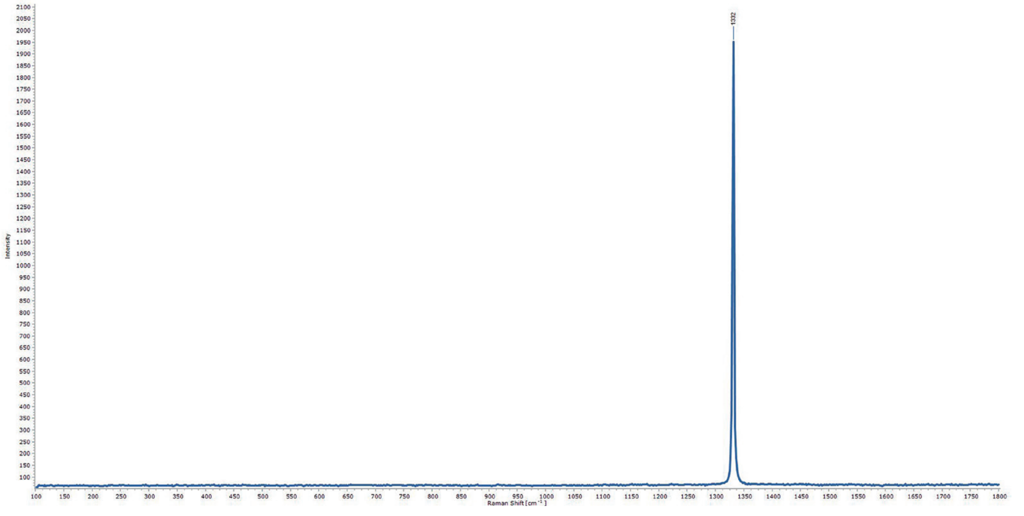
Formation of Diamonds and Lonsdaleite Diamonds in the Earth's Mantle

The minimum formation pressure of diamond in the mantle is a complex issue. Although a single value is not explicitly mentioned in the sources (Litvin, 2017; Spivak and Litvin, 2019; Simakov *et al.*, 2019; Kaminsky, 2017; Dobrzhinetskaya *et al.*, 2012; Sorokhtin, 2016; and Tappert and Tappert, 2011), it can be inferred from the information provided. Cr-in-Cpx barometry, used to estimate the formation pressure of diamonds with clinopyroxene inclusions, begins to un-

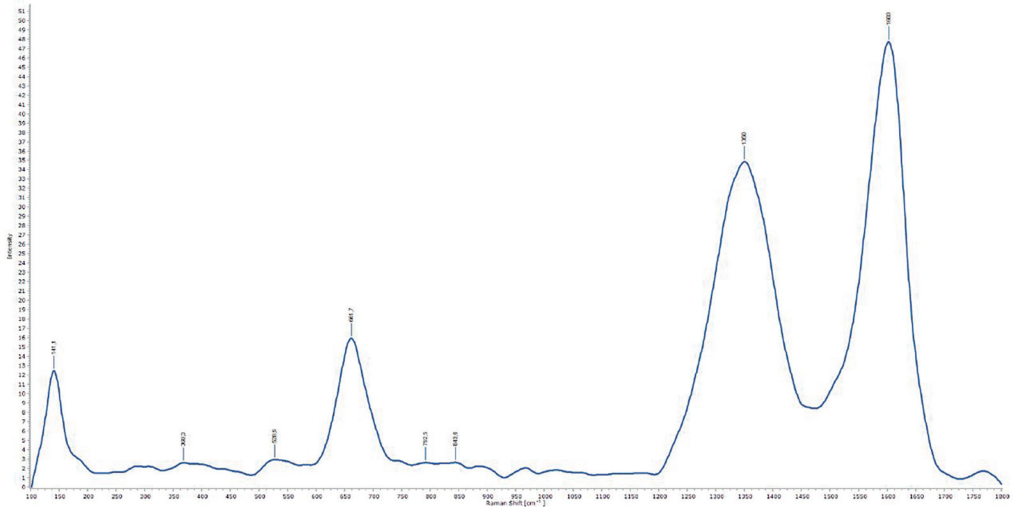
Table 1. FWHM calculation with different softwares: I, Spectragryph; II, ArDI; III, RCH and IV, Fityk. All diamonds except Capii-1 (Presser & Sikder, 2022 and Presser, 2024 and references) and number 11 (literature without exact reference) were compiled from RRuFF.

