

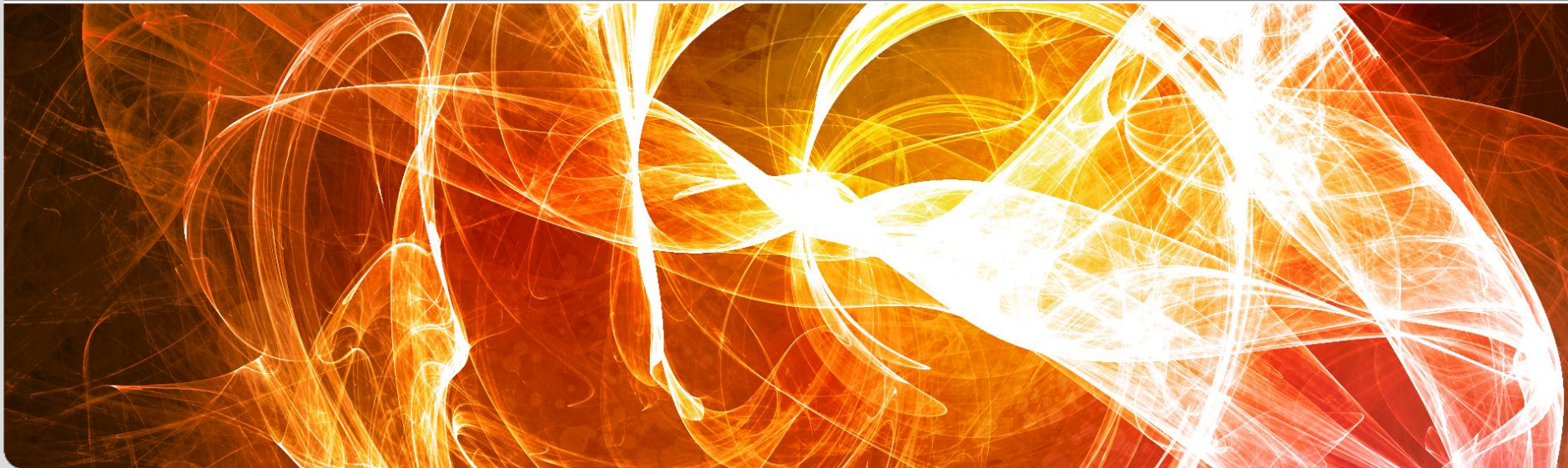
Investigation of irradiation effects in artificial diamond – new irradiation results

US-EU-JPN-RF-WS 2026, San Diego CA (USA)

