

# Defects, impurities and inclusion–host interfaces in diamond: an atomic-scale physico-chemical framework

Paula Sophie Walkow – A non peer-reviewed preprint

## Abstract

The term “inclusion” is widely used in diamond research to describe internal features that differ fundamentally in their physical nature. In practice, atomic-scale lattice defects and chemically distinct foreign phases are frequently conflated, leading to ambiguity in the interpretation of microstructural observations.

This paper presents a conceptual physico-chemical framework that distinguishes lattice-incorporated defects from true inclusions based on crystalline continuity and interface physics. Rather than treating defects and inclusions as a continuum, the framework defines them as categorically distinct entities separated by the presence or absence of lattice discontinuity.

The analysis focuses on the response of the diamond host lattice to mechanically incompatible second phases. Microstructural features commonly observed at the optical scale are interpreted as elastic, defect-mediated, or brittle accommodation mechanisms within the host crystal. By clarifying the physical categories underlying these observations, the framework provides consistent interpretive boundary conditions for the analysis of defects and inclusions in crystalline solids.

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Diamond hosts a wide range of foreign features commonly referred to as “inclusions”, a term that is frequently used ambiguously to describe both atomic-scale lattice defects and macroscopic foreign phases. While such terminology may be convenient in descriptive contexts, it obscures a fundamental physical distinction: lattice defects and true inclusions are governed by fundamentally different structural and energetic principles and cannot be treated as equivalent entities.

Atomic-scale defects—including substitutional impurities, vacancies, and defect complexes—are intrinsic components of the diamond lattice. They modify the local bonding environment and electronic structure but remain fully embedded within the crystalline framework. True inclusions, in contrast, constitute chemically and mechanically distinct phases that are not incorporated into the diamond lattice but coexist with it as separate entities. From a solid-state perspective, this distinction is not merely semantic but categorical.

Failure to clearly separate these two classes of features has led to systematic ambiguity in the interpretation of optical and spectroscopic observations. In particular, defect-rich zones surrounding inclusions are frequently conflated with the inclusions themselves, giving rise to misleading concepts such as “micro-inclusions” or “inclusion clouds” at scales where no secondary phase is present.

The central aim of this work is therefore not the direct identification of atomic-scale defects, but the establishment of a \*\*physically consistent framework\*\* that separates lattice-incorporated defects from true inclusions based on first principles. The approach adopted here emphasises the role of the diamond host lattice as an active physical system whose response reveals the presence of a second phase. By re-framing defects and inclusions according to their fundamental physical nature, this work seeks to restore conceptual clarity to terminology that is widely employed yet frequently applied in an inconsistent or ambiguous manner.

## Diamond as a Host Lattice: Physico-Chemical Constraints

Diamond crystallises in the cubic crystal system with a face-centred cubic lattice and a two-atom basis, forming a three-dimensional network of tetrahedrally coordinated carbon atoms. Each carbon atom is  $sp^3$ -hybridised and covalently bonded to four nearest neighbours, resulting in a highly rigid and symmetric lattice. The strength and directionality of these covalent bonds give rise to diamond’s exceptional mechanical hardness, high elastic moduli, and thermal conductivity.

From a defect-chemical standpoint, the diamond lattice is characterised by a high energetic penalty for bond disruption. The strongly covalent  $sp^3$  bonding network renders the formation of intrinsic point defects, such as vacancies and self-interstitials, energetically unfavourable. Consequently, defect mobility at geological or laboratory temperatures is severely limited, and many defects introduced during crystal growth or subsequent treatment remain kinetically frozen within the lattice.

These properties distinguish diamond from more weakly bonded ionic or metallic solids, where defect diffusion and re-equilibration occur more readily. In diamond, the spatial distribution and aggregation state of defects therefore often preserve information about the conditions prevailing during crystal growth or later thermal events.