Nº	Analysis	Raman shift [1/cm]	Intensity	FWHM [1/cm]	II	III	IV
1	Eric Van Valkenburg-Diamond__R050204__Broad_Scan__532__0__unoriented__Raman_Data_RAW__12743	1335,3	3124	10,8	10	10	4
2	Eric Van Valkenburg-Diamond__R050204__Broad_Scan__532__0__unoriented__Raman_Data_RAW__12743	1336,2	68031	14,8	15	15	6
3	Eric Van Valkenburg-Diamond__R050204__Broad_Scan__532__0__unoriented__Raman_Data_RAW__12743	1335,5	175550	10,3	10	10	4
4	Eric Van Valkenburg-Diamond__R050204__Broad_Scan__532__0__unoriented__Raman_Data_RAW__12743	1335,9	87859	15	15	8	6
5	Bushimaie River, Belgian Congo-Diamond__R150108__Broad_Scan__532__0__unoriented__Raman_Data_RAW__24047	1337,2	9324	10,7	11	10	4
6	Cullinan-Diamond__R150106__Broad_Scan__532__0__unoriented__Raman_Data_RAW__24041	1373,8	33411	11,3	11	8	4
7	Zaire-Diamond__R150107__Broad_Scan__532__0__unoriented__Raman_Data_RAW__24044	1337,3	6529	14,2	15	8	6
8	Capii-2_P_new1	1331,5	1893	3,5	3	3	2
9	Diamond__R150106__Broad_Scan__532__0__unoriented__Raman_Data_RAW__24041	1337	33185	11,3	11	8	4
10	Diamond__R150107__Broad_Scan__532__0__unoriented__Raman_Data_RAW__24044	1337,3	6529	14,2	15	8	6
11	Diamond-spectra, literature reference	1331	37714	4,7	4,4	5	2
12	Gemological Institute of America 28754-sinthetiC-diamond__X080011__Broad_Scan__532__0__unoriented__Raman_Data_RAW__19274	1335,9	20405	14,9	15	8	6
13	Michael Scott-Diamond__R150086__Broad_Scan__532__0__unoriented__Raman_Data_RAW__24014	1337,3	15098	9,4	9,4	8	4
14	Plumas County, California, USA-Diamond__X050052__Raman__785__0__unoriented__Raman_Data_Processed__6472	1330,9	27500	5,7	5,6	5	2
15	Synthetic, DeBeers Element6-Diamond__X070001__Broad_Scan__532__0__unoriented__Raman_Data_RAW__14079	1337,4	11809	17,5	18	8	7
16	Synthetic, General ElectriC-diamond__X050053__Raman__514__0__unoriented__Raman_Data_Processed__6522	1334,9	9228	19,7	19	20	8

