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# RAMAN AND FTIR SPECTRA ANALYSIS OF RADIATION EFFECTS ON NEUTRON-IRRADIATED CVD DIAMOND CRYSTALS

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# RESEARCH RELEVANCE



The research is supported by *Latvian Research Program «High-energy Physics and Accelerator Technologies»* (Agreement No: VPP-IZM-CERN-2022/1-0001).

The project is focused on assessing the radiation resistance of CVD diamond, a material employed as a detector at CERN. We investigate its structural response to radiation exposure, crucial for its suitability on CERN's challenging environment. Additionally, we analyze the impact of varying radiation levels on its properties, providing insights into its sensitivity.

This research aims to determine CVD diamond's efficacy as a detector in high-energy experiments at CERN and its potential applications in fields such as nuclear engineering and medical radiation therapy. Ultimately, our goal is to ascertain its ability to withstand high levels of radiation, contributing to the development of improved detectors and versatile materials.

The research partners of this project are **Karlsruhe Institute of Technology** (Germany), **Institute of Solid State Physics**, University of Latvia (Latvia) and **Institute of Physics, University of Tartu** (Estonia).



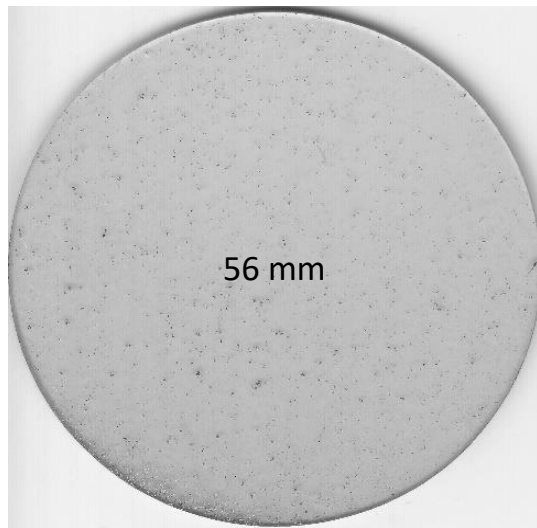
# RESEARCH OBJECTIVES

- To characterize defects in non-irradiated and neutron-irradiated diamond crystal samples by measuring and analyzing their Raman and FTIR spectra;
- To analyze the correlation between the spectral properties of the samples and the radiation dose;
- To compare the spectra of neutron-irradiated and non-irradiated samples and determine the impact of radiation on the sample structure.



# RESEARCH METHODS AND SAMPLES

In this research, using Raman and FTIR spectroscopy, the effect of neutron radiation on functional ceramics synthesized on a synthetic diamond crystal base was examined.



Undoped polycrystalline diamond optical window

The samples were obtained from research partners of the Karlsruhe Institute of Technology in Germany, but their irradiation was carried out in Sweden.

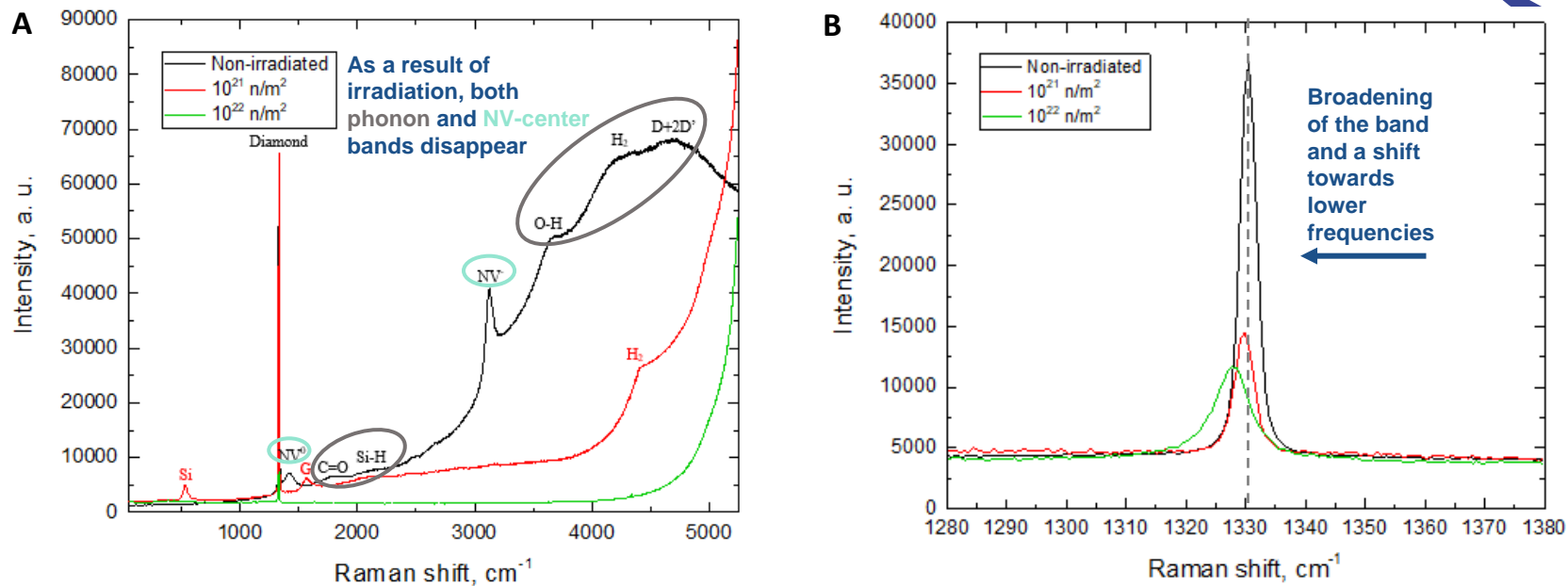
The sample price is up to 100 000€ (one average-sized non-irradiated diamond optical window).



