

High-performance diamond “Supertools” with extreme tool-life

I.S. Durazo-Cardenas^a, Saurav Goel^{b,c,*}, P. Shore^a, L. Kirkwood^a, Graham L.W. Cross^d

^a Faculty of Engineering and Applied Sciences, Cranfield University, MK43 0AL, UK

^b School of Engineering and Design, London South Bank University, London SE10, AA, UK

^c University of Petroleum and Energy Studies, Dehradun 248007, India

^d Advanced Materials and Bioengineering Research (AMBER) Centre (CRANN) and School of Physics, Trinity College, Dublin 2, Ireland

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ABSTRACT

The use of diamond as a cutting tool is pervasive in modern ultra-high-precision machining applications, particularly for generating sub-micron accurate features through the Single Point Diamond Machining (SPDM) method. Beyond SPDM, diamond is also widely employed in contact profilometry (imaging), nanoindentation, nanoimpact, nanoscratching, and lithography applications.

Interestingly, a particular type of diamond, commonly used in what the fabrication industry calls “supertools,” consistently demonstrates a lifespan up to 300% longer than that of standard diamond tools. Despite this remarkable performance, the reasons behind the enhanced durability of these unique diamond tools have remained unclear.

This paper provides the first experimental explanation for the exceptional properties of these “supertools”. Using Fourier Transform Infrared Spectroscopy (FTIR), we establish that such diamond possess higher overall concentration of nitrogen, particularly Defect Type A (type IaA) and Defect Type C (type Ib). Counterintuitively, they also exhibit lower residual stresses, as revealed through cross-polar examination. Moreover, the diamond tip misalignment error, estimated using Laue backscattering analysis, was found to be insignificant in governing the tool wear resistance. These findings suggest that the wear resistance of natural diamonds can be predicted by screening for high levels of nitrogen defects (combination of Type A and Type C). This insight offers valuable potential for selecting superior diamonds for high-value manufacturing.

1. Introduction

Wear-resistant diamond tools, often referred to as “supertools” play a critical role in enabling uninterrupted fabrication of large, free-form shapes and lightweight optical components. These tools are particularly essential for the ultra-high-precision fabrication process known as Single Point Diamond Machining (SPDM), widely used in machining optical elements for infrared applications [1,2].

Certain materials with high chemical affinity to carbon pose significant challenges for diamond machining, leading to severe tool wear. As shown in Fig. 1 [3], various metals classified as non-machinable by diamond cutting tools are highlighted in red. Despite the diamond's extreme hardness, the frictional contact with metals like tungsten (W), iron (Fe), and tantalum (Ta) results in rapid degradation of the diamond's edge radius.

Conversely, materials highlighted in green, such as copper (Cu) and germanium (Ge), exhibit high machinability. Diamond tools can be used

to cut these materials uninterruptedly, achieving cutting lengths of several kilometers without significant wear.

Previous case studies have suggested that the rapid wear of diamonds during the machining of “non-machinable” metals and certain other materials may be attributed to the presence of unpaired d-shell electrons in the substrate being cut [4]. However, notable exceptions challenge this argument. For instance, materials such as beryllium (in machining CuBe) and silicon cause severe chemical wear on diamond tools, despite neither possessing unpaired d-shell electrons [5]. An alternative explanation lies in the electronic structure of diamonds. The diamond lattice has four valence electrons, but only a maximum of three can form stable surface bonds. This leaves one or two “dangling bonds,” which are highly reactive and prone to interactions with elements like silicon, iron, and beryllium [6]. Despite significant research efforts over the years, the precise mechanisms underlying diamond tool wear remain elusive. Understanding the origins of diamond wear requires further investigation to achieve a comprehensive explanation of these complex wear

* Corresponding author at: School of Engineering and Design, London South Bank University, London SE10, AA, UK.

E-mail address: Goels@LSBU.ac.uk (S. Goel).

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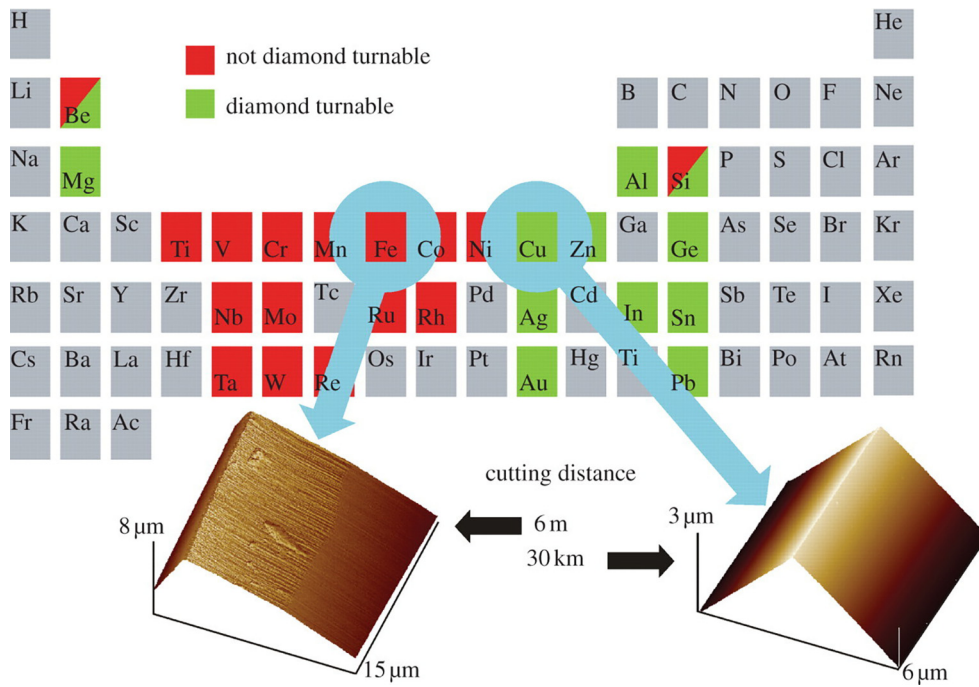


Fig. 1. Microscopic inspection of the diamond tool cutting edge in case of machining (left) iron and (right) copper [3].