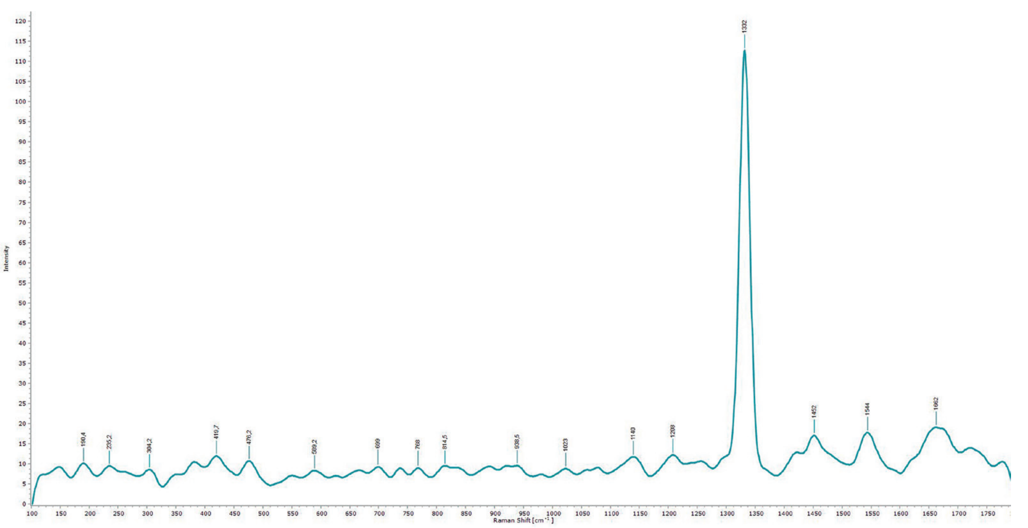
6



7

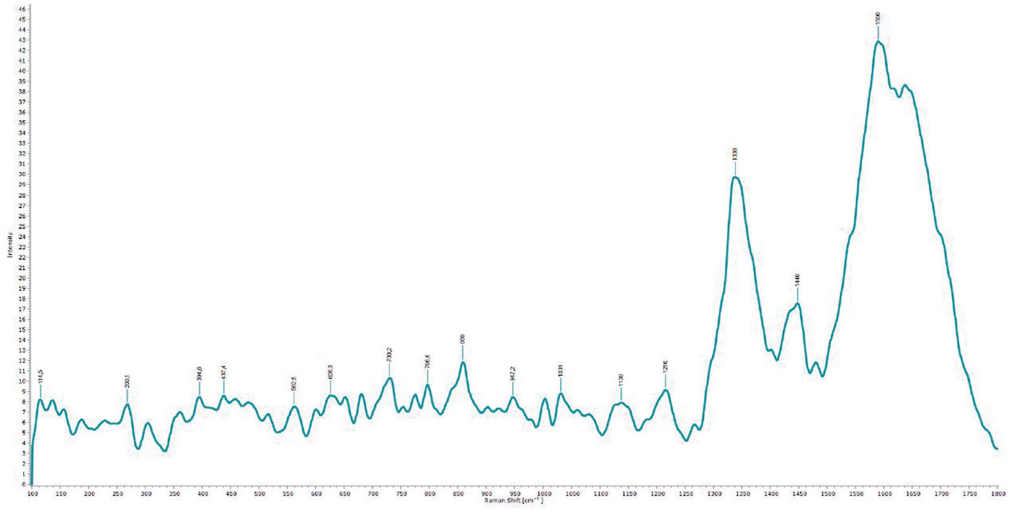


8

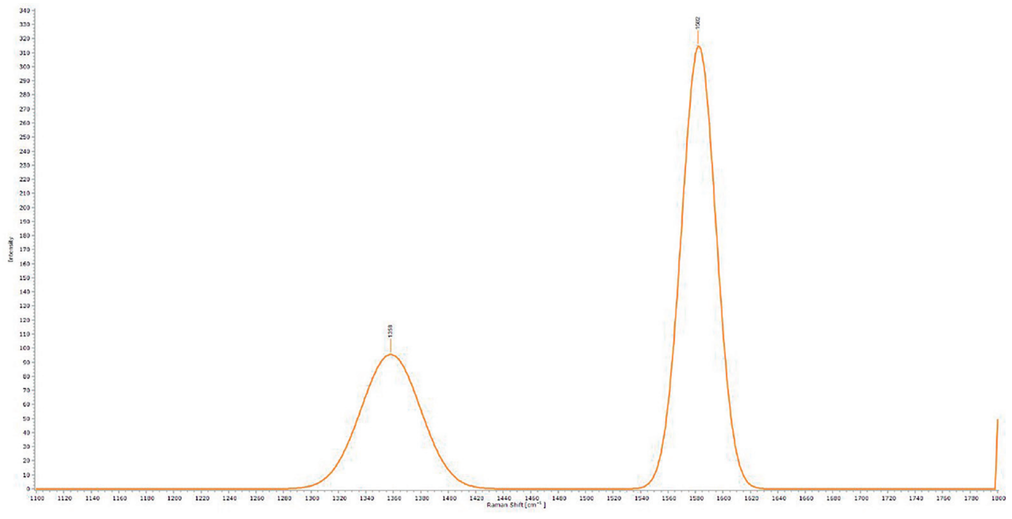


Lower mantle lonsdaleite

9



10



Previous and current page: Figures 6-10. Raman spectra. **6)** Of cratonic diamond. **7-9)** Of lonsdaleite diamonds. **10)** Of lonsdaleite. **6-9)** Data from Presser & Sikder, 2022. **6)** Raman spectrum of Capii02_P_new1, with its characteristic peak 1332 cm^{-1} (Table 1). **7)** Raman spectrum of Capii-6, with its broad D peak (FWHM 129 cm^{-1}) and shifted to 1350 cm^{-1} and also showing a pronounced graphite peak (1602 cm^{-1}) to its right and a characteristic ferropericlase peak (662 cm^{-1}) to its left. **8)** Raman spectrum with a different configuration from the previous figure (Capii-10), with its somewhat broad D peak (FWHM 22 cm^{-1}) and at 1332 cm^{-1} and also showing a smooth diaphite peak (1452 cm^{-1}). **9)** Raman spectrum with a different configuration from the previous two figures (Capii-15), with its broad D peak (FWHM 81 cm^{-1}) and at 1338 cm^{-1}, also showing a smooth diaphite peak (1448 cm^{-1}) and a pronounced graphite peak (1590 cm^{-1}) to its right. **10)** Raman of lonsdaleite from the Canyon Diablo meteorite (scanned from Karczemska *et al.*, 2008) with its broad D peak (FWHM 52 cm^{-1}) and at 1358 cm^{-1}, also showing a pronounced graphite peak (1582 cm^{-1}) to its right.

derestimate pressure at values above 4.5 GPa (Litvin, 2017). This suggests that the minimum pressure for diamond formation in the mantle could be in the range of 4.5 GPa or higher. Nimis (2022) in a modal pressure approach estimates that the diamond formation pressure would be at ~6 GPa.

Experimental Formation of Diamonds

The formation of diamonds from amorphous carbon and graphite in the presence of COH fluids has been investigated experimentally using laser-heated diamond anvil cells (DACs) in situ at high pressure and temperature. These experiments seek to simulate the extreme conditions found in the Earth's mantle where diamonds form naturally.

