Optical Defects in Diamond: A Quick Reference Chart

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Gem diamonds owe much of their value to their color, or lack thereof. Defects in the atomic structure of diamond are responsible for this color and are important for the identification of color treatments. This article and its tables are intended as a quick reference for gemologists as they read about various common diamond defects in the gemological literature.

Despite the commercial value of natural-color diamonds, distinguishing them from treated diamonds remains a significant identification challenge. While some diagnostic visual features exist (inclusions, color or growth zoning, and absorption bands seen with a spectroscope), the separation of natural from synthetic or treated diamonds is not always possible using standard gemological methods. In such cases, advanced spectroscopic analysis at a professional gem-testing laboratory is required. Imaging of luminescence distribution patterns is also a helpful tool for recognizing synthetic diamonds (Martineau et al., 2004; Shigley et al., 2004).

In a laboratory setting, the identification of diamonds is based mainly on the detection of tiny imperfections in the atomic lattice. These "defect centers" may include foreign impurity atoms (typically nitrogen, and occasionally boron or hydrogen); carbon atom vacancies in the lattice (either single or clusters of neighboring vacancies); carbon atoms positioned in between normal lattice locations (interstitials); and dislocations where planes of carbon atoms are offset from one another due to plastic deformation. Not all of these lattice imperfections create spectroscopic features, but several do so by allowing the diamond to absorb particular energies of incident light or radiation. Defects can occur randomly or in particular locations within the lattice. Diamonds can contain more than one type of defect, and in natural diamonds, defects can be altered over geologic time in the earth or by exposure to heat or radiation during color treatment.

So-called optical defects (or optical centers) cause absorption in the visible or near-visible portions of the electromagnetic spectrum, often producing coloration (e.g., figure 1). Luminescence reactions result when defects absorb higher-energy incident radiation and then reemit lower-energy radiation as visible light. Optical defects occur in very low concentrations in all diamonds, and their presence can be detected using spectroscopic techniques. A theoretically "pure and perfect" diamond containing no such defects would appear colorless.

Figure 1. The red color of the graining in this Fancy red diamond from Brazil is caused by absorption related to the 550 nm band. This band, the most common cause of pink to red color in natural, untreated diamonds, is thought to be the result of a defect created by plastic deformation. Photomicrograph by Jian Xin (Jae) Liao; magnified 50×.