Table I
Classification of diamonds [8].

	Type I		Type II (Extremely good heat conductors)	
	I _a	I _b	II _a	II _b
Nitrogen (ppm)	~200–2400	~40	~8–40	~5–40
Boron (ppm)	None	None	None	~0.5
Remarks	Nitrogen exists in small geometrically clustered groups	Nitrogen exists as isolated substitution atoms	Chemically pure with very little nitrogen	Little nitrogen but contains substantial boron impurities

processes.

What makes this field particularly fascinating is the observation that even when cutting the same material under similar conditions, different diamond tools exhibit varying wear patterns [7]. No clear explanations currently exist in the literature to account for why the machining of a given material results in inconsistent diamond wear.

A prior study conducted by the authors of this paper [7] revealed a remarkable finding: one specific diamond tool demonstrated significantly stronger wear resistance, lasting approximately 300 % longer than other diamonds tested. Extensive additional testing confirmed this tool's superior performance, showing it to be independent of coolant type, machining parameters, and tool edge refurbishment. This exceptional tool, later dubbed the mysterious “supertool” remained an unexplained phenomenon for over a decade. The quest to unravel the mystery of the “supertool” became the primary motivation behind this research, aiming to uncover the origins of its unparalleled durability.

The current industrial practice for screening diamonds primarily relies on the *gem's* colour, which serves as a basic indicator of quality. While more sophisticated optical characterization methods can provide a quantitative assessment of diamond properties, these techniques are both time-consuming and costly.

As outlined in Table I, diamonds can be broadly classified based on

the presence of trace impurities such as boron and nitrogen. These impurities significantly influence the behaviour and performance of diamond tools, affecting their wear resistance, thermal conductivity, and machinability.

Type IIb diamonds are widely recognised to offer consistent repeatability in their operational lifetimes. Diamonds may also contain planar precipitates, commonly referred to as platelets, which lie on the (100) crystallographic plane. These platelets can be detected using X-ray topography and Fourier Transform Infrared Spectroscopy (FTIR) [9].

Type I diamonds, in contrast to Type II, are characterised by low dislocation density and a high density of two-dimensional platelet defects [10], which limits dislocation mobility. Nitrogen atoms in diamonds can exist as single substitutional impurities, characteristic of Type Ib diamonds, or aggregate into clusters over time. In Type Ia diamonds, nitrogen commonly forms A-centers, consisting of paired nitrogen atoms, or B-centers, comprising four nitrogen atoms surrounding a vacancy. Platelet defects are hypothesized to arise from the interaction of nitrogen aggregates with vacancies or interstitial carbon atoms, resulting in planar structures within the diamond lattice. High-temperature and high-pressure conditions facilitate the migration and clustering of nitrogen atoms, thereby promoting the development of platelet defects. These defects are typically aligned parallel to the (111) crystallographic planes, which represent the densest atomic packing in the cubic diamond lattice. There are other types of defects observed in diamonds and a summary of these defects along with their corresponding FTIR spectra can be seen from Fig. 2.

Primarily, the main defects observed in diamond are:

- Defect type A: Pairs of nitrogen atoms substituting for two adjacent carbon atoms in the diamond lattice (type IaA diamond).
- Defect type B: Clusters of four nitrogen atoms surrounding a single carbon vacancy (type IaB diamond).
- Defect type C: Single substitutional nitrogen atoms replacing individual carbon atoms in the lattice (type Ib diamond).
- Defect type D (Platelet): They are planar defects typically associated with nitrogen aggregates, often aligned parallel to the (111) planes (Mostly type Ia diamond).