Diamond Formation in the Earth's Mantle

Diamonds (from cratonic environments) are a deep mineral often associated with kimberlites, lamproites, lamprophyres, and mantle xenoliths. The study of lithospheric diamonds has allowed us to better understand the stabilization of continents and their mantle keels, the onset of plate tectonics, and the nature of continental margin subduction, especially in the ancient past.

Diamonds form in the Earth's mantle at depths of ~150 to ~800 km. During the growth of diamond crystals, fragments of minerals, melts, and volatile compounds from the parent medium are captured and preserved as inclusions in the diamonds. Inclusions in diamonds provide information about the multi-component and multiphase composition of the parent medium where the diamonds formed. Diamonds can contain, fundamentally, peridotite or eclogite inclusions, indicating their origin in different parts of the mantle. See synthesis in Harris *et al.* (2022) and Stachell *et al.* (2022).

Importance of Physical-Chemical Experiments

The methodology of physical-chemical experiments is crucial to solve the genetic problems of diamonds and associated phases. These experiments allow the reproduction of the actual PT conditions in the upper mantle, the transition zone, and the lower mantle. By recreating these conditions in the laboratory, scientists can investigate the formation, growth, and transformations of diamonds and associated minerals in a controlled environment. As a synthesis of references see Luth *et al.* (2022).

Lonsdaleite Diamond Formation Pressure

Now, the minimum formation pressure of lonsdaleite or lonsdaleite diamond in the mantle is an even more complex and partly taboo subject. Addressing more directly the issue of lonsdaleite (or the mixture of cubic and hexagonal diamond) formation pressure and temperature, and how it is determined, below is a summary of some of the key studies in the literature that have addressed this issue. In addition, the experimental techniques that have been used are mentioned.

Studies on lonsdaleite formation

Lonsdaleite Formation at Low Pressures (15-20 GPa) One of the earliest works on lonsdaleite formation was carried out in the 15-20 GPa pressure range. These studies were based on compression experiments using diamond anvil cells (DACs) and showed that the mixture of cubic and hexagonal diamond began to form at these pressures.

Key reference: Mao, *et al.* (1996). This work reported that cubic diamond transformed into a mixture of lonsdaleite at pressures above 15 GPa, with an increase in the proportion of the hexagonal phase as pressure increased. Noteworthy is the work of Yang *et al.* (2021), who synthesized lonsdaleite from graphite using high pressures (20 GPa; i.e., ~Lower Mantle pressure) and temperatures, confirming its unique structure and superior mechanical properties.

Lonsdaleite Formation at Higher Pressure (50-60 GPa) Other studies have pointed out that lonsdaleite formation can occur at much higher pressures, between 50 GPa and 60 GPa, which is attributed to high-pressure conditions and the transition of structural phases.

Key reference: Gregoryanz, *et al.* (2004). This study showed that lonsdaleite began to form in a more significant mixture of hexagonal and cubic phases at pressures close to 50-60 GPa, indicating a gradual transition towards pure lonsdaleite as pressures increase. However, a very important pillar can be referred to with the work of He *et al.* (2002) who achieved the transformation of cubic diamond to lonsdaleite using shock wave compression (50-200 GPa), highlighting the importance of shear stress and kinetics in the transformation. See also the findings of De Carli *et al.* (2002) and Jones *et al.* (2016). Shag *et al.* (2023) successfully synthesized an almost pure sp3 amorphous carbon sample using C70 fullerene as a precursor under high pressure and high temperature (HPHT) conditions. This material exhibits improved short/medium-range structural order and superior physical properties compared to amorphous carbon synthesized from C60. Work from which it is rescued that sp3 amorphous carbon was synthesized from fullerenes C70 under high pressures (18-30 GPa) and high temperatures (900-1200°C). The resulting material exhibited structural characteristics similar to hexagonal diamond (HD) at the medium-range order (MRO) level. These studies contribute significantly to understanding the formation of lonsdaleite, a material with enormous potential in various technological applications.

Now, from the works of Yang *et al.* (2021) and Shag *et al.* (2023) it was possible to obtain FWHM and P values (in GPa) that, when plotted on a GPa Vs FWHM graph, showed a direct linear relationship between P and the FWHM values. To this, the FWHM value of a cratonic diamond (Presser & Sikder, 2022 and Presser, 2024) was added, which presented the lowest FWHM value and was assigned a reference formation P (based, for example, on Litvin, 2017) of 4.56 GPa; (Table 2), which came to perfectly add to what was previously found with the data of Yang *et al.* (2021) and Shag *et al.* (2023), as shown in Figure 11.

Thus, based on Figure 11, the equation: ***P (GPa) = (0.3416xFWHM) + 3.2044*** was

Table 2. FWHM values and the operating/estimated pressure in GPa in diamonds (type C and type H) found experimentally and inferred. The FWHM estimation method has been governed by the protocol discussed in the Methodology Item. 1-Presser & Sikder (2022), 2- Shag *et al*. (2023) and 3- Yang *et al*. (2022).