October 19 – 21, 2026

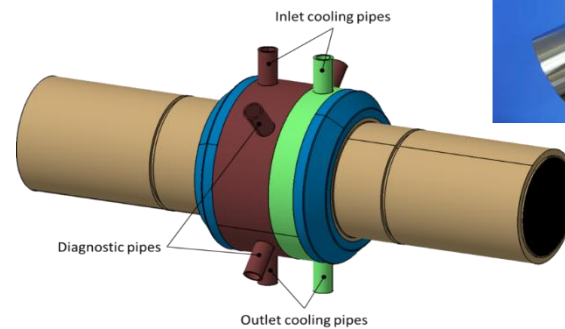
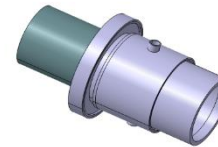
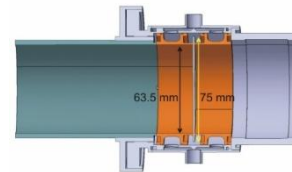
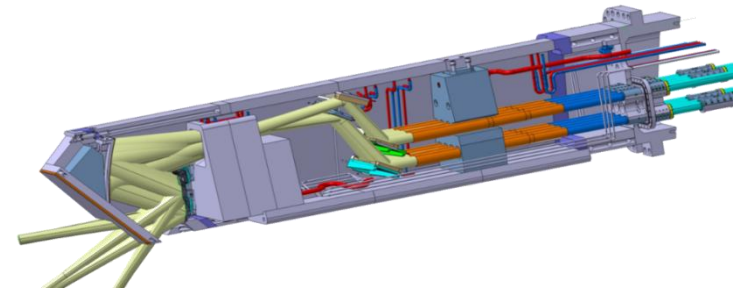
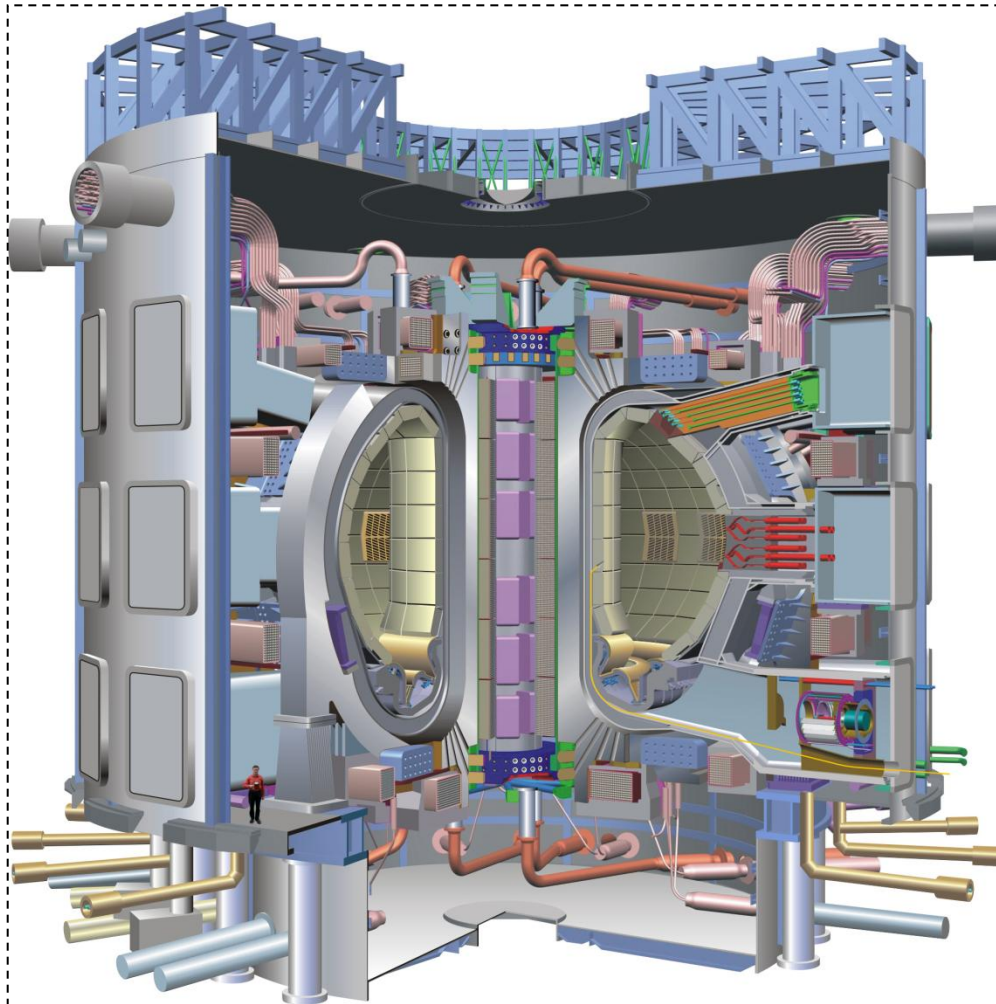
Prof. Dr. Theo A. Scherer, Dr. F. Mazzocchi (PROXIMA Fusion)

Karlsruhe Institute of Technology – Institute for Applied Materials (KIT-IAM)