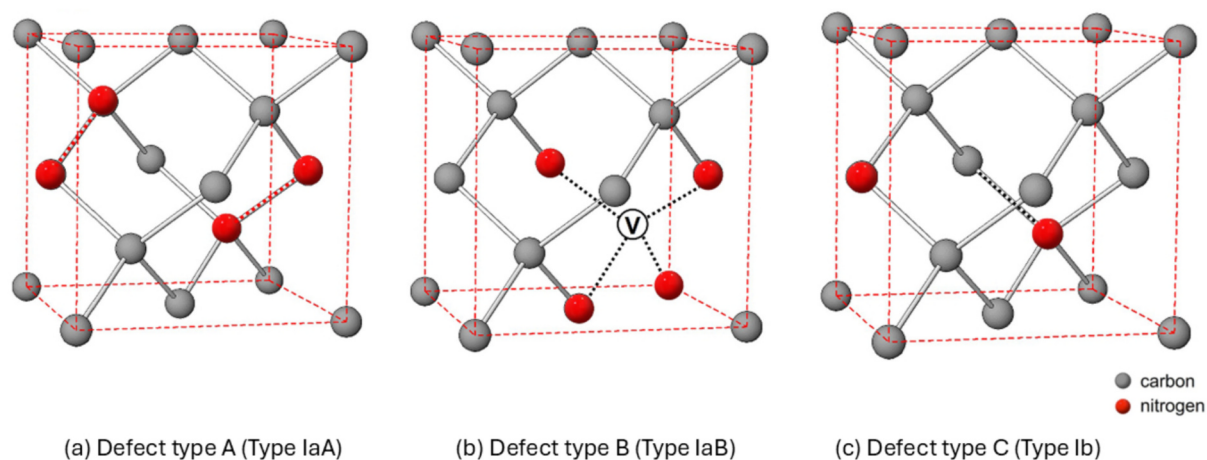
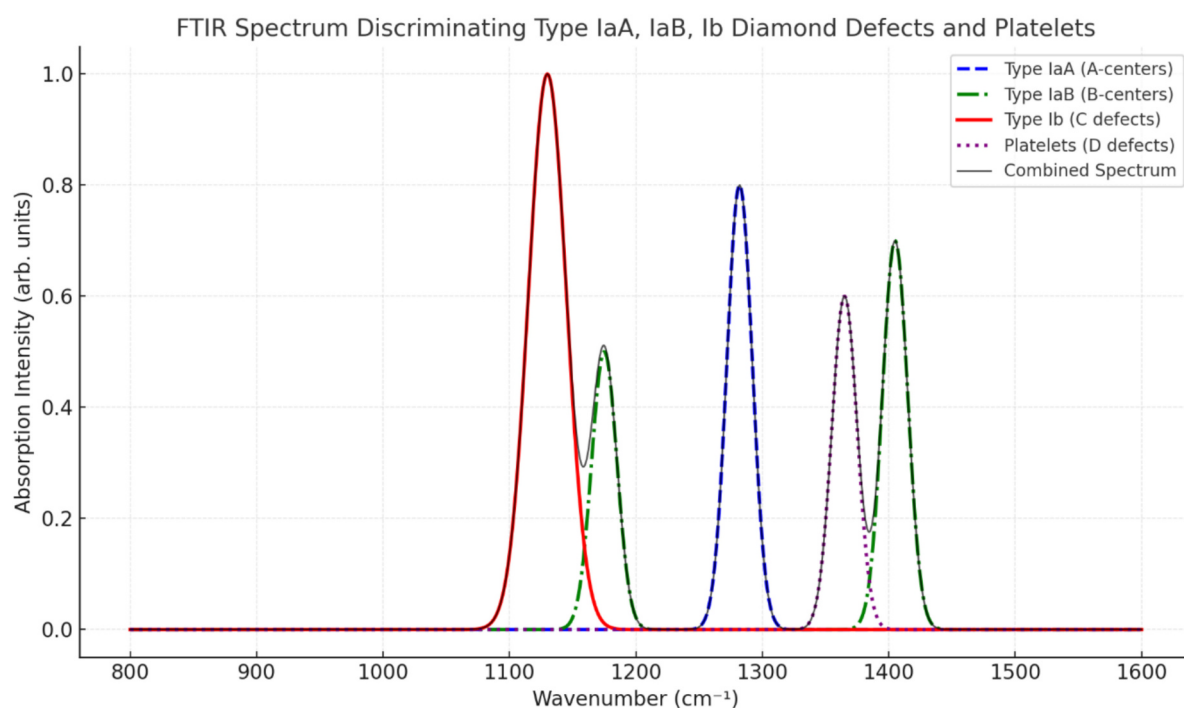


Fig. 2. Structural configuration of various extrinsic defects observed commonly in diamond [11] and a graph showing how FTIR spectra will discriminate different types of defects in diamond.