Raman shift [1/cm]	Intensity	FWHM [1/cm]	II	III	IV
1335,3	3124	10,8	10,1	10	4,4
1336,2	68031	14,8	15	15	5,6
1335,5	175550	10,3	10,2	10	4,4
1335,9	87859	15,0	15	7,5	6
1337,2	9324	10,7	10,6	10	4,4
1373,8	33411	11,3	11,2	7,5	4,4
1337,3	6529	14,2	14,8	7,5	5,6
1331,5	1893	3,5	3	2,5	2
1337,0	33185	11,3	11,2	7,5	4,4
1337,3	6529	14,2	14,8	7,5	5,6
1331,0	37714	4,7	4,4	5	2
1335,9	20405	14,9	14,8	7,5	6
1337,3	15098	9,4	9,4	7,5	4
1330,9	27500	5,7	5,6	5	2
1337,4	11809	17,5	17,6	7,5	7,2
1334,9	9228	19,7	19,2	20	8

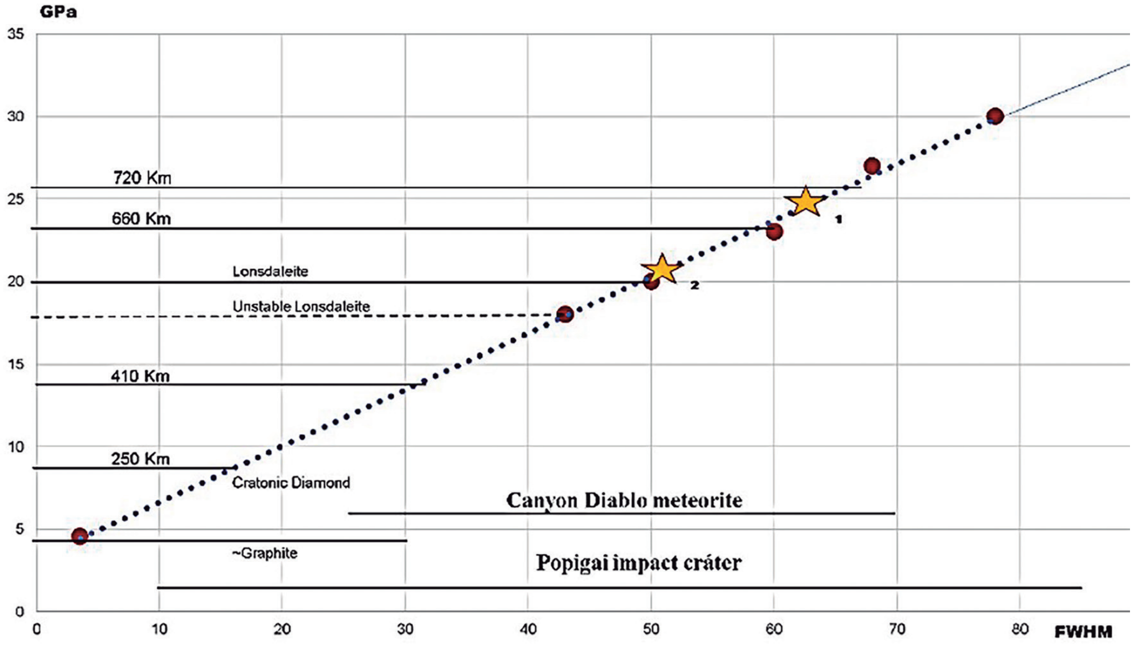


Figure 11. Pressure (GPa) versus FWHM for experimental results of diamonds (type c and type C/H) according to the data in Table 2. Where the data were plotted: 1 (star) impact diamond from the Canyon Diablo meteorite (Karczemska *et al.*, 2008); and as a star with the number 2 representing: Capii-6: Ferropericlase-bridgmanite-(Ferropericlase 25.786 Gpa)-bridgmanite-enstatite-corundum=Xray). Capii-1: Retro bridgmanite. Capii-3: Retro bridgmanite. Capii-5, Capii-7, Capii-10: Retro brigmanite (bridgmanite-corundum-enstatite-ferropericlase -27 GPa=X-ray)-enstatite-Ca-perovsquite. Capii-16 (*cf.* Presser, 2024). To which data were also added from: Canyon Diablo meteorite with FWHM from ~25 to 70 (Miyamoto, 1998); Popigai impact crater impact diamonds, with FWHM from ~10 to 85 (Ovsyuk *et al.*, 2019). Lonsdaleite unstable according to He, *et al.* (2002) and is taken as stable lonsdaleite from >20 GPa (according to Yang *et al.* 2022; i.e., ~Lower Mantle pressure).

obtained. The FAWHM value corresponds to the D peak (as C-diamond or H-diamond; more properly c+h or lonsdaleite diamonds =Diamond Band). This formula would allow the estimation of the formation depth of cratonic diamonds (or typically C-diamond) to ultra-deep diamonds (super deep diamonds and lonsdaleite diamonds).