Non-irradiated and neutron-irradiated diamond samples

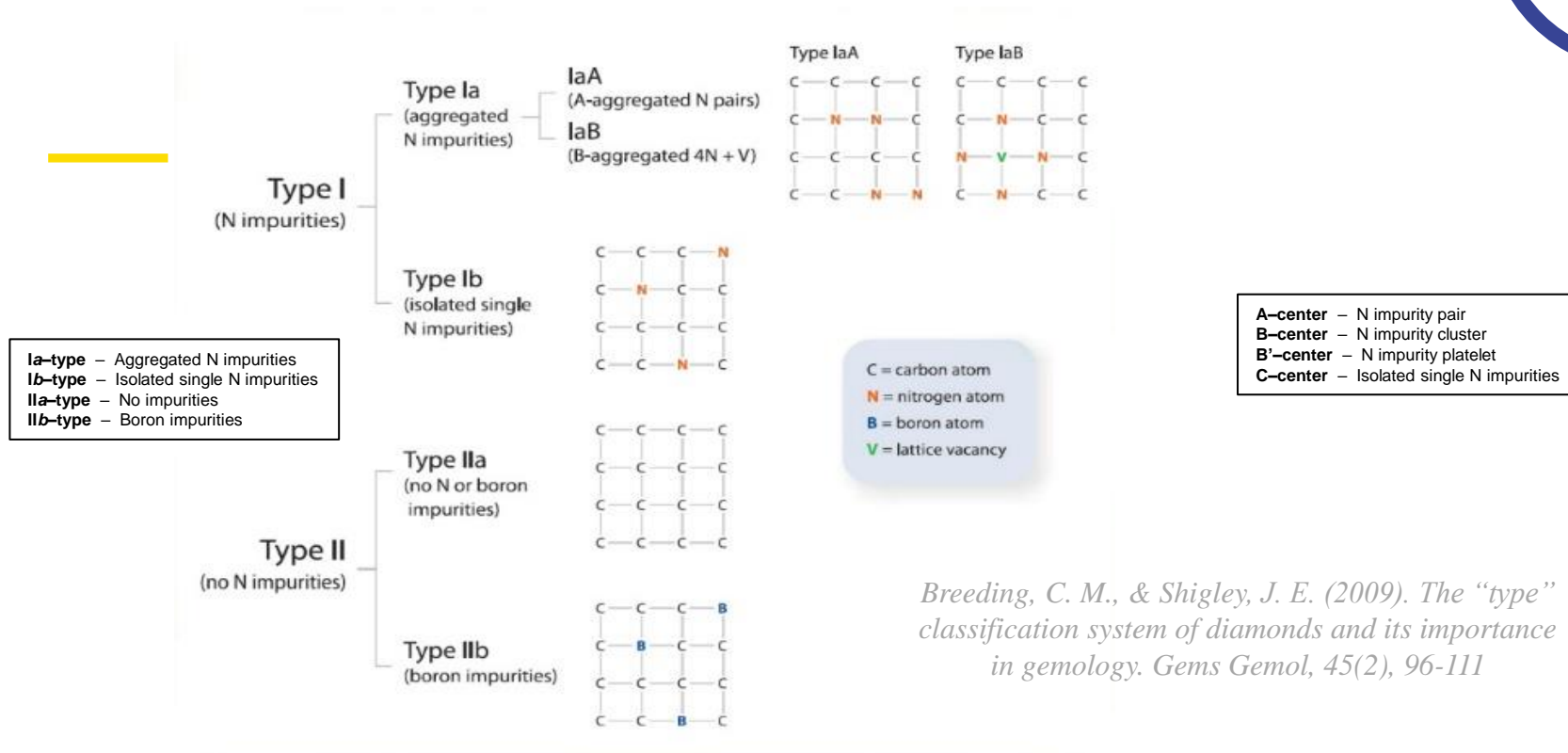


# RESULTS: DIAMOND RAMAN SPECTRA



Non-irradiated and neutron-irradiated diamond Raman spectra (A) and its enlargement in the 1280-1380  $\text{cm}^{-1}$  range (B) at 532 nm laser excitation