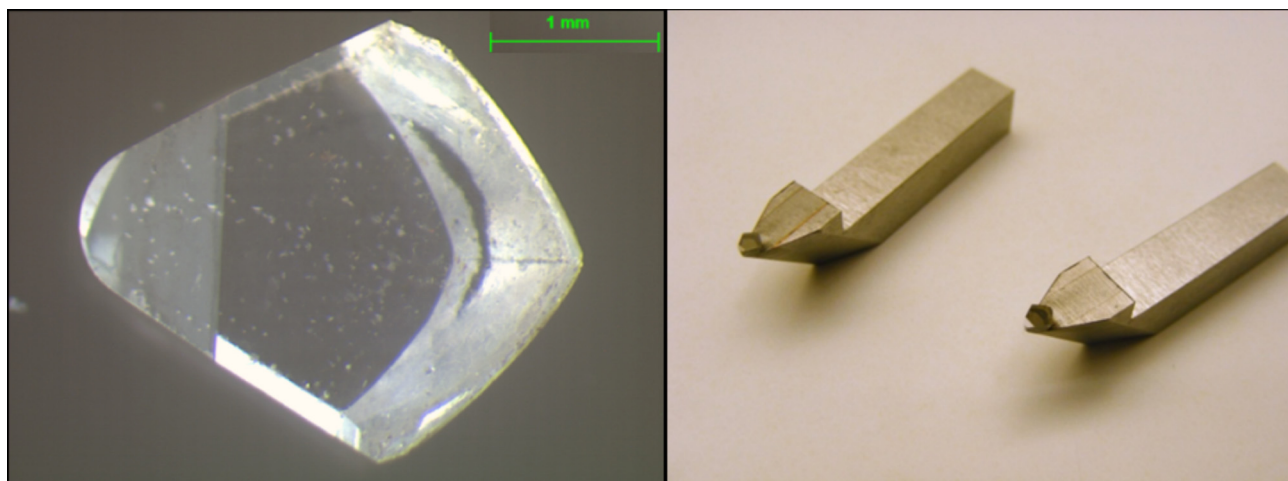
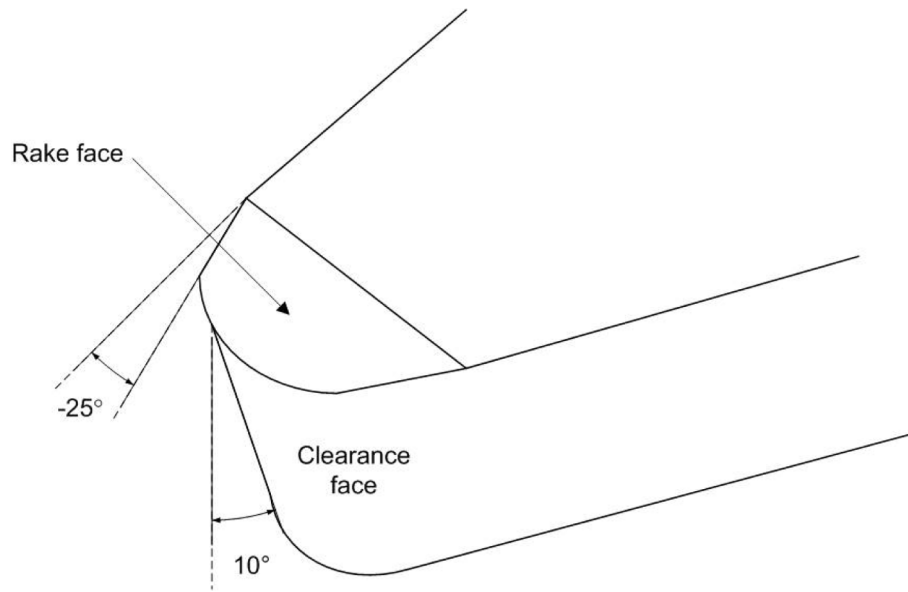
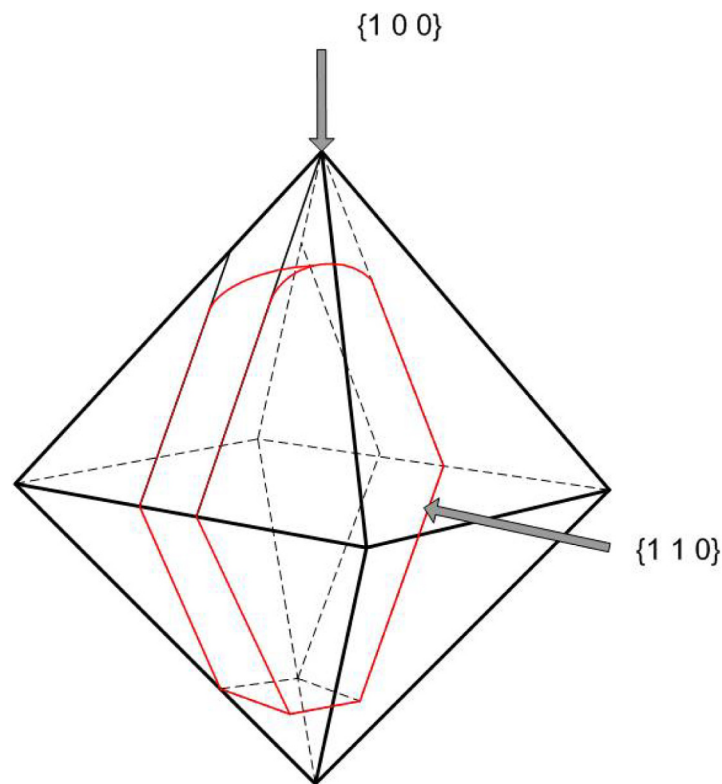


Fig. 3. (Left) micro-photograph of typical gemstone used for SPDT diamond tools. (Right) Natural gemstone diamond tools.



(a)



(b)

Fig. 4. (a) Schematic of the typical geometry of a diamond tool used for SPDT of optical grade silicon. The tools have a radius, a top rake face at -25° and a clearance face at 10° (b) schematic of the dodec tool ($1\ 1\ 0/1\ 1\ 0$ orientation) [17,18].

- Defect type X: Complex aggregates of nitrogen and possibly other impurities or lattice vacancies (Mostly Type Ib diamonds or Type IaB diamonds).

The plastic deformation, abrasion resistance and mechanical

properties of diamonds are frequently linked to nitrogen content [12] and the presence of platelets [13]. Another factor influencing diamond tool performance is the crystal lattice orientation of the diamond relative to the tool cutting geometry [10,14,15].

Additionally, birefringence caused by internal stress has been

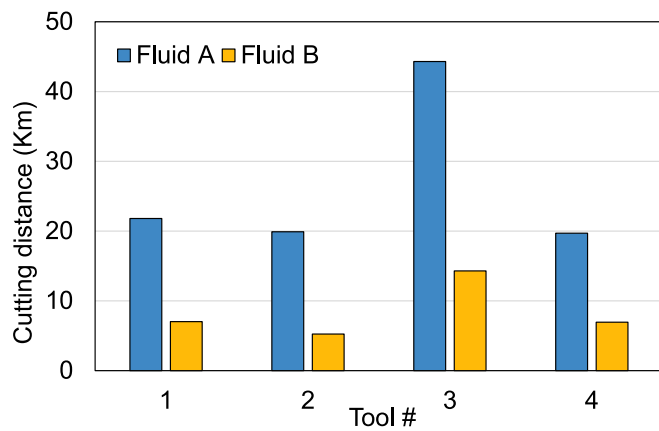


Fig. 5. Cutting distance in km achieved before the onset of brittle fracture by diamond tool [7]. The chart clearly illustrates the longer life achieved by tool #3. A feed rate of 1 $\mu\text{m}/\text{rev}$, a depth of cut of 10 μm and a spindle speed of 600 rpm were used. Fluid A is a water-based coolant, while fluid B is oil based.

suggested as an indicator of mechanical instability [16], which may impact performance. Building on the existing literature, the subsequent sections of this study focus on comparing the wear-resistant “supertool” with standard diamond tools exhibiting average performance. The key parameters used for experimental comparison include nitrogen content, defect type, orientation and residual stress within the tools.