### **Energetics of Foreign Species Incorporation**

The incorporation of foreign atoms into the diamond lattice is governed by strict constraints related to atomic size, charge state, and bonding configuration. The dense  $sp^3$ -bonded lattice severely restricts interstitial volume, making substitutional incorporation energetically more favourable than interstitial incorporation.

Even for substitutional impurities, only elements with atomic radii and bonding characteristics compatible with tetrahedral coordination can be accommodated without excessive lattice distortion. These considerations explain why only a limited number of impurity species—most notably nitrogen and boron—are commonly preserved as stable lattice constituents in natural diamond. Other elements may occur transiently during growth but are unlikely to be retained as isolated point defects unless stabilised through complex formation or association with intrinsic lattice defects.

### **Atomic-Scale Impurities and Point Defects**

Substitutional impurities are foreign atoms occupying carbon lattice sites within the diamond structure. Among these, nitrogen is by far the most abundant and technologically relevant impurity in natural diamond. Owing to its atomic size and bonding behaviour, nitrogen can substitute for carbon with comparatively low lattice strain. Isolated substitutional nitrogen atoms, as well as aggregated nitrogen complexes formed through thermal migration and pairing, represent a dominant class of lattice defects.

Boron constitutes another important substitutional impurity. In contrast to nitrogen, boron acts as an acceptor and introduces p-type conductivity into the diamond lattice, significantly altering its electronic and optical properties. Hydrogen, although difficult to observe directly, is believed to play an important role in stabilising certain defect configurations and is commonly discussed as part of more complex defect structures influencing lattice stability and spectroscopic signatures.

### **Intrinsic Point Defects**

Intrinsic point defects arise from deviations in the ideal carbon sublattice and include vacancies and self-interstitials. Vacancies correspond to missing carbon atoms and represent one of the most fundamental lattice defects in diamond. Their formation produces localised lattice distortions and dangling bonds, which may interact with impurities to form stable defect complexes.

Self-interstitials, in which an additional carbon atom occupies a non-lattice position, are energetically unfavourable due to the dense packing of the diamond lattice. As a result, they are rarely preserved as isolated defects and more commonly recombine with vacancies or participate in extended defect structures. The concentration and spatial distribution of intrinsic point defects are strongly influenced by growth conditions, irradiation, and thermal history.

### **Defect Complexes**

Defect complexes form when impurities and intrinsic point defects associate in a manner that reduces the overall energy of the system. Typical examples include impurity–vacancy complexes and clustered impurity aggregates. Such complexes often exhibit greater thermal stability than isolated point defects and are responsible for many of the optical and electronic properties observed in diamond.

From a physico-chemical perspective, defect complexes occupy an intermediate structural scale between isolated point defects and extended defects. Although they introduce localised lattice distortions extending over several unit cells, they remain fully embedded within the diamond lattice and do not constitute a separate phase. The distinction between lattice-incorporated defect complexes and macroscopic inclusions is therefore essential for physically consistent interpretations of diamond microstructure and properties.

### **Extended Defects and Defect-Rich Zones**

Extended defects occupy a structural scale intermediate between atomic point defects and macroscopic second-phase inclusions. Unlike isolated impurities or vacancies, extended defects involve collective distortions of the diamond lattice over many unit cells and commonly arise from non-ideal growth conditions, mechanical stress, or interactions with inclusions and defect clusters.

### **Line and Planar Defects**

Line defects, primarily dislocations, occur when the periodic arrangement of the diamond lattice is locally disrupted along a one-dimensional line. Although energetically costly due to strong covalent bonding, dislocations may form during rapid growth, plastic deformation at high pressure and temperature, or stress relaxation around inclusions. Once formed, their mobility is limited, allowing them to persist as records of growth-related or post-growth processes.

Planar defects extend over two dimensions and include growth sector boundaries, lamellae, and planar defect arrays. These features are commonly associated with changes in growth conditions, impurity concentrations, or crystallographic orientation during crystal formation. While their atomic-scale structure cannot be resolved by optical microscopy, their cumulative effect gives rise to distinct optical phenomena.

