MD Technical Review Letter –

Study of Natural and Synthetic Diamonds in Single-crystal X-ray Diffraction

H. Y. TSANG, K. W. CHENG and Tony K. C. HUI

Master Dynamic Ltd.

Dr. Holger Ott

Bruker AXS GmbH

Introduction

Diamond, well-known to be one of the hardest natural materials in the world, is formed of carbon in the Earth's mantle under extreme temperature and pressure conditions. Unlike the other carbon allotrope graphite, the carbon atoms in diamond connect with one another to form a giant covalent network of tetrahedrally bonded carbon. Due to this atomic arrangement, diamonds have a remarkable hardness [1,2] in contrast to graphite. in which carbon atoms are arranged in hexagonal layers. Each layer is only weakly connected to the next by van der Waal's forces.

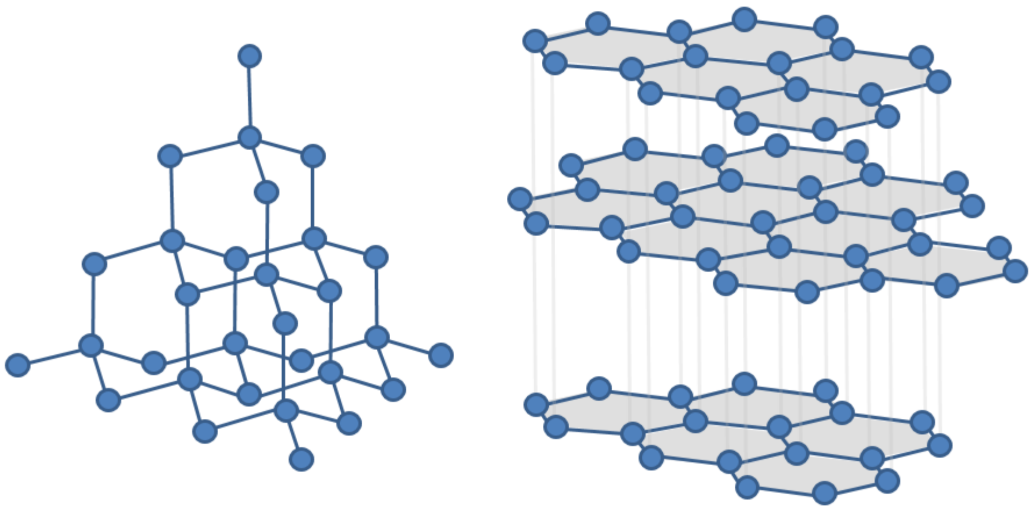

Fig 1. Crystal structures of diamond (left) and graphite (right)

While diamond grows in the nature, it captures nitrogen or other impurities to go inside the diamond lattice. [3,4] Depending on the impurities content, diamond can be classified into two main types:

- Type I diamonds contain nitrogen as main impurities. Nitrogen atoms may substitute the carbon atoms or occupy interstitial sites either as individual atoms (Ib type) or in clusters (Ia type).
- Type II diamonds show either no nitrogen impurities (IIa type) or very low concentrations of nitrogen in the lattice but other impurities such as boron (IIb type). [4]

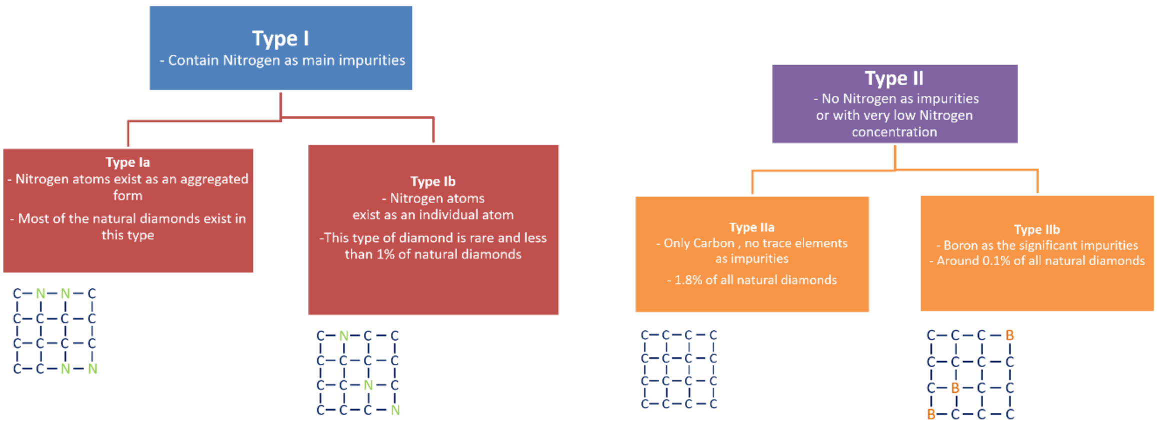

Fig2. (a) Schematics diamond types

Due to the physical and chemical properties of diamond, scientists developed manufacturing methods to produce diamond films or bulk samples for different applications e.g. electronic and health applications. [5, 6] Synthetic diamonds are laboratory-grown diamonds that are made by two common methods - high-pressure high-temperature (HPHT) or chemical vapor deposition(CVD). HPHT diamonds are created from graphite under extremely high temperature and pressure, which imitates the natural process of diamond formation in the earth crust. [7] CVD diamonds are produced from a mixture of hydrogen and hydrocarbon gases (i.e. methane). [8]

In this letter, the differences between natural and synthetic diamonds are elucidated by single-crystal X-ray diffraction (SC-XRD). This technique provides deep insight into the crystal structure of different types of diamonds by interpreting the diffraction patterns.