2. Material and analytical methods

Several natural single-crystal diamond tools with identical specifications, including the previously identified “Supertool” were prepared in a controlled manner. The nitrogen content was examined using FTIR analysis while Laue scattering was used to examine the alignment error

while polarised light microscopy was used to estimate the presence of residual stresses in the specimens.

2.1. Diamond tool specimens

The diamond tools were produced from high-quality industrial grade single crystal gemstones and prepared by a well-known diamond tool fabricator company (*Contour Fine Tooling*) to be of the same specifications. The tool geometry was that of a 0.5 mm nose radius, -25° top rake angle and 10° clearance angle (Fig. 3 and Fig. 4).

In this configuration, the cutting-edge radius was contoured on the (100) plane, while the top rake surface was polished onto the (110) plane, as depicted in Fig. 4. Notably, no characterization of the gemstones' nitrogen content, orientation, or strain patterns was conducted before fabricating the tools. Additionally, the geographical and geological origins of the gemstones were unknown. The wear resistance of the diamond tools against silicon was evaluated based on the cutting distance (in kilometers), as previously reported [7] and shown in Fig. 5, where several tools were compared and a particular tool showed exceedingly good performance. Among the tested specimens, specimen #3 demonstrated the longest cutting distance, indicating superior wear resistance.

2.2. Fourier transform infra-red spectroscopy

Infrared absorbance spectra of the diamond tools were measured using a *spectrum One* Perkin Elmer FTIR spectrometer. The spectra plots were used to estimate the nitrogen content from its aggregation state by measuring the absorption coefficient at 1282 cm^{-1} [19,20]. The spectra were acquired from 100 scans over a spectral range from 4000 to 400 cm^{-1} . The infrared spectral envelopes were de-convoluted into components generated by the different centres, using a linear least-squares regression program that determines the nitrogen aggregation. In addition, the average radius of the platelet defects was obtained from the

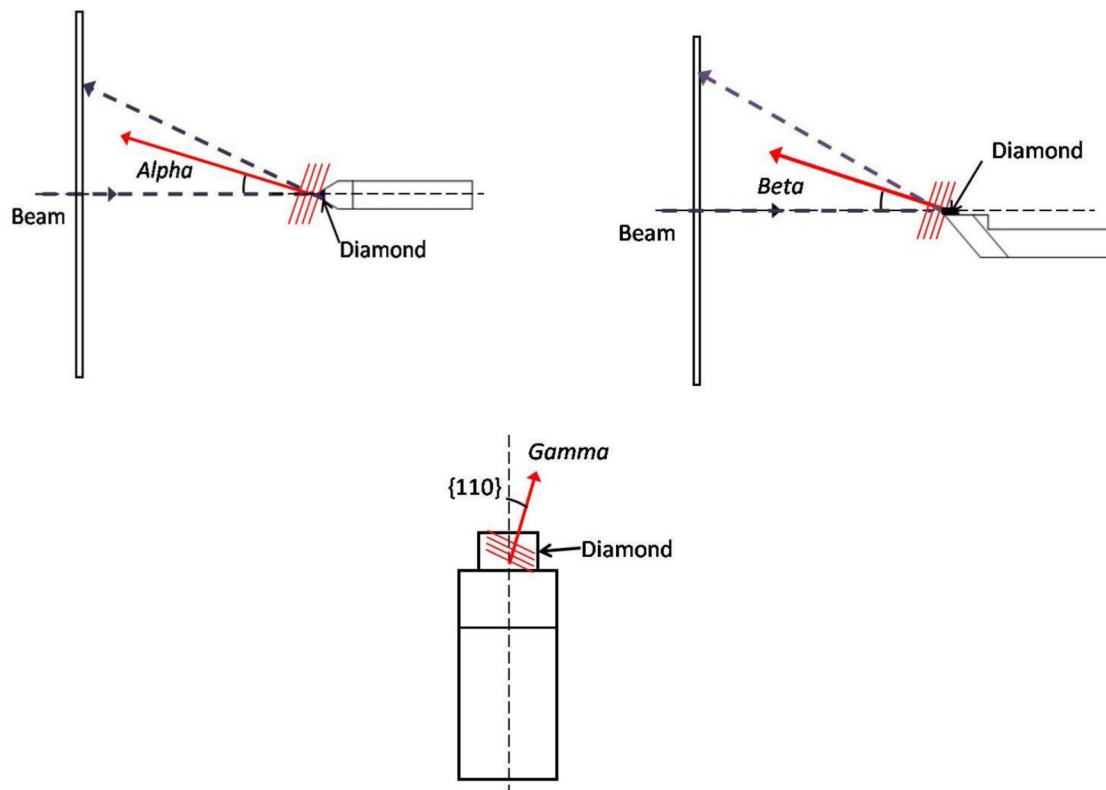


Fig. 6. Laue backscattering analysis set up showing the measurement of Alpha, Beta and Gamma.