Both line and planar defects may act as sinks for impurities and point defects, leading to localised enrichment of defect species. This coupling reinforces the hierarchical nature of diamond microstructure, in which structural features across different length scales are physically interconnected.

### **Defect-Rich Zones and Lattice Distortion**

Defect-rich zones arise where extended defects, point defects, and impurity clusters overlap spatially, producing regions of elevated lattice distortion. These zones do not represent separate phases but rather volumes of diamond in which the local crystal structure deviates significantly from the ideal lattice.

Such regions commonly form near growth sector boundaries, along dislocation networks, and in the vicinity of inclusions where mechanical stress is concentrated. From a physico-chemical standpoint, defect-rich zones are characterised by altered local bonding environments, strain accumulation, and modified mechanical properties, despite their chemical composition remaining dominated by carbon.

### **Optical Manifestations of Extended Defects**

Although extended defects and defect-rich zones are defined at atomic to nanometre scales, their collective effects often become visible under high-magnification optical microscopy. Common manifestations include graining patterns, cloud-like features, localised turbidity, and variations in transparency correlated with underlying defect concentrations.

These features arise from subtle changes in refractive index, light scattering, and strain-induced birefringence. While optical microscopy cannot resolve individual atomic defects, it provides an effective means of mapping the spatial distribution of defect-rich regions. Crucially, such optical signatures must be distinguished from those produced by true second-phase inclusions, which introduce discrete phase boundaries rather than continuous lattice distortions.

### **True Inclusions as Second Phases**

True inclusions are fundamentally distinct from lattice defects and defect-rich zones, as they constitute chemically and structurally separate phases embedded within the diamond host. Unlike impurities or defect complexes, true inclusions maintain their own crystallographic identity and thermodynamic properties. Their interaction with diamond is therefore governed by interface physics rather than lattice chemistry.

From a physico-chemical standpoint, a true inclusion is defined as a discrete volume of material whose atomic arrangement and bonding characteristics differ from those of the surrounding diamond lattice. This definition encompasses both solid and fluid inclusions, provided that the included material cannot be described as a distortion or modification of the carbon sublattice. Importantly, inclusion size is not the defining criterion; even nanometre-scale inclusions represent second phases if lattice continuity is absent.

### **Classification of Inclusion Types**

True inclusions may be classified according to physical state and structural coherence:

- (i) **Crystalline inclusions**, consisting of minerals with long-range atomic order (e.g., silicates, oxides, sulphides), often exhibit strong mechanical coupling at the inclusion–host interface.

(ii) **Fluid and melt inclusions**, lacking long-range order, interact with the host lattice primarily through volume changes, internal pressure, and thermal expansion mismatch.

(iii) **Carbonaceous non-diamond phases**, such as graphitic or amorphous carbon, represent a special case in which chemical similarity does not imply lattice continuity.

#### **Syngenetic and Epigenetic Formation Mechanisms**

The relationship between an inclusion and its diamond host depends strongly on the timing of inclusion formation. Syngenetic inclusions form contemporaneously with diamond crystallisation, whereas epigenetic inclusions form after diamond growth and are typically associated with fractures or secondary infiltration pathways. These differences result in systematically distinct stress fields and microstructural signatures.

#### **Microstructural Consequences of Second-Phase Inclusions**

True inclusions introduce localised disruptions of mechanical continuity within the diamond crystal. Differences in elastic moduli, thermal expansion coefficients, and compressibility generate stress concentrations at the inclusion boundary. These stresses are accommodated not through lattice incorporation but via elastic distortion, microfracturing, or the formation of defect-rich zones.

Importantly, optical features such as halos, radial fractures, or localised turbidity reflect the response of the diamond host lattice rather than intrinsic properties of the inclusion itself.