Experimental Results

The diamonds were first classified into the different diamond types using *BRUKER TENSOR 37 Fourier Transform Infrared (FTIR) Spectrometer*. Afterwards, the single crystal X-ray diffraction measurements were carried out utilizing a *BRUKER D8 VENTURE* with Mo X-ray source. Table 1 summarizes the crystallographic results of different diamond samples:

Type I Diamond				
	Diamond	Type	Lattice Parameter [Å]	Bravais type
01	Natural	Type IaAB	3.562(7)	Cubic F
02	Synthetic	Type IaA	3.569(5)	Cubic F
03	Synthetic	Type IaA	3.564(2)	Cubic F

Table 1. Summary of Type I diamonds

Type II Diamond				
	Diamond	Type	Lattice Parameter [Å]	Bravais type
04	Natural	Type IIa	3.513(12)	Cubic F
05	Synthetic	Type IIa	3.526(13)	Cubic F
06	Synthetic	Type IIa	3.555(8)	Cubic F
07	Synthetic	Type IIa	3.547(12)	Cubic F

Table 2. Summary of Type II diamonds

The rotation frames of all the diamond samples were recorded with the *Bruker APEX3* software package:

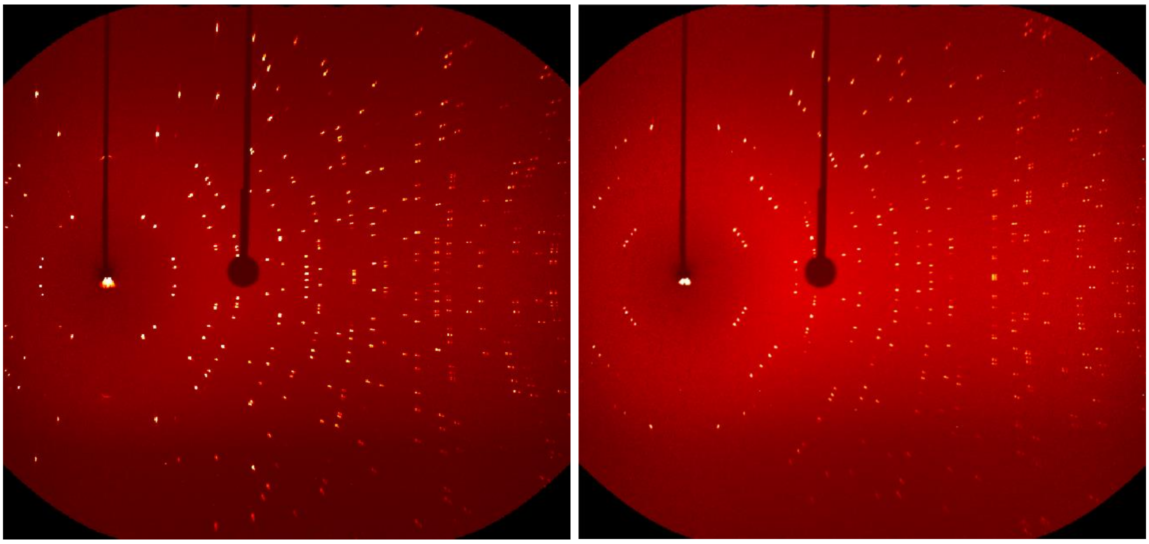

Fig3. Diffraction pattern of the Type IaAB natural diamond (a) and a Type IaA CVD synthetic diamond (b)