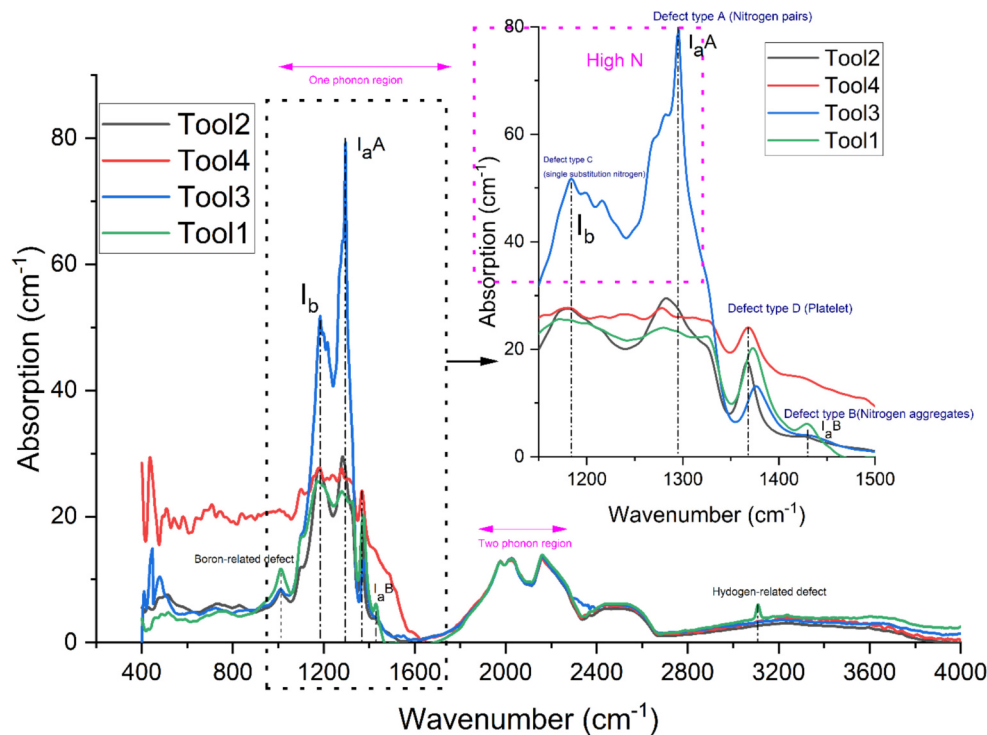


Fig. 7. The FTIR spectra of all four diamond tools investigated in this work labelled to highlight various defects. Tool 3 (high wear resistant) showed a significantly high content of N atoms present both in Defect Type A (type IaA) and Defect Type C (type Ib).

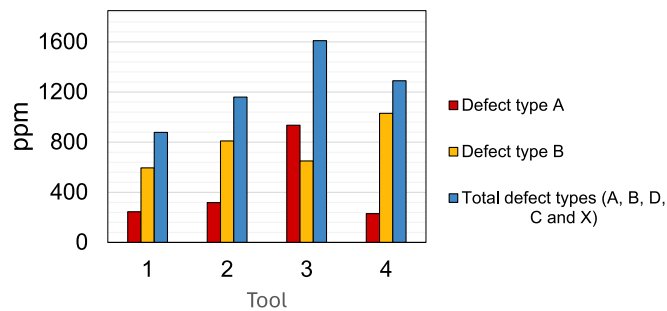


Fig. 8. FTIR analysis results showing the estimates of Defect type A, Defect Type B and number of cumulative defects (A, B, D, C and X) in the four diamond tools used in the study.

FTIR spectra. The precise location of the absorption peak around 1370 cm^{-1} is known to be related to average platelet radius [19]. For this measurement, higher resolution scans were performed at $\pm 5\text{ cm}^{-1}$ off the observed peak for each diamond tool.

2.3. Laue scattering photography

The Laue scattering photographic technique was performed on each tool to determine the orientation error of the diamond gem concerning the tool's geometry. Orientation error has traditionally been considered a factor in the performance of diamond tools because of diamond's anisotropic nature [10,19,20].

The deviation or incorrect positioning of the diamond tip orientation (referred to as misalignment error) with respect to the geometry of the tool is expected to significantly influence the diamond tool's wear resistance. Misalignment errors are primarily introduced during the fabrication process.

In this investigation, misorientation error was measured with respect to the three most significant directions: vertical axis (Alpha), horizontal

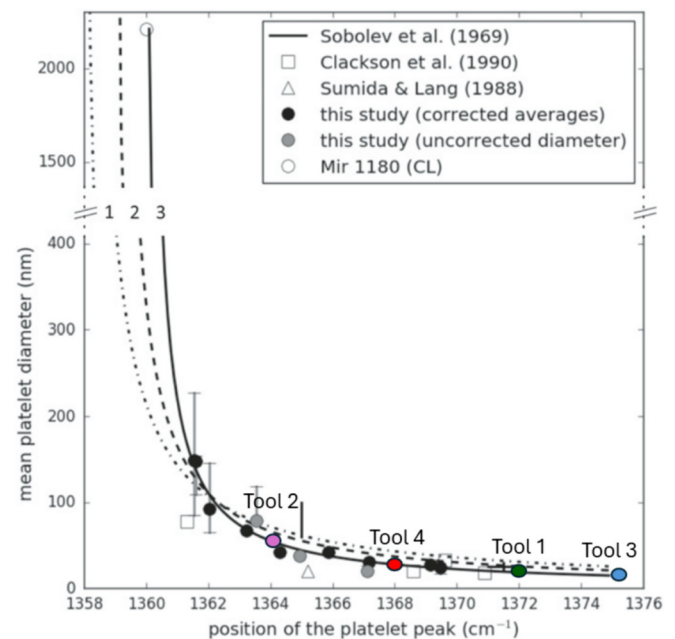


Fig. 9. Variation of platelet peak position in the FTIR spectra with mean platelet diameter [22].

axis (Beta) and the lattice rotational misorientation (Gamma). The accuracy of the measurement was 0.5° , 0.5° and 1° , respectively. The tool was aligned with each measured axis being parallel to the photographic film, and the diamond's cutting edge facing the film. Fig. 6 illustrates the setup used to determine the orientation of the diamond gem with respect to the tool geometry.

Table II

Results of Laue scattering showing the misorientation error with respect to alpha, beta and gamma.