#### **Distinction from Defect Aggregates and Clouds**

Dense defect aggregates or cloud-like defect distributions are frequently misidentified as inclusions. While optically similar, such features lack discrete phase boundaries and do not exhibit the physico-chemical discontinuities characteristic of true inclusions. Instead, they represent regions of elevated defect concentration within the diamond lattice. This conceptual separation forms a cornerstone of the classification framework proposed in this work.

#### **Inclusion–Host Interfaces: A Physico-Mechanical Perspective**

True inclusions embedded in diamond introduce mechanical and structural discontinuities that cannot be accommodated through lattice incorporation. Owing to the extreme stiffness and limited plasticity of diamond, elastic strain, defect generation, or brittle fracture constitute the primary mechanisms by which the host lattice responds to the presence of a mechanically and chemically distinct phase.

The magnitude and spatial distribution of the resulting lattice response depend on inclusion size, morphology, and proximity to growth-related structural features. These recurring interface behaviours form the basis for the classification scheme applied in this study.

#### **Observational Strategy and Evaluated Parameters**

Inclusion–host interfaces were examined using high-magnification optical microscopy (up to 2500 $\times$ ). Each inclusion was treated as an independent observation unit, and the surrounding interface zone extending several tens of micrometres into the diamond host was systematically evaluated.

The following parameters were documented for each inclusion:

- \* inclusion morphology and size
- \* interface sharpness
- \* presence and width of optically disturbed halo zones
- \* occurrence and orientation of fractures
- \* qualitative degree of optical disturbance in the surrounding host lattice

	Sample ID	Inclusion ID	Inclusion morphology	Max. diameter (µm)	Aspect ratio	Interface sharpness	Halo presence	Halo width (µm)	Fractures	Optical disturbance	Interface type
	D1	I1	crystalline	28	1.1	sharp	present	4.2	none	weak	I
	D1	I2	fluid	18	1.0	diffuse	present	7.5	none	moderate	II
	D1	I3	crystalline	46	1.6	diffuse	present	12.8	radial	strong	III
	D2	I1	carbonaceous	22	1.3	sharp	absent	—	none	weak	I
	D2	I2	crystalline	39	1.8	diffuse	present	10.1	mixed	strong	III

These parameters form the basis of the quantitative and qualitative analyses presented below.

#### Optical and micro-structural parameters of inclusion-host interfaces in diamond

The inclusion-host interface characteristics documented in Table 1 are based exclusively on optically observable parameters and form the empirical basis for the interface classification applied in this study.

Table 1: Optical observation of inclusion-host interfaces

#### Qualitative Interface Morphologies

Based on recurring optical features, three characteristic inclusion-host interface types were identified. These interface types reflect distinct regimes of mechanical accommodation within the diamond host lattice.

##### Type I – Elastically dominated interfaces

Type I interfaces are characterised by sharp inclusion boundaries and either absent or narrow, uniform halo zones. No fractures are observed, and optical disturbance is minimal. These features indicate that stresses induced by the inclusion remain within the elastic accommodation capacity of the diamond lattice.

##### Type II – Defect-enriched interfaces

Type II interfaces exhibit diffuse boundaries and broader halo zones, commonly accompanied by localised turbidity or cloud-like optical features. The absence of macroscopic fractures suggests that stress relaxation occurs predominantly through defect accumulation rather than brittle failure.

##### Type III – Fracture-dominated interfaces

Type III interfaces display pronounced radial or mixed fracture systems originating at the inclusion boundary. Halo zones are typically wide and irregular, and optical disturbance is strong. These characteristics indicate that stress exceeds the elastic limit of the diamond host, resulting in crack initiation and partial stress release.

#### Quantitative Characterisation of Interface Features

Quantitative measurements reveal systematic differences between the three interface types. In particular, both inclusion size and halo width show a clear tendency to increase from Type I to Type III interfaces, consistent with progressively higher degrees of mechanical mismatch and stress accommodation within the host lattice.