Conclusions

Lonsdaleite, initially considered a simple hexagonal polytype of diamond, has proven to be a much more complex material thanks to recent research using modern analytical techniques such as HRTEM and Raman spectroscopy. This nanocomposite, characterized by highly disordered cubiC/Hexagonal (C/H) stacking of intergrown (or not) diamond with diaphite, forms at significantly higher pressures than conventional cubic diamond.

Raman spectroscopy and X-ray diffraction (XRD) are essential tools for distinguishing lonsdaleite from cubic diamond. An FWHM greater than 58.1 cm^{-1} at the Diamond Band of the Raman spectrum, along with XRD patterns showing shifted peaks (below 43.9 2-theta), such as the "triplet" or "doublet" between 40° and 50° (100-111-101) 2-theta, are indicators of the presence of lonsdaleite.

The linear relationship observed between formation pressure and FWHM value in type c and C/H diamonds has led to a crucial equation for research: P (GPa) = (0.3416xFWHM) + 3.2044. This equation, supported by experimental data presented in Figure 11 and Table 2, allows the estimation of diamond formation depth, opening new possibilities for the study of impact diamonds, cratonic and ultra-deep diamonds.

The redefinition of lonsdaleite as a complex nanocomposite has significant implications for understanding its formation, properties, and potential in various technological applications. Future research should focus on fully unraveling its mysteries and harnessing its potential in fields such as materials science and technology.

Acknowledgments

The author of this work sincerely acknowledges and deeply appreciates the thorough review provided by the peers of this manuscript. Their insightful comments and constructive suggestions significantly contributed to improving the quality of this research.

Literature

Afanasiev, V., Gromilov, S., Sonin, V., Zhimulev, E. & Chepurov, A. (2019). Graphite in rocks of the Popigai impact crater: Residual or retrograde?. *Turkish Journal of Earth Sciences*, 28(3): 470–477.

Afanasiev, V.P., Pruuel, É.R., Kurepin, A.E., Gromilov, S.A. & Vityazev, P.A. (2022). Comparative characteristics of impact diamonds of the Popigai astrobleme and synthetic diamonds produced by explosion. *Journal of Engineering Physics and Thermophysics*, 95(1): 1697–1702.

Baek, W., Gromilov, S.A., Kuklin, A.V., Kovaleva, E.A., Fedorov, A.S., Sukhikh, A.S., Hanfland, M., Pomogaev, V.A., Melchakova, I.A., Avramov, P.V. & Yusenko, K.V. (2019). Unique nanomechanical properties of diamond–lonsdaleite biphases: Combined experimental and theoretical consideration of Popigai impact diamonds. *Nano Letters*, 19(3): 1570–1576.

Chepurov, A., Goryainov, S., Gromilov, S., Zhimulev, E., Sonin, V., Chepurov, A., Karpovich, Z., Afanasiev, V. & Pokhilenko, N. (2023). HPHT-treated impact diamonds from the Popigai Crater (Siberian Craton): XRD and Raman spectroscopy evidence. *Minerals*, 13(2)154: 1–21.

De Carli, P.S., Bowden, E., Jones, A.P. & Price, G.D. (2002). Laboratory impact experiments versus natural impact events. Pp. 32–33, in Lunar and Planetary Institute. (Ed.). *Catastrophic events and mass extintions: impacts and beyond*. Houston: Lunar and Planetary Institute. xv + 242 pp.

Denisov, V.N., Mavrin, B.N., Serebryanaya, N.R., Dubitsky, G.A., Aksenenkov, V.V., Kirichenko, A.N., Kuzmin, N.V., Kulnitskiy, B.A., Perezhogin, I.A. & Blank, V.D. (2011). First-principles, UV Raman, X-ray diffraction and TEM study of the structure and lattice dynamics of the diamond–lonsdaleite system. *Diamond and Related Materials*, 20(7): 951–953.

Dobrzhinetskaya, L., Faryad, S.W., Wallis, S. & Cuthbert, S. (Eds.). (2012). *Ultrahigh-pressure metamorphism: 25 years after the discovery of coesite and diamond*. London & Burlington: Elsevier Inc. 696 pp.

El Mendili, Y., Orberger, B., Chateigner, D., Bardeau, J-F., Gascoin, S. & Petit, S. (2022). Raman investigations and *ab initio* calculations of natural diamond-lonsdaleite originating from New Caledonia. *Chemical Physics*, 559(111541): 1–7.

Garvie, L.A.J & Németh, P. (2009). The structure of Canyon Diablo "diamonds". *Abstracts of the 40th Lunar and Planetary Science Conference*, 1346. The Woodlands: Lunar and Planetary Institute. 2 pp.