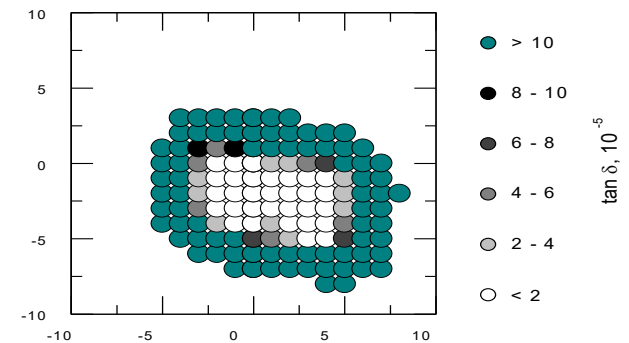
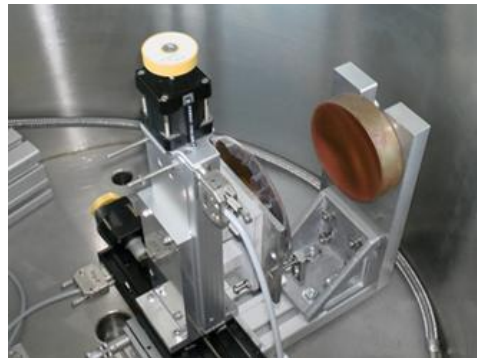
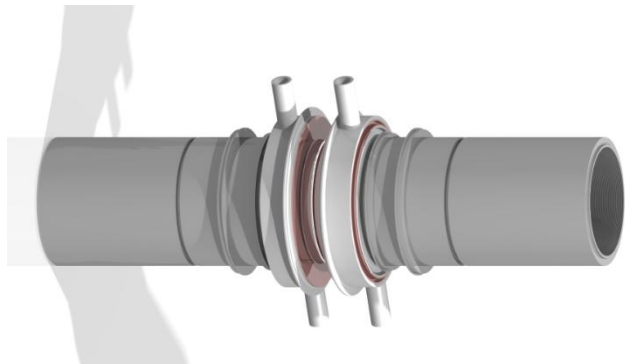


- ITER ECRH
- Diamond window characterization: FABRY-PEROT-Resonators
- Loss mechanisms
- Irradiated/non-irradiated insulators – dielectric results
- ERDA / composition
- RAMAN, IR measurements
- N-Irradiation experiments
- Diamond wafers available
- Theoretical calculations (ab initio)
- Functional materials : LaAlO_3 and NdGaO_3

ITER ECRH



Diamond Windows Characterization



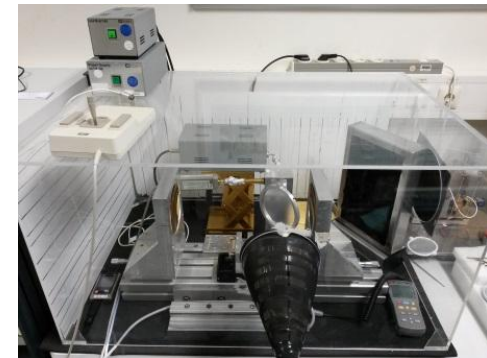
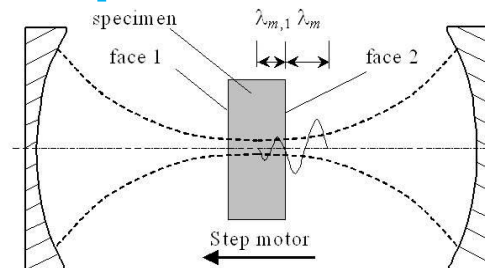
- ECRH waveguides are equipped with **diamond windows** that act as a barriers against the diffusion of tritium from the vacuum vessel, while retaining **exceptional transparency in the mm-wave range**.
- Characterization of diamond (ϵ_r and **tan δ**) have so far relied on Fabry-Perot resonators, **tan δ** meas. resolution limited to 10^{-5} by resonator dimensions, sufficient for polycrystalline diamond.
- Increase in ECRH power of the second generation plants will require even better transparency (single crystal diamond) → **higher Q resonators needed to resolve the losses**.

Measurements of $\tan\delta$ in the diamond disc

- Fabry-Perot resonators are used to measure the dielectric properties of the diamond disc: ϵ_r and $\tan\delta$.
- The measured ϵ_r and $\tan\delta$ are then used in the FEM analyses to model the power absorbed in the diamond disc during the beam transmission.

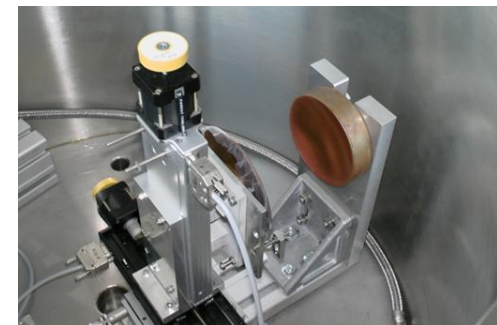
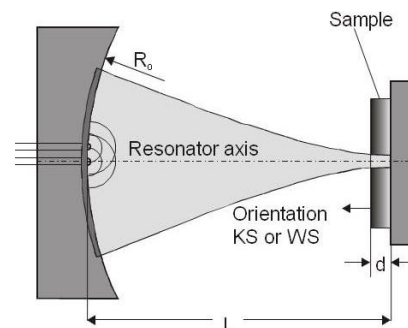
Spherical measurement setup

Determination of $\tan\delta$ at the center of the diamond disc.