Tool#	Alpha	Beta	Gamma
1	-3.5	0.5	0
2	-8.5	4.5	2
3	3.5	-3	0
4	-7	-4	0

2.4. Polarised light microscopy

Strain patterns in the structure of diamonds can be detected using polarised light microscopy, between cross polars. Diamond as a crystal is not birefringent and is optically isotropic. However, strain introduced by dislocations, lattice distortion (elastic strain), inclusions, plastic deformation, and fracture during growth or from applied stress, may result in the structure of the diamond becoming anisotropic [19], causing birefringence. Polarised light microscopy is a qualitative technique used [16,20] to find a correlation between the observed strain patterns and the performance of SPDM diamond tools.

3. Results and discussions

The FTIR spectra of all four diamonds showed strong absorption at the A and B defect peaks of 1282 cm^{-1} and 1174 cm^{-1} , respectively, as illustrated in Fig. 7. These confirmed that the gemstones used for the diamond tools were of a mixed type IaB with nitrogen aggregates comprising 2 atoms as well as 4 atom clusters both present.

The FTIR spectra were de-convoluted and further decomposed into a total of five sub-spectra, the three main components for defects A, B and D (platelet related) and two additional components: C and X. These sub-spectra reveal the quantity of each defect type, which are then added to

give the total amount of nitrogen in each sample (see Fig. 8).

De-convolution of the FTIR spectra revealed total nitrogen concentrations ranging from 912 to 1648 ppm. The diamond belonging to tool #3 possessed the highest nitrogen content, as much as 318 ppm more than any other tool, as shown in Fig. 8. This was clearly a difference between Tool #3 (the wear resistant tool) and the other diamonds with average wear resistance. However, the defect type that appears most significant resulting from the FTIR analysis is the two-nitrogen substitutional type-A defect present in diamond #3 with a total of 966.4 ppm, or 275 % more than any other of the tools studied.

Meanwhile, tool #3 had reduced levels of the four nitrogen with vacancy type-B defect than tools #2 and #4, and a similar amount to that of tool #1. We conclude therefore that the influence of type-B defects on the wear resistance of the cutting tool during SPDM of silicon is a less dominant factor.

The wear of diamond tools during SPDM of silicon [7] was reported to be arising due to the atom-by-atom attrition that gradually leads to significant micro-cracks and chipping [13] with location of these chips playing a significant role in governing the tool life [21].

Type IaA diamonds are associated with an additional anomalous peak in the region of 1372 cm^{-1} , related to the development of platelets (Fig. 2). The position of these platelet peaks in Fig. 7 varied slightly from specimen to specimen with values ranging from 1367 to 1376 cm^{-1} . The platelet peak position is inversely correlated to platelet size, where larger platelets correspond to the lower peak positions ($\leq 1367\text{ cm}^{-1}$) and smaller platelets of about 20 nm in radius correspond to high peak positions ($\sim 1374\text{ cm}^{-1}$) [9].

There are different empirical formulations to obtain information about platelet size from the FTIR spectra. For instance, one of the works [9] suggest that the average platelet diameter “D” in a diamond can be estimated using the eq. $D = ax - b$ where “x” is the position of the platelet in the IR spectrum while “a” is a constant and “b” is the minimum

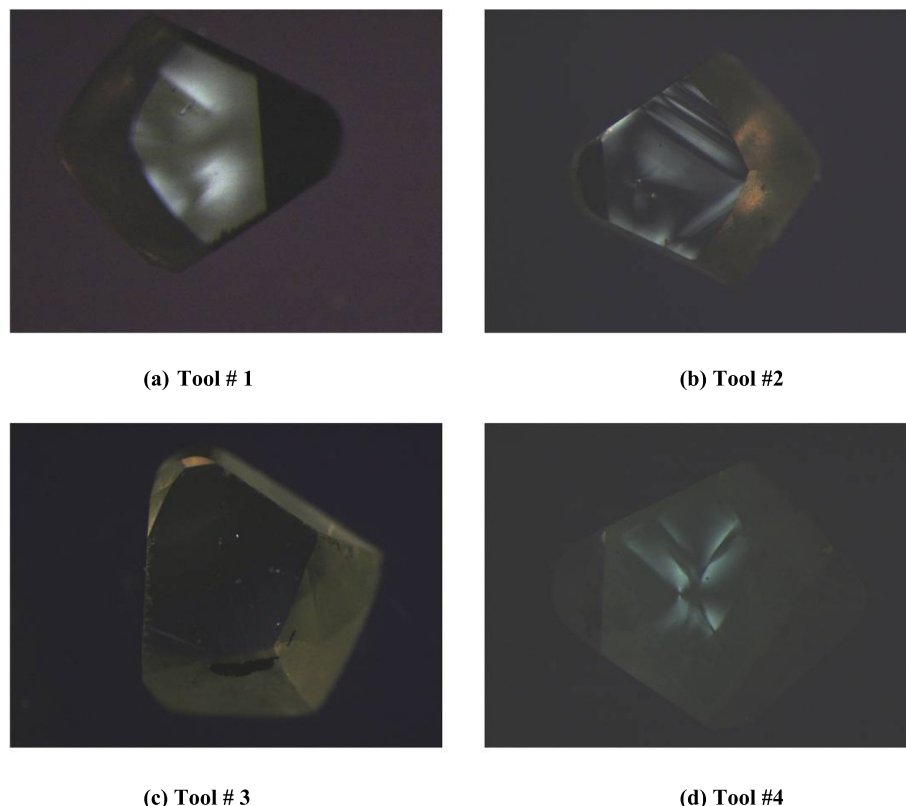


Fig. 10. Cross-polar images of the diamond tools shown in (a), (b), (c) and (d). Tool #3 (c) was seen free from the strain patterns.

position of the platelet peak. More recent works used FTIR together with TEM to develop a generic plot, which was used here to obtain the estimated size of the platelets from the FTIR spectra (See Fig. 9).