Goryainov, S.V., Likhacheva, A.Y. & Ovsyuk, N.N. (2018). Raman scattering in lonsdaleite. *Journal of Experimental and Theoretical Physics*, 127(1): 20–24.

Gregoryanz, E., Somayazulu, M. & Hemley, R.J. (2004). The synthesis of lonsdaleite and its relationship to diamond. *Nature Materials*, 3(1): 29–32.

Harris, J.W., Fedortchouk, Y. & Moore, M. (2022). Morphology of monocrystalline diamond and its inclusions. *Reviews in Mineralogy & Geochemistry*, 88(1): 119–166.

He, H., Sekine, T. & Kobayashi, T. (2002). Direct transformation of cubic diamond to hexagonal diamond. *Applied Physics Letters*, 81(4): 610–612.

Jones, A.P., McMillan, P.F., Salzmann, S.G., Alvaro, M., Nestola, F., Prencipe, M., Dobson, D., Hazael, R. & Moore, M. (2016). Structural characterization of natural diamond shocked to 60 GPa; implications for Earth and planetary systems. *Lithos*, 265: 214–221.

Kaminsky, F.V. (2017). *The Earth's lower mantle composition and structure*. Cham: Springer International Publishing. xiii + 331 pp.

Karczemska, A., Szurgot, M., Kozanecki, M., Szynkowska, M.I., Ralchenko, V., Danilenko, V.V., Louda, P. & Mitura, S. (2008). Extraterrestrial, terrestrial and laboratory diamonds — Differences and similarities. *Diamond and Related Materials*, 17(7-10): 1179–1185.

Litvin, Y.A. (2017). *Genesis of diamonds and associated phases*. Cham: Springer International Publishing. xiv + 137 pp.

Luth, R.W., Palyanov, Y.N. & Sokol, A.G. (2022). Petrología experimental aplicada al crecimiento natural del diamante. *Reviews in Mineralogy & Geochemistry*, 88(1): 755–808.

Mao, H.K., Hemley, R.J., Williams, Q., Bassett, W.A. & Downs, R.T. (1996). Pressure-induced transformations of carbon at high pressures. *Science*, 271(5245): 1607–1609.

Miyamoto, M. (1998). Micro Raman Spectroscopy of diamonds in the Canyon Diablo iron meteorite: implication for the shock origin. *Antarctic Meteorite Research*, 11: 171–177.

Murri, M., Smith, R.L., McColl, K., Hart, M., Alvaro, M., Jones, A.P., Németh, P., Salzmann, C.G., Corà, F., Domeneghetti, M.C., Nestola, F., Sobolev, N.V., Vishnevsky, S.A., Logvinova, A.M. & McMillan, P.F. (2019). Quantifying hexagonal stacking in diamond. *Scientific Reports*, 9(10334): 1–8.

Németh, P., Garvie, L.A.J. & Salzmann, C.G. (2023). Canyon Diablo lonsdaleite is a nanocomposite containing C/H stacking disordered diamond and diaphite. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 381(20220344): 1–20.

Németh, P., Lancaster, H.J., Salzmann, C.G., McColl, K., Fogarassy, Z., Garvie, L.A.J., Illés, L., Pécz, B., Murri, M., Corà, F. [et al.] (2022a). Shock-formed carbon materials with intergrown sp3- and sp2-bonded nanostructured units. *Proceedings of the National Academy of Sciences*, 119(28)e2203672119: 1–9.

Németh, P., McColl, K., Garvie, L.A.J., Corà, F., Salzmann, C.G. & McMillan, P.F. (2022b). Impact-formed complex diamond-graphite nanostructures. *Resolution and Discovery*, 6(2021)1: 1–6.

Németh, P., McColl, K., Garvie, L.A.J., Corà, F., Salzmann, C.G. & McMillan, P.F. (2020). Diaphite-structured nanodiamonds with six- and twelve-fold symmetries. *Diamond and Related Materials*, 119(108573): 1–2.

Németh, P., McColl, K., Garvie, L.A.J., Salzmann, C.G. & McMillan, P.F. (2022c). Impact-formed complex diamond-graphite nanostructures. *Resolution and Discovery*, 6(1)2051: 1–6.

Nimis, P. (2022). Pressure and temperature data for diamonds. *Reviews in Mineralogy & Geochemistry*, 88(1): 533–566.

Ohfuji, H., Irifune, T., Litasov, K.D., Yamashita, T., Isobe, F., Afanasiev, V.P. & Pokhilenko, N.P. (2015). Natural occurrence of pure nano-polycrystalline diamond from impact crater. *Scientific Reports*, 5(14702): 1–8.

Ohfuji, H., Nakaya, M., Yelisseyev, A.P., Afanasiev, V.P. & Litasov, K.D. (2017). Mineralogical and crystallographic features of polycrystalline yakutite diamond. *Journal of Mineralogical and Petrological Sciences*, 112: 46–51.