Hemispherical measurement setup

Determination of $\tan\delta$ distribution over the diamond disc surface.



Loss mechanisms in diamond

Loss tangent increase by free charge carriers:

$$\tan \delta = \frac{\sigma}{\operatorname{Re}\{\varepsilon\} \cdot \varepsilon_o \cdot \omega} \quad \sigma \propto T^{\frac{3}{2}} \cdot \exp\left[-\frac{E_{\text{gap}}}{2k_B T}\right]$$

$$\tan \delta \propto 1/f \quad E_{\text{gap}} = 5.6 \text{ eV}$$

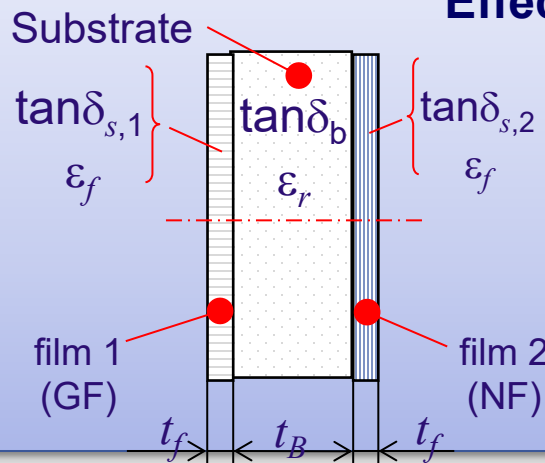
Loss tangent increase by intrinsic lattice/phonon interaction:

$$\tan \delta \propto \frac{f^2}{T} \cdot \frac{1}{\sinh^2\left(-\frac{T_D}{2T}\right)} \quad T_D = 1860 \text{ K}$$

Loss tangent increase by scattering on bulk defects (Rayleigh)

$$I(d, \lambda, \theta) = \frac{I_{\text{inc}}}{r^2} \cdot \frac{1 + \cos^2 \theta}{2} \cdot \left(\frac{2\pi}{\lambda}\right)^4 \cdot \left(\frac{n^2 - 1}{n^2 + 2}\right)^2 \cdot \left(\frac{d}{2}\right)^6 \propto \frac{d^6}{\lambda^4} \propto d^6 \cdot f^4$$

Effective loss of the disk:



$$\tan \delta_{\Sigma} = \underbrace{\tan \delta_b}_{\text{bulk term}} + \underbrace{\tan \delta_{s,1} + \tan \delta_{s,2}}_{\text{surface term}}$$

where $\tan \delta_{s,1}$ and $\tan \delta_{s,2}$ relate to the growth (GF) and nucleation (NF) faces:

$$\tan \delta_{s,i} = a \frac{t_{f,i} \cdot \tan \delta_{f,i}}{t_B}$$

$a = 1.7 \dots 2$ weight factor; $\tan \delta_f$ film loss.