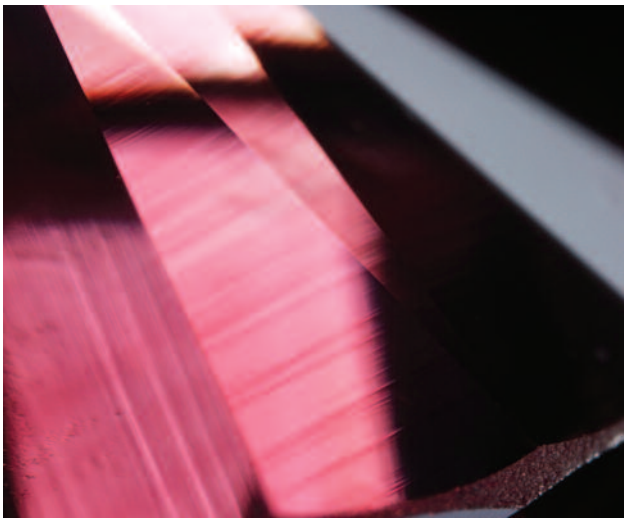

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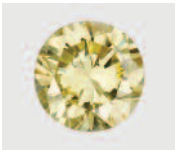
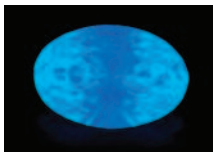
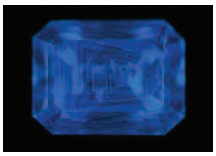
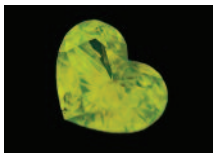
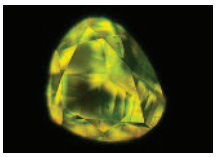
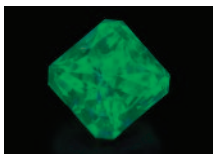
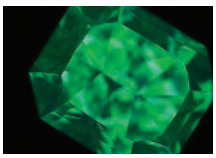
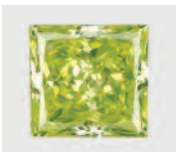
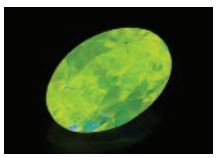
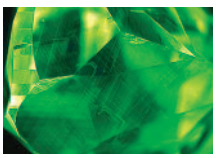
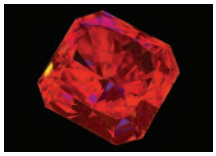
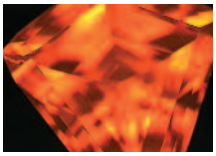
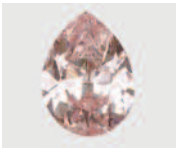
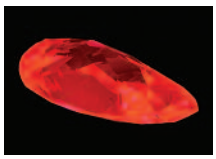
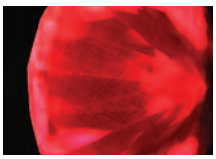
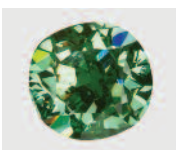
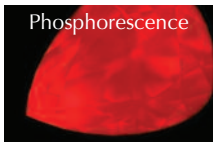
TABLE 1. Important optical defects in diamond and their effect on color and luminescence.

Color	Optical defect and spectroscopic means of detection	LWUV fluorescence (~365 nm lamp)	DiamondView luminescence (<220 nm source)
No effect	**ND1:** A defect with an absorption line at **393.6 nm** (3.150 eV). Thought to consist of a vacancy in the negative charge state (V^-). Produced by natural or artificial irradiation. *UV*	No effect	No effect
	**N3:** An impurity and intrinsic defect with an absorption line at **415.2 nm** (2.985 eV) and associated bands. Thought to consist of three substitutional nitrogen atoms surrounding a vacancy (3N+V). Often occurs with the associated N2 (477.2 nm) and several other related bands (465, 452, 435, and 423 nm) in "Cape" diamond spectra. All are naturally occurring. *UV, PL, EPR*		
	**480 band:** A naturally occurring optical defect of uncertain structure (sometimes attributed to substitutional oxygen) in type I diamonds with a broad absorption band centered at **480 nm** (2.580 eV). *UV*		
	**H4:** An impurity and intrinsic defect with an absorption line at **496.2 nm** (2.498 eV). Thought to consist of four substitutional nitrogen atoms surrounding two vacancies (4N+2V). Occurs naturally or can be produced by irradiation followed by annealing. *UV, PL*		
	**H3:** An impurity and intrinsic defect with an absorption line at **503.2 nm** (2.463 eV) and associated bands. Thought to consist of two substitutional nitrogen atoms separated by a vacancy in a neutral charge state $(N\text{-}V\text{-}N)^0$. Occurs naturally or can be produced by irradiation followed by annealing or by high-pressure, high-temperature annealing. *UV, PL*		
May contribute to a green color	**3H:** A defect with an absorption line at **503.4 nm** (2.462 eV). Thought to be related to interstitial carbon (I). Produced by natural or artificial irradiation. *UV, PL*	No effect	No effect
	**550 band:** An optical center of uncertain structure with a broad absorption band centered at **550 nm** (2.250 eV). Thought to result from plastic deformation of the lattice structure. Occurs naturally. *UV*	No effect	No effect
	**NV^0:** An impurity and intrinsic defect with an absorption line at **575 nm** (2.156 eV) and associated bands. Thought to consist of a single substitutional nitrogen atom associated with a vacancy in a neutral charge state (NV^0). Occurs naturally or can be produced by irradiation followed by annealing. *PL, EPR, UV*		
May contribute to other colors	**595 band:** An optical defect of uncertain structure with an absorption band at **594.4 nm** (2.086 eV). Thought to be related to nitrogen. Occurs naturally or can be produced by irradiation followed by annealing. *UV*	No effect	No effect
	**NV^-:** An impurity and intrinsic defect with an absorption line at **637 nm** (1.945 eV) and associated bands. Thought to consist of a single substitutional nitrogen atom associated with a vacancy in a negative charge state (NV^-). Occurs naturally or can be produced by irradiation followed by annealing or by high-pressure, high-temperature annealing. *PL, EPR, UV*		
	**GR1:** A defect with a pair of absorption lines at **740.9 nm** (1.673 eV) and at **744.4 nm** (1.665 eV) and associated bands. Thought to consist of a vacancy in a neutral charge state (V^0). Produced by natural or artificial irradiation. *UV, PL*	No effect	No effect