# CLASSIFICATION OF DEFECTS IN DIAMOND

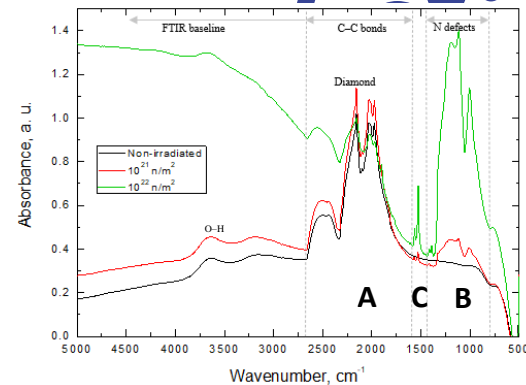
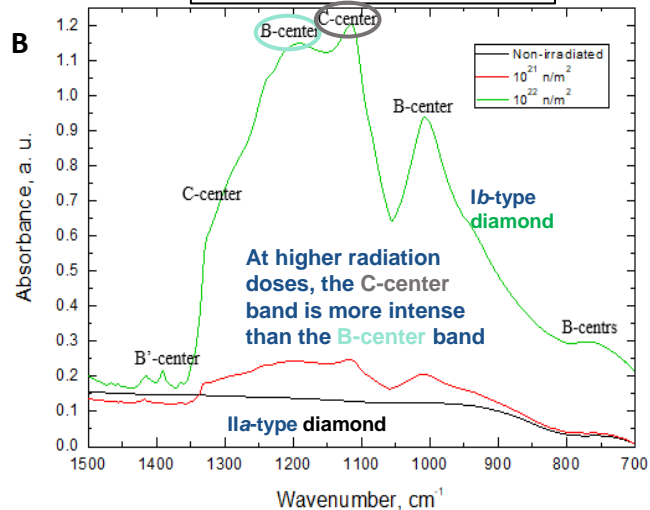
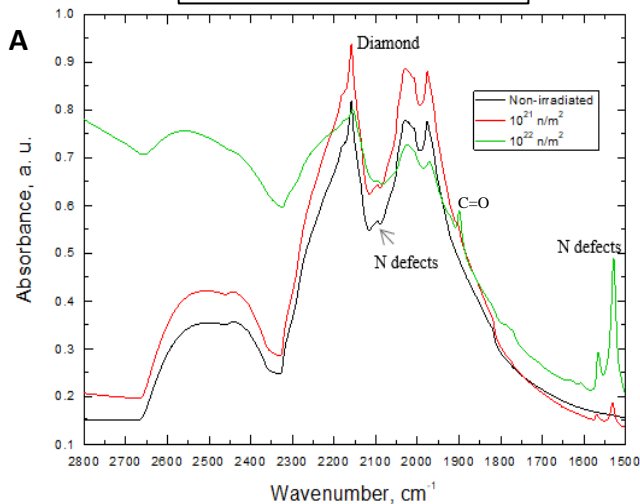


Breeding, C. M., & Shigley, J. E. (2009). The “type” classification system of diamonds and its importance in gemology. *Gems Gemol*, 45(2), 96-111

# RESULTS: DIAMOND FTIR SPECTRA

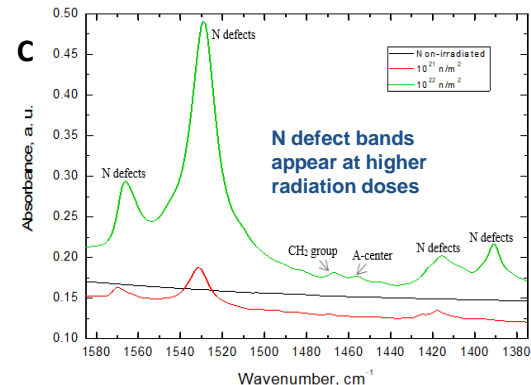
**Ia-type** – Aggregated N impurities  
**Ib-type** – Isolated single N impurities  
**Ila-type** – No impurities  
**Ilb-type** – Boron impurities

**A-center** – N impurity pair  
**B-center** – N impurity cluster  
**B'-center** – N impurity platelet  
**C-center** – Isolated single N impurities