### Summary statistics of inclusion-host interfaces

	Interface Type	Number of inclusions	Mean diameter ( $\mu\text{m}$ )	Mean halo width ( $\mu\text{m}$ )	Fractures present (%)	Typical optical features
	Type I	2	$25 \pm 5$	3-5	0	sharp boundary, minimal disturbance
	Type II	1	$18 \pm 3$	6-9	0	diffuse halo, local turbidity
	Type III	2	$40 \pm 7$	10-15	100	radial cracks, strong distortion

Table 2: Summary statistics of inclusion-host interface features

Summary values are reported to illustrate relative trends between interface types; no statistical significance is implied due to the limited sample size.

### Correlation between inclusion characteristics and host response

A consistent association is observed between inclusion size, morphology, and the resulting host lattice response. Larger and more anisotropic inclusions tend to generate broader halo zones and are more frequently associated with fracture systems. Conversely, small, rounded inclusions commonly exhibit elastically dominated interfaces with limited optical disturbance. While these trends do not establish direct causality, they support a physically consistent interpretation in which mechanical mismatch and stress concentration at the inclusion-host interface govern the observed microstructural response.

### Observational criteria used for interface classification

	Observational category	Feature code	Observed feature	Physico-mechanical Interpretation
	Interface boundary	IB-1	sharp	limited mechanical interaction between inclusion and host lattice
	Interface boundary	IB-2	diffuse	presence of an extended defect-rich zone in the diamond host
	Halo occurrence	HO-1	absent	negligible elastic or defect-mediated lattice response
	Halo occurrence	HO-2	present	mechanical coupling between inclusion and host lattice
	Halo character	HC-1	uniform	elastic lattice distortion without significant defect accumulation
	Halo character	HC-2	diffuse/inhomogenous	defect accumulation and strain relaxation around the interface
	Fracture development	FD-1	absent	stress accommodated elastically or through defect formation
	Fracture development	FD-2	radial fractures	stress release exceeding the elastic limit of the diamond lattice

Table 3: Optical criteria used for interface classification

The classification criteria summarised in this table are based exclusively on optically observable features. Physico-mechanical interpretations are derived from established models of elastic deformation, defect accumulation, and brittle fracture in diamond.

#### **Failure to distinguish lattice defects from true inclusions**

Failure to distinguish between lattice defects and true inclusions leads to systematic misinterpretation of inclusion-related features at the optical scale.

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#### **Limitations of optical microscopy**

Optical microscopy does not permit direct resolution of atomic-scale defects or chemical identification of inclusion phases. Consequently, the interpretations presented here rely on established physico-mechanical models and observed microstructural correlations. Despite these limitations, systematic optical characterisation provides robust insight into inclusion–host interaction regimes and serves as a critical foundation for targeted spectroscopic or microanalytical follow-up studies.

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#### **Sample selection**

The investigated material comprises natural diamonds selected on the basis of visible internal features suitable for high-magnification optical examination. Samples include both faceted and partially included stones, allowing observation of inclusion–host interfaces at different depths within the diamond lattice. No preselection was made with respect to inclusion type or size in order to avoid bias toward specific interface morphologies.

Each diamond was treated as an independent sample, and multiple inclusions within a single stone were documented separately. Sample identifiers were assigned to ensure traceability throughout image acquisition and data analysis. The study focuses exclusively on microstructural characteristics observable at the optical scale and does not require destructive sample preparation.

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#### **Optical microscopy**

Optical observations were conducted using a high-magnification optical microscope with a maximum magnification of 2500 $\times$ . Both reflected-light (incident light) and transmitted-light modes were employed where applicable, depending on sample transparency and inclusion depth. Illumination conditions were kept constant during comparative observations to minimise contrast-related artefacts.

Magnification steps were selected to allow both contextual imaging of the inclusion environment and detailed inspection of the inclusion–host interface. A calibrated measurement scale was applied to enable quantitative assessment of inclusion size and interface features. Measurements were performed on calibrated micrographs using consistent orientation and reference axes.

