Infrared Absorption Study of Pink-colored Lab-Grown Diamonds

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For the past decade, the interest on lab-grown diamonds is increasing. The demand on fancy-colored diamonds, in particular pink, is growing. With its popularity on the rise, a more detailed understanding on what makes a diamond pink is of utmost importance. For this study, a total of 41 lab-grown diamonds from New World Diamonds are used to determine the concentration of color centers that make up a pink diamond. Table 1 summarizes the distribution of the colors and hues. The weight of samples ranged from 0.28 to 3.02 ct. All samples were characterized using Nicolet IS 5 Fourier-Transform Infrared (FTIR) spectrometer. The FTIR spectra were acquired from 400 to 4000 cm^{-1} at 128 scans and using a resolution of ~2 cm^{-1}. The measured IR absorption coefficient were initially baseline corrected. To reduce the influence of carat weight and cut, we normalized the spectra using the intensity at 2000 cm^{-1} such that the absorption coefficient is 12.3 cm^{-1}, which is the expected value for diamond. In this work, we focused our study on the following IR-active nitrogen, hydrogen and vacancy-related impurities in lab-grown diamonds namely: substitutional nitrogen in their neutral charge state (Ns0) and positive charge state (Ns^+) as shown in Figure 1. Additional peaks such as NVH (centered at 3123 cm^{-1}) and VN3H (centered at 3107 cm^{-1}) were also compared and analyzed. We believed that these main peaks contribute to the final color and hue of the colored CVD diamond.

From the normalized FTIR spectra, we calculated the integrated intensity, that is the area under each IR-active defect peak. The integrated intensity centered at 1130 and 1344 cm^{-1} can be used to estimate the concentration of Ns0, while the intensity at 1332 cm^{-1} is proportional to Ns^+. The total nitrogen impurities present in the diamond were estimated by adding the integrated intensity from each impurity as: $N_{total} = Ns0 + Ns^+ + NVH + VN3H$. The sum of all the calculated intensity from each defect is plotted in Figure 2 as a function of color and hue. We observed that pink and yellow diamonds show significantly higher N_{total} compared to the other colored diamonds. Colorless diamonds showed the lowest N_{total}, which is indicative of the low level of impurities. Pink colored diamonds, on the other hand, revealed the highest with an average total intensity of 995.5 $\pm$ 454 a.u. However, we found that the N_{total} alone is not enough to distinguish it from yellow-colored diamonds. Figure 2 shows the variation of NVH + VN3H with color and hue. We observed that the total amount of vacancies in yellow diamonds are statistically lower compared to pink-colored diamonds. These results indicate that the diffusion and capture of vacancies play a role in distinguishing pink from yellow diamonds. It is important to note that the results presented applies only to lab-grown diamonds.

Color	Hue	Number of Samples
Brown	Brown	1
Colorless	Colorless	4
Orange	Brownish	2
	Orange	1
Pink	Grayish Orange	2
	Orangy	3
	Pink	14
Purple	Pinkish	3
Yellow	Yellow	11

Table 1. Breakdown of lab-grown diamonds

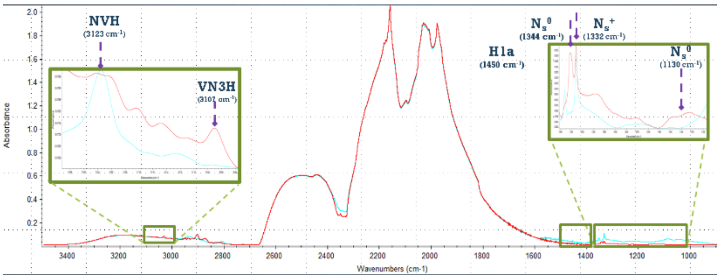

Figure 1. Typical FTIR spectrum of a lab-grown diamond.

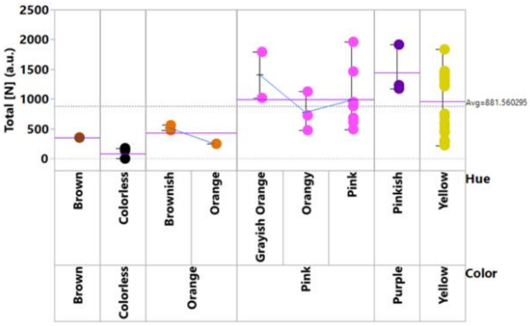

Figure 2: Total nitrogen variation with color and hue.

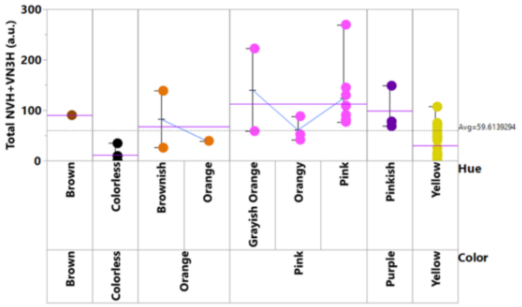

Figure 3: Total NVH+VN3H variation with color and hue.