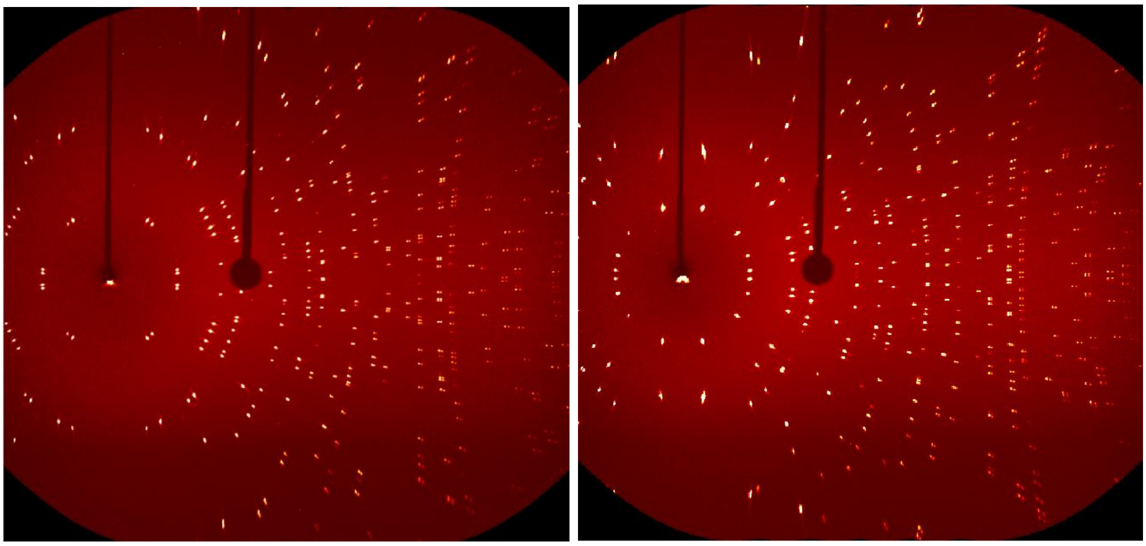

Fig4. Diffraction Pattern of Type IIa natural diamond (a) and Type IIa CVD synthetic diamond (b)

All diffraction patterns were integrated in a 2θ range of 15° - 55° (corresponding to 2.72 - 0.77 Å resolution) to give a 1D diffractogram and analyzed with the *Bruker DIFFRAC.EVA* software. All diamonds show the same number of diffraction peaks. Their positions are compared to the diffraction peaks of diamond in PDF database (PDF-01-071-3649).

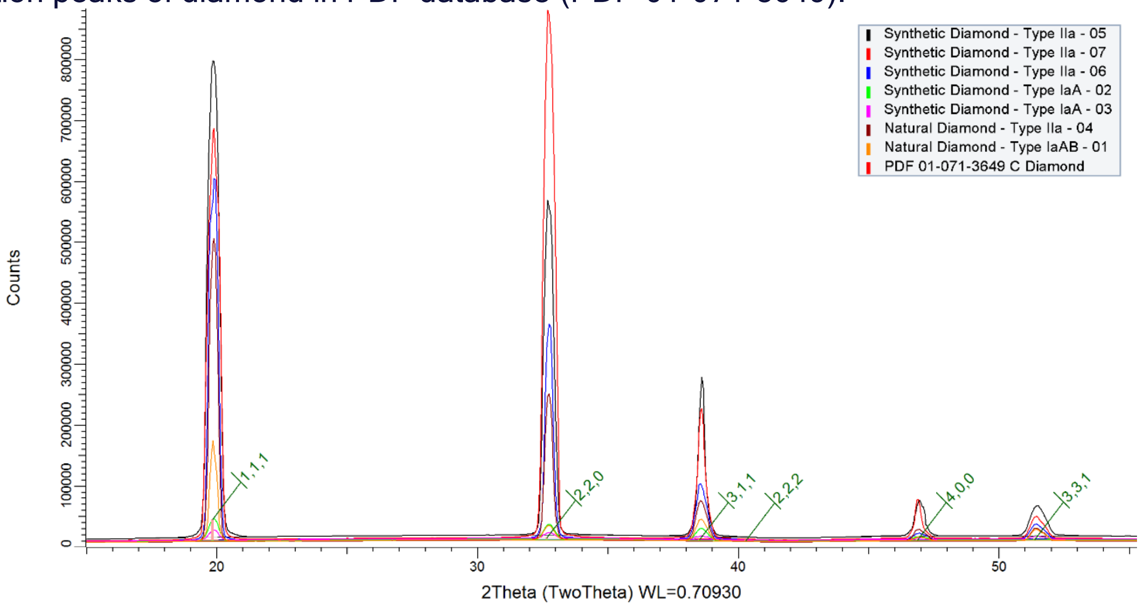

Fig5. Diffractograms of all diamond samples

In the above results, the type I natural diamond has the sharp diffraction spots then the type I synthetic diamond. Diffraction spots are arranged more closely-packed in CVD synthetic diamonds. The lattice parameters of the natural and the corresponding synthetic diamonds are close to each other. The presence of the nitrogen atoms in the type I diamonds expand the diamond lattice resulting in larger lattice parameters.[9]

Even though the value of the lattice constants between the same type of natural diamonds and CVD diamonds are very close to each other, there is a subtle difference. The packing of carbon atoms seems to be slightly different between natural and synthetic diamonds.[10]

Conclusion

The crystal structures and the differences between natural and synthetic diamonds were studied and compared by X-ray diffraction techniques in terms of the lattice constants derived from the diffraction patterns. The difference between the lattice parameters of type I and type II diamond can be attributed to the impurities.

About the Authors

Miss H. Y. Tsang is Process Engineer, Mr. K.W. Cheng is Technical Manager and and Mr. Tony K.C. Hui is Senior Director of Nanotechnology Development & Applications Centre (NTAC) at Master Dynamic Limited in Hong Kong.

Dr. Holger Ott is the Global Application Coordinator SC-XRD (Single Crystal X-ray Diffraction) and Senior Application Scientist at the Bruker AXS GmbH in Germany.

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