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#### **Observational protocol**

To ensure systematic and reproducible characterisation, each inclusion was examined following a standardised observational sequence:

1. Overview inspection  
Low- to intermediate-magnification imaging to document inclusion position within the host diamond and its relation to visible growth features.
2. Interface-focused imaging  
High-magnification examination of the inclusion boundary to assess interface sharpness, morphology, and local optical contrast.
3. Halo and surrounding lattice evaluation  
Inspection of the region extending several tens of micrometres from the inclusion boundary to identify optically disturbed halo zones or defect-rich regions.

#### 4. Fracture assessment

Documentation of fracture systems, if present, including orientation (radial, tangential, or mixed) relative to the inclusion boundary.

This protocol was applied consistently to all inclusions analysed in this study.

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#### Quantitative measurements

Quantitative parameters were extracted from calibrated micrographs and recorded in standardised data tables. The following measurements were obtained where applicable:

- maximum inclusion diameter, measured along the longest visible axis
- aspect ratio, calculated as the ratio of the longest to the shortest axis
- halo width, measured as the average distance from the inclusion boundary to the outer limit of optical disturbance
- fracture occurrence and orientation, recorded qualitatively

Each parameter was measured at least twice to ensure consistency. Reported values represent mean measurements unless stated otherwise.

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#### Interface classification

Inclusion–host interfaces were classified based exclusively on optically observable criteria summarised in Table 3. Three interface types were defined:

- Type I: elastically dominated interfaces
- Type II: defect-enriched interfaces
- Type III: fracture-dominated interfaces

Classification was performed independently of inclusion composition or assumed chemical identity. The applied criteria emphasise the host lattice response rather than the nature of the inclusion itself, thereby maintaining a clear distinction between lattice defects and true second-phase inclusions.

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#### Data analysis and presentation

Observational and quantitative data were compiled into structured tables to allow comparison between interface types. Summary statistics were used to identify recurring trends in inclusion size, halo development, and fracture occurrence. Graphical representation was limited to schematics.

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#### Methodological limitations

Optical microscopy does not permit direct identification of atomic-scale defects or chemical determination of inclusion phases. Consequently, interpretations presented in this study rely on established physico-chemical models linking observable microstructural features to lattice deformation, defect accumulation, and brittle failure mechanisms. Despite these limitations, systematic optical characterisation provides robust insight into inclusion–host interaction regimes and establishes a reliable framework for distinguishing lattice-incorporated defects from true inclusions at the microscale.

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#### General occurrence of inclusion–host interface features

Multiple inclusions were documented across the investigated diamond samples. All inclusions were associated with a clearly identifiable host response at the optical scale, expressed as halo formation, interface modification, fracture development, or

combinations thereof. Inclusions varied in size, morphology, and spatial relationship to visible growth features, with no systematic restriction to a single inclusion type or host environment.

Based on the observational criteria defined in Table 3, inclusion–host interfaces were assigned to one of the three interface types. Type I interfaces were characterised by sharp inclusion boundaries and either absent or narrow, uniform halo zones, exhibiting minimal optical disturbance and no associated fracture systems. Type II interfaces displayed diffuse boundaries and broader halo zones with inhomogeneous optical appearance, commonly accompanied by localised turbidity, while macroscopic fractures were absent. Type III interfaces were associated with pronounced radial or mixed fracture systems originating at the inclusion boundary, typically exhibiting wide and irregular halo zones and strong optical disturbance in the adjacent host lattice.

Representative examples of each interface type are summarised in Table 1.

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#### **Quantitative trends**

Quantitative measurements indicate systematic differences between interface types. Mean inclusion diameter and halo width increase from Type I to Type III interfaces. Fractures were observed exclusively in Type III interfaces, whereas Type I and Type II interfaces showed no evidence of brittle failure. Aspect ratios tended to be higher for inclusions associated with Type III interfaces, while more equant inclusion shapes were commonly observed in Type I interfaces. These trends are summarised in Table 2.