From Fig. 9, the mean platelet diameter (D) for tools 1, 2, 3 and 4 were obtained as 60.5 nm, 181 nm, 49.8 nm and 89 nm respectively. In contrast to the present research's findings, a recently published study of SPDT of copper [13] showed that larger platelet radius and lower nitrogen content were related to higher wear resistance. It is believed, however, that these differences are mainly attributable to the different wear mechanisms observed for the different substrate materials of copper vs. silicon. The wear of diamond during SPDM of optical silicon is typical of an atom-by-atom attrition nature, which leads to micro-cracking and subsequently micro-chipping [21]. In contrast, the wear characteristics observed during SPDM of copper was typically have craters on the rake face of the diamond tool [8]. The underlying reason appears to be straightforward. Materials with a higher affinity for reacting with carbon in diamond, such as silicon, tend to form carbides and predominantly exhibit flank wear. In contrast, materials like copper, which have a greater affinity for environmental oxygen rather than carbon, primarily fail on the rake face, resulting in crater wear.

Table II shows the misorientation error results using the Laue scattering technique. These showed there was a wide scattering of Alpha (12°) and Beta (8.5°), the alignment error with respect to the vertical and horizontal axis, respectively. Only tool #2 showed a misalignment error with respect to Gamma of 2° . However, this did not appear to be significant.

It has been argued [23,24] that misorientation error may affect the quality of diamond tools. The range of misorientation error observed for tools 1, 2 and 4 was of 5 and 8.5° for Alpha and Beta, respectively. Despite the scatter observed, all these tools showed very similar levels of wear resistance (see earlier Fig. 5). Whereas diamond tool #3, the wear-resistant tool, showed an Alpha misalignment of 3.5° , which is similar in magnitude to tools 1, 2 and 4. From these results, it is concluded that misorientation error within these parameters is not a dominant factor in tool performance during SPDT of silicon.

Comparison of the cross-polar analyzer photographs obtained by polarised light microscopy, revealed significant differences between diamond #3, the wear resistant tool, and the other tools. The wear resistant tool showed minimal strain patterns (Fig. 10) that were only appreciable around the cutting edge. In contrast, tools 1, 2 and 4 showed clearly distinguishable strain patterns. The geological background and growth conditions of diamond #3 were unknown, therefore establishing the reasons for the minimal strain patterns observed has not been possible.

The causes of strain in diamonds are well-documented [19]; with plastic deformation being very significant. A recent study [25] reports that the presence of nitrogen defects stiffens the diamond lattice against distortion caused by plastic deformation. Similarly, it is believed that the relative abundance of nitrogen type-A defects in diamond #3 prevented its structure from distorting widely. Therefore, this tool's exceptional wear resistance and the lack of obvious strain patterns may be linked.

In contrast to the polarised light microscopy cross-polar findings, a previous tool wear study [26] found no apparent relationship between internal stresses and wear of tools whilst SPDM of copper and aluminium. The differences with the present work are mainly attributable to the wear mechanisms experienced whilst SPDM of optical silicon and those of copper or aluminium. In the case of copper and aluminium substrates, nitrogen inclusions do not seem to have an appreciable positive effect.

In summary the present study, three of the principal factors suggested to influence tool wear resistance during SPDT of brittle materials such as optical silicon have been investigated. Four gemstones, one of which had observed superior wear resistance, were subjected to FTIR analysis for nitrogen content, Laue scattering X-ray diffraction for misorientation and polarised light microscopy for residual stresses. The results showed that nitrogen content and specifically the number of

type-A defects was the most significant factor relating to tool wear resistance. The size of average platelet radius did not produce a significant influence. Misorientation of the gemstone with respect to the tool geometry also showed not to be a dominant factor. Lower strain patterns were linked to high nitrogen content and may also be related to wear resistance.

We suggest from our analysis here that the abundance of type-A defects accounts for the improved wear resistance observed, by making diamond #3 less brittle and therefore retarding the formation of micro-cracks and chipping along the tool's cutting edge.

4. Conclusions

- (i) The most notable difference between the wear-resistant "super-tool" and standard diamond tools lies in its nitrogen content. The wear-resistant tool contains a higher overall concentration of nitrogen, particularly Defect Type A (type IaA) and Defect Type C (type Ib). The abundance of Defect Type-A is strongly correlated with the previously observed three times tool life than ordinary diamond tool life.
- (ii) The average radius of platelets does not appear to significantly influence the wear resistance of natural single-crystal diamonds used for machining optical materials.
- (iii) Laue backscattering analysis confirms that the deviation or incorrect positioning of the diamond tip orientation (referred to as misalignment error) is not a significant factor influencing the wear resistance of natural single-crystal diamonds.
- (iv) The wear-resistant tool exhibited minimal internal strain, which could be attributed to its higher nitrogen content. This likely enhances lattice stiffness, reducing susceptibility to plastic deformation and distortion.

CRediT authorship contribution statement

I.S. Durazo-Cardenas: Writing – original draft, Investigation, Conceptualization. **Saurav Goel:** Writing – original draft, Visualization, Formal analysis. **P. Shore:** Supervision, Project administration. **L. Kirkwood:** Writing – review & editing. **Graham L.W. Cross :** Writing – review & editing, Methodology.

Declaration of Generative AI and AI-assisted technologies in the writing process

During the preparation of this work, the author(s) used AI assistance to improve the readability and language of the manuscript. The authors reviewed and edited the final content and took full responsibility for the content of the published article.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

The datasets used and/or analysed during the current study are available from the corresponding author on reasonable request.

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