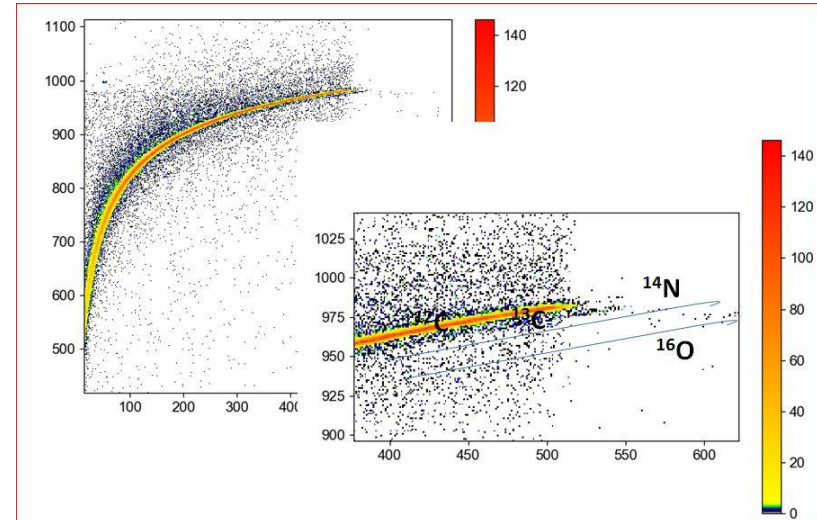
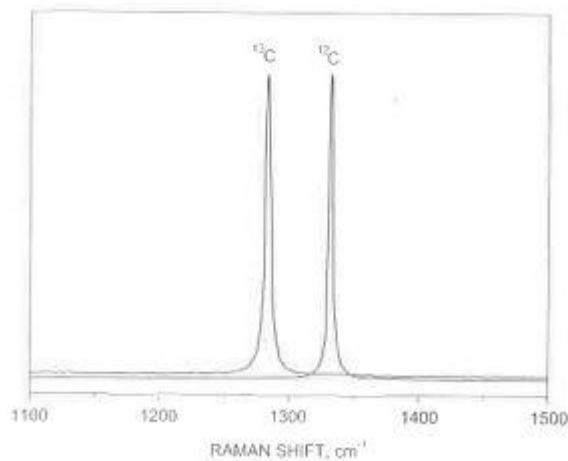
Investigation of defects in poly- and single crystalline diamond related to dielectric losses

1. Detailed characterization of non-irradiated and irradiated diamond samples by $\tan \delta$ and ϵ_r
2. Characterization of single crystalline diamond by $\tan \delta$ and ϵ_r
3. RAMAN investigation of sp^2/sp^3 distribution, especially at the grain boundaries in poly-materials.
4. Detailed determination of influence of nitrogen content to $\tan \delta$ and ϵ_r (N-V effects)

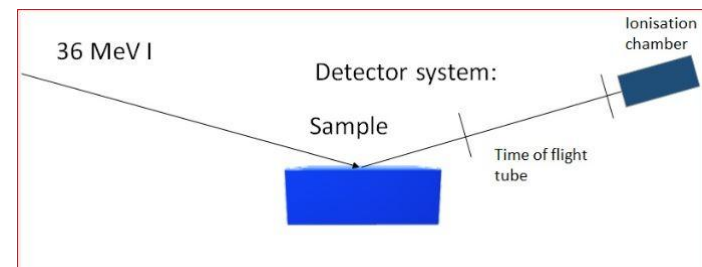
n-irradiated/non-irradiated samples : $\tan\delta$

Sample No.	Material	Diameter	Thickness	Irradiation	Remarks	Dielectric losses	Frequency	Thickness
		mm	mm	n/m ²		tand		
ERIV_62-1	polycrystalline CVD-Diamond	30	0,69	1E+22		6,80E-05	188,76	0,6669
ERIV_56-1	polycrystalline CVD-Diamond	30	1,31	1E+21		1,00E-05	192,21	1,3097
ER_Lot10	polycrystalline CVD-Diamond	30	1,11	1E+24	broken	-		
ER_Lot01	polycrystalline CVD-Diamond	30	1,11	0	broken	-		
3Qu04	Silica	30	1,005	1E+22	4 marks	7,70E-04	152,66	1,007
4Qu04	Silica	30	3,041	1E+22	4 marks	4,60E-04	151,63	3,042
3Qu07	Silica	30	1	1E+21	3 marks	5,20E-04	153,07	1,0046
4Qu07	Silica	30	3	1E+21	3 marks	4,50E-04	152,17	3,031
4Qu09	Silica	30	3	0		4,40E-04	151,51	3,044
Al_146	Alumina	40	4	0	1 mark	3,30E-04	90-100	4,014
Al_166	Alumina	40	4	0	2 marks	4,50E-03	90-101	4,015

Characterization of virgin/irradiated materials



ToF-ERDA spectrum of diamond.