Color	Optical defect and spectroscopic means of detection	LWUV fluorescence (~365 nm lamp)	DiamondView luminescence (<220 nm source)
May contribute to a green color	**H2:** An impurity and intrinsic defect with an absorption line at **986.3 nm** (1.256 eV, 10125 cm^{-1}) and associated bands. Thought to consist of two substitutional nitrogen atoms separated by a vacancy in a negative charge state $(N\text{-}V\text{-}N)^{-}$. Occurs naturally or can be produced by irradiation followed by annealing or by high-pressure, high-temperature annealing. *IR, PL*	No effect	No effect
No effect	**H1c:** An impurity and intrinsic defect of uncertain structure with an infrared absorption line at **1934 nm** (0.6408 eV, 5171 cm^{-1}). Thought to be associated with nitrogen B centers. Occurs naturally or can be produced by irradiation followed by annealing. *IR*	No effect	No effect
No effect	**H1b:** An impurity and intrinsic defect of uncertain structure with an infrared absorption line at **2024 nm** (0.612 eV, 4941 cm^{-1}). Thought to be associated with nitrogen A centers. Occurs naturally or can be produced by irradiation followed by annealing. *IR*	No effect	No effect
	**Hydrogen:** Defect(s) of uncertain structure with many related infrared absorption lines, most notably at **3107 cm^{-1}** (0.385 eV). Occurs naturally. This defect can also produce yellow and violet colors. *IR, UV*	No effect	No effect
	**Boron:** A defect with a primary infrared absorption line at **2803 cm^{-1}** (0.348 eV) and associated lines, and a band extending into the visible region. Thought to consist of single substitutional boron atoms. Occurs naturally. This defect produces red phosphorescence. *IR*		
	**A center:** A defect with an infrared absorption band at **1282 cm^{-1}** (0.159 eV). Thought to consist of two adjacent substitutional nitrogen atoms (N-N). Occurs naturally. *IR*	Quenches luminescence	Quenches luminescence
	**B center:** A defect with an infrared absorption band at **1175 cm^{-1}** (0.146 eV). Thought to consist of four adjacent substitutional nitrogen atoms surrounding a vacancy (4N+V). Occurs naturally. *IR*	No effect	No effect
	**C center:** A defect with an infrared absorption band at **1130 cm^{-1}** (0.140 eV). Thought to consist of a single substitutional nitrogen atom (N). Occurs naturally or can be produced by high-pressure, high-temperature annealing of diamonds containing A or B centers. *IR, UV, EPR*	No effect	No effect
No effect	**H1a:** An impurity and intrinsic defect of uncertain structure with an infrared absorption line at **1450 cm^{-1}** (0.180 eV). Thought to be associated with interstitial nitrogen. Occurs naturally or can be produced by irradiation followed by annealing. *IR*	No effect	No effect
No effect	**Platelet:** An impurity and intrinsic defect of uncertain structure with an infrared absorption line at about **1360 cm^{-1}** (0.169 eV). Thought to be associated with groups of interstitial carbon atoms. Occurs naturally. *IR*	No effect	No effect
	**Vacancy cluster:** A defect of uncertain structure with increasing absorption toward the blue end of the spectrum. Thought to consist of groups of vacancies. Occurs naturally. *UV*	No effect	No effect

UV = Ultraviolet-visible absorption spectroscopy
IR = Infrared absorption spectroscopy
PL = Photoluminescence spectroscopy
EPR = Electron paramagnetic resonance spectroscopy

TABLE 2. Spectroscopic techniques for characterizing lattice defects in diamond.