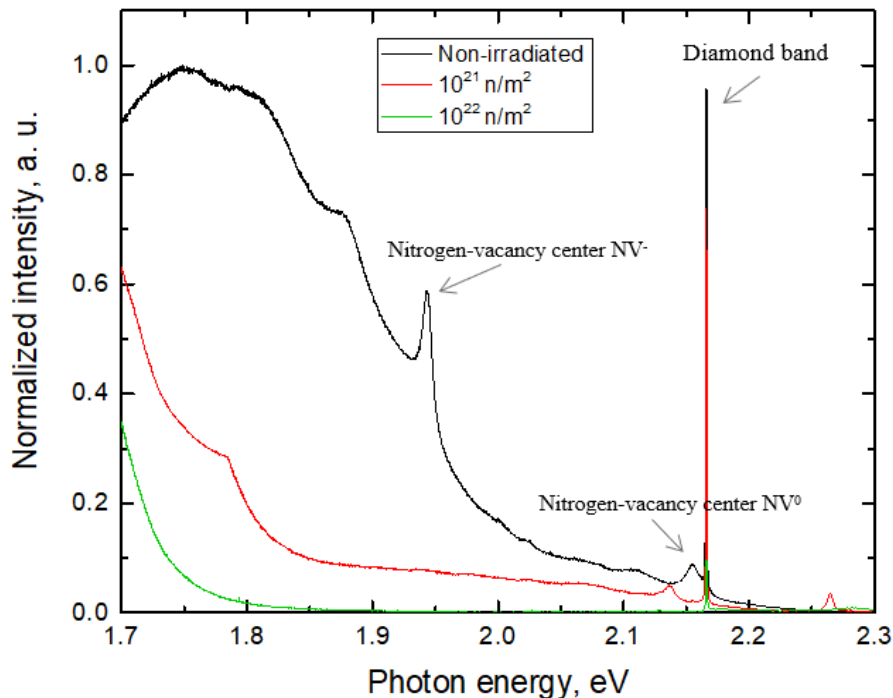
Non-irradiated and neutron-irradiated diamond FTIR absorption spectra

Enlarged non-irradiated and neutron-irradiated diamond FTIR absorption spectra in the C-C bond (A) and N defect (B) regions



Enlarged non-irradiated and neutron-irradiated diamond FTIR absorption spectra in the N defect region (1580-1380  $\text{cm}^{-1}$ )

# RESULTS: DIAMOND PL SPECTRA



Normalized luminescence spectra of non-irradiated and neutron-irradiated diamond at 532 nm laser excitation

The spectral band positions of NV-centers in diamond photoluminescence spectra

	Obtained position, eV	Literature position [1, 2, 3], eV
NV <sup>-</sup>	1.943	1.945
NV <sup>0</sup>	2.155	2.156

[1] Ganesan, K., Ajikumar, P. K., Ilango, S., Mangamma, G., & Dhara, S. (2019). Si and N-Vacancy color centers in discrete diamond nanoparticles: Raman and fluorescence spectroscopic studies. *Diamond and Related Materials*, 92, 150-158.

[2] Iakubovskii, K., & Adriaenssens, G. J. (2000). Luminescence excitation spectra in diamond. *Physical review B*, 61(15), 10174.

[3] Su, Z., Ren, Z., Bao, Y., Lao, X., Zhang, J., Zhang, J., ... & Xu, S. (2019). Luminescence landscapes of nitrogen-vacancy centers in diamond: quasi-localized vibrational resonances and selective coupling. *Journal of Materials Chemistry C*, 7(26), 8086-8091.

$$\omega_{eV} = \frac{\omega_{cm^{-1}}}{8065.6} = \frac{\omega_L - \omega_R}{8065.6} = \frac{18797 - \omega_R}{8065.6}$$

$\omega_{eV}$  – band position [eV]

$\omega_{cm^{-1}}$  – band position [ $cm^{-1}$ ]

$\omega_L$  – laser frequency [ $cm^{-1}$ ]

$\omega_R$  – Raman shift [ $cm^{-1}$ ]

$$1 \text{ eV} \approx 8065.6 \text{ cm}^{-1}$$





# CONCLUSIONS

- No new spectral bands arising from radiation-induced defects were observed in the diamond Raman spectra after neutron irradiation.
- The diamond crystal synthesized using the CVD method belongs to the *Ia* type of synthetic diamond group. When irradiating *Ia*-type synthetic diamonds with neutron radiation, its modification into type *Ib* diamond occurs, resulting in the formation of nitrogen defects (A, B, and C centers).
- At lower neutron radiation doses, diamonds exhibit a high concentration of N impurity clusters. However, with increasing neutron radiation dose, the N atoms become more isolated from each other.
- Increasing the neutron radiation dose results in the broadening of the diamond Raman “1332  $\text{cm}^{-1}$ ” band and a shift to lower frequencies, as well as the disappearance of practically all phonon bands in the diamond Raman spectrum due to the structural disordering of the diamond.
- Nitrogen-vacancy NV luminescent centers are observed only in non-irradiated diamond, as radiation-induced recombination occurs for these defects.



# THANK YOU

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