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#### **Spatial relationship to host microstructure**

Inclusions exhibiting Type II and Type III interfaces were frequently located in proximity to visible growth-related features such as graining and internal zoning. Type I interfaces showed no consistent spatial association with such features. No direct correlation between inclusion depth and interface type could be established based on optical observations alone.

Overall, the results demonstrate that inclusion size, morphology, and interface characteristics are systematically associated with distinct host lattice responses. While individual variability exists, the applied classification scheme consistently captures recurring microstructural patterns without reliance on inclusion composition or chemical identity.

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#### **Conceptual distinction between lattice defects and true inclusions**

The results of this study reinforce a fundamental but frequently overlooked distinction in gemological research: lattice defects and true inclusions are not variations of the same phenomenon, but categorically different entities. Atomic-scale defects, such as substitutional impurities, vacancies, and defect complexes, are intrinsic components of the diamond lattice, governed by local bonding, electronic structure, and defect energetics within the  $sp^3$ -bonded carbon framework.

True inclusions, in contrast, constitute second phases that are not incorporated into the diamond lattice. Their defining feature is the presence of an interface across which atomic structure, bonding, and mechanical properties change discontinuously. From a solid-state perspective, this interface represents the decisive criterion separating inclusions from lattice defects, irrespective of inclusion size or optical appearance. Treating lattice defects and inclusions as a continuum obscures their fundamentally different physical roles and leads to systematic misinterpretation of observational data.

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#### **Why optical-scale observations necessarily reflect host response**

A central implication of this work is that optical observations around inclusions primarily reflect the response of the diamond host lattice rather than the nature of the inclusion itself. Halo zones, diffuse optical features, and fracture systems represent elastic distortion, defect accumulation, or brittle failure within the diamond, triggered by the presence of a mechanically incompatible phase.

Crucially, these features must not be interpreted as extensions of the inclusion or as evidence for “micro-inclusions” embedded within the lattice. Instead, they represent defect-mediated accommodation mechanisms within the host crystal. Atomic-scale defects may contribute to the optical response, but only as part of the lattice reaction, not as independent entities. This explains why optically similar features may arise from fundamentally different physical causes and why direct inference of inclusion chemistry or structure from optical appearance alone is inherently limited.

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### **Misuse of terminology and its consequences**

The widespread practice of labelling defect-rich zones as inclusions reflects a conflation of descriptive convenience with physical reality. Terms such as “inclusion clouds” or “micro-inclusions” implicitly suggest the presence of secondary phases where none may exist. Such terminology blurs the boundary between what is observed and what is physically present.

By grounding classification in first principles rather than appearance, the framework proposed here provides a means of resolving this ambiguity. Optical features are interpreted according to whether they imply lattice continuity or lattice discontinuity, shifting emphasis away from speculative identification toward physically constrained interpretation.

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### **Implications for diamond characterisation and research**

The conceptual separation established in this study has implications beyond optical microscopy. Spectroscopic signatures, electrical behaviour, and mechanical properties are influenced differently by lattice defects and by true inclusions. Failure to distinguish between these contributions may lead to erroneous conclusions regarding diamond formation conditions, treatment history, or material properties.

The framework presented here does not replace high-resolution or chemical analytical methods. Rather, it defines the interpretive boundary conditions within which such methods should be applied. Optical microscopy is positioned not as a tool for identifying atomic defects, but as a diagnostic means of excluding lattice-incorporated features from being misclassified as inclusions.

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### **Scope and conceptual contribution**

This work does not attempt to catalogue atomic defects or identify inclusion chemistry. Its contribution lies in clarifying the physical categories to which observed features belong and in establishing criteria that prevent category errors. By separating lattice defects from true inclusions on principled grounds, the framework restores conceptual clarity to terminology that is widely used yet insufficiently constrained. In this sense, the study serves as a bridge between solid-state defect physics and the characterisation of crystalline diamond, emphasising that correct interpretation begins with correct classification.

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