Technique	Type of spectroscopy	Typical scan range	Commonly detected features and defects	Test conditions	Advantages	Disadvantages	Comments
Ultraviolet/ visible/near-infrared (UV-Vis-NIR)	Absorption (transmission)	250–800 nm	ND1, N3, N2, H3, H4, 595 nm, and GR1	~77 K temperature	Evaluation of color-causing defects; relatively inexpensive	Large samples absorb too much light, causing detector saturation; difficulty quantifying results from faceted stones because of the uncertain path length of light travel	Staple technique in gemological laboratories; can be performed with scanning or dispersive detector
Mid- to near-infrared (IR)	Absorption (transmission)	400–11,000 cm^{-1}	A and B aggregate centers, C centers, various hydrogen-related defects, H1a, H1b, H1c, H2, and "amber centers"	Room temperature	Determination of diamond type; relatively inexpensive; defect concentrations can be quantified by normalization	Large samples absorb too much light, causing detector saturation	Staple technique in gemological laboratories
Raman	Luminescence	100–2000 cm^{-1} Raman shift	Diamond Raman line (1332 cm^{-1})	Room temperature	Identification of diamond; analysis of internal strain	Expensive; yields little information regarding treatment; difficulty analyzing strongly fluorescent samples	Typically used for diamond vs. non-diamond identification (provides little other information)
Photoluminescence (PL)	Luminescence	350–1000 nm	N3, 490.7 nm, H4, H3, NV^0, NV^-, GR1, H- and Ni-related defects	~77 K temperature or lower	Detection of HPHT treatment; characterization of low-concentration defects; small analysis area allows for detailed investigation	Expensive; difficulty analyzing strongly fluorescent samples; variety of laser excitations required to activate various defects; requires carefully controlled cryogenic test temperatures	Lasers of various wavelengths used for excitation (most commonly 325, 488, 514, 532, and 633 nm); required for effective treatment detection
Cathodoluminescence (CL)	Luminescence	400–700 nm	A band, B band, N3, H3, and H4	Room temperature	Evaluation of internal structure; detection of defects causing luminescence	Requires an electron beam and a vacuum; provides little information about color treatment	Rarely used, limited data obtainable
Electron-spin/paramagnetic resonance (ESR, EPR)	Resonance absorption in a changing magnetic field		C centers, NV defects	Room temperature	Detection of very low-concentration defects; evaluation of specific defect structures and charges	Very expensive; long sample run times; provides little information about color treatment	Typically used for defect research

As a quick reference for gemologists, table 1 lists the most common lattice defects, including those that can create color and/or luminescence reactions in diamond. The scientific name of the defect, as well as the wavelength (or wavenumber) and electron volt (eV) positions of the main and associated spectral bands, are shown along with photos of representative diamonds. The most common spectroscopic technique used to detect the defect center is indicated by a code shown in italics.

Some precautions should be kept in mind when using this table. Each lattice defect is known to produce a particular diamond color or luminescence. For instance, the GR1 center produces green or blue-green color. But the reverse is not necessarily true—for example, not all green diamonds owe their color to the GR1 center. In fact, there are several causes of green color. In some cases, a diamond contains more than one optical defect, and its color stems from a combination of defects. In other cases, a diamond's

color may arise from absorption caused by one optical center, while its luminescence may result from another optical center.

Table 2 provides a comparison of the most common spectroscopic techniques for diamond characterization. For further reading on color in diamond, the Additional Reading list serves as a reference guide to access the much larger range of gemological and technical literature on diamond identification.

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