Ovsyuk, N.N., Goryainov, S.V. & Likhacheva, A.Y. (2019). Raman scattering of impact diamonds. *Diamond and Related Materials*, 91: 207–212.

Presser, J.L.B. (Ed.). (2024). *The Capiibary "Diamonds": A window to the lower mantle*. Chisinau: Eliva Press. 325 pp.

Presser, J.L.B., Monteiro, M. & Maldonado, A. (2020). Impact diamonds in an extravagant metal piece found in Paraguay. *Historia Natural*, 3(10)2: 5–15.

Presser, J.L.B. & Sikder, A. (2022). Raman spectroscopic analysis of diamonds and his mineral inclusions from "lamproites" in the Capiibary, San Pedro Dpto., Paraguay. *Historia Natural*, 3(12)3: 5–19.

Presser, J.L.B. & Sikder, A. (2024). Impact diamonds in an extravagant metal piece found in Paraguay: Published Raman spectra revisited. *Revista de la Sociedad Científica del Paraguay*, 29(1): 22–42.

Presser, J.L.B., Sikder, A.M. & Connelly, D.P. (2024a). The Musgrave impact diamonds from MAPCIS very probable impact basin, West Central Australia. *Boletín del Museo Nacional de Historia Natural del Paraguay*, 28(e2024009): 47–57.

Presser, J.L.B., Sikder, M.A. & Meyer, C. (2024b). Onset XRD analysis of lonsdaleite diamonds from "lamproites" in the Capiibary, San Pedro Dpto, Paraguay. Pp. 157–209, *in* Presser, J.L.B. (Ed.). *The Capiibary "Diamonds": A window to the lower mantle*. Chisinau: Eliva Press. 325 pp.

Presser, J.L.B., Sikder, M.A. & Meyer, C. (2024c). Lonsdaleite diamonds from "lamproite" in the Capiibary, San Pedro Dpto, Paraguay. Pp. 2010–233, in Presser, J.L.B. (Ed.). *The Capiibary "Diamonds": A window to the lower mantle*. Chisinau: Eliva Press. 325 pp.

Saitoh, Y., Aoki, K., Matsumoto, T. & Takehana, Y. (1999). Raman spectroscopy of lonsdaleite and diamond under high pressure. *Physical Review B*, 59(5): 3120–3126.

Salzmann, C.G., Murray, B.J. & Shephard, J.J. (2015). Extent of stacking disorder in diamond. *Diamond and Related Materials*, 59: 69–72.

Shames, A.I., Mogilyansky, D., Panich, A.M., Sergeev, N.A., Olszewski, M., Boudou, J.P. & Osipov, V.Y. (2015). XRD, NMR, and EPR study of polycrystalline micro- and nano-diamonds prepared by a shock wave compression method. *Physica Status Solidi A – Applications and Materials Science*, 212(11): 2400–2409.

Simakov, S., Scribano, V., Melnik, N., Pechnikov, V., Drozdova, I., Vyalov, V. & Novikov, M. (2019). Nano and micro diamond formation in nature ultrafine carbon particles on earth and space. Cham: Springer International Publishing. viii + 132 pp.

Sorokhtin, N.O. (2016). *The origins of natural diamonds*. Beverly: Wiley-Scrivener. 532 pp.

Spivak, A.V. & Litvin, Y.A. (2019). *Evolution of magmatic and diamond-forming systems of the Earth's lower mantle*. Cham: Springer International Publishing. xii + 95.

Stachel, T., Brey, G.P. & Harris, J.W. (2022). Inclusiones minerales en diamantes litosféricos: Una revisión. *Reviews in Mineralogy and Geochemistry*, 88(1): 307–391.

Tappert, R. & Tappert, M.C. (2011). *Diamonds* *in nature: A guide to rough diamonds*. Berlin & Heidelberg: Springer-Verlag. xii + 142.

Yang, L., Lau, K.C., Zeng, Z., Zhang, D., Tang, H., Yan, B., Gou, H., Yang, Y., Xiao, Y., Luo, D., Srinivasan, S., Sankaranarayanan, S., Yang, W., Wen, J. & Mao, H. (2021). Lonsdaleite: The diamond with optimized bond lengths and enhanced hardness. *ArXiv*, 2111.09176. [Consulted: 30.iv.2025]. <https://arxiv.org/abs/2111.09176>.

Yelisseyev, A., Gromilov, S., Afanasiev, V., Sildos, I. & Kiisk, V. (2019). Effect of lonsdaleite on the optical properties of impact diamonds. *Diamond and Related Materials*, 101(107640).

Yelisseyev, A., Khrenov, V., Afanasiev, V., Pustovarov, S., Gromilov, A., Panchenko, N., Pokhilenko & Litasov, K. (2015). Luminescence of natural carbon nanomaterial: Impact diamonds from the Popigai crater. *Diamond and Related Materials*, 58: 69–77.