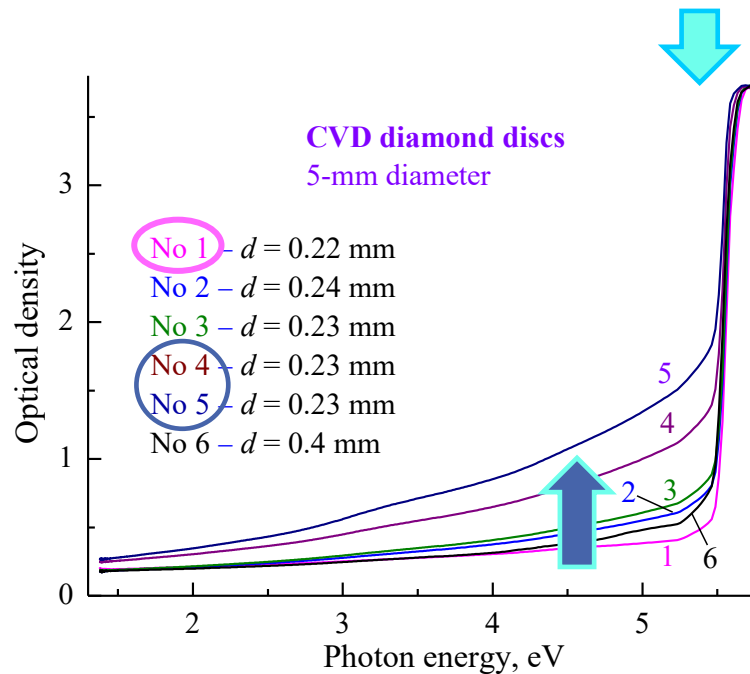
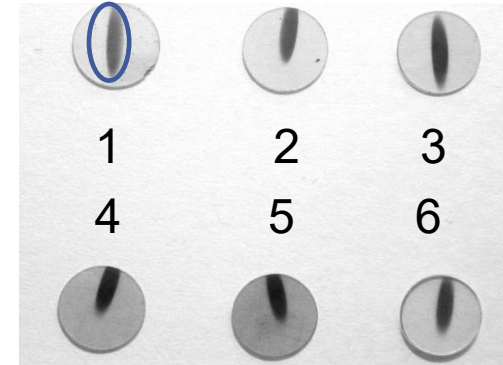


Schematic Setup of ERDA-irradiation for diamond with 36 MeV Iodine in Uppsala/Sweden.

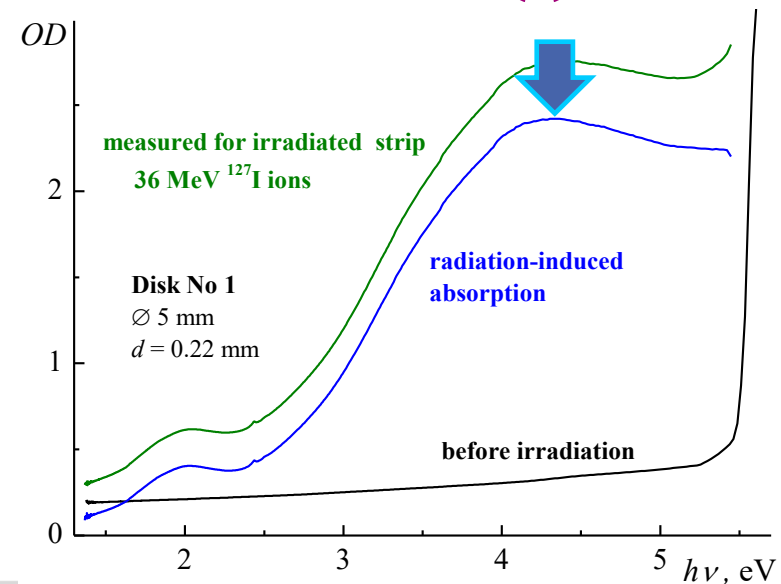
Characterization of virgin/irradiated materials (UT, ISSP-UL)

Six 5-mm-diameter discs of CVD diamond have been analyzed **before and after** irradiation with 36-MeV ^{127}I ions (Elastic Recoil Detection Analysis (ERDA) measurements using Tandem accelerator in Angström-Lab, Uppsala).

Optical absorption spectra for nonirradiated Diamond discs, JASCO-V660 spectrophotometer



$$OD(\lambda) = \frac{1}{d} \log\left(\frac{1}{T(\lambda)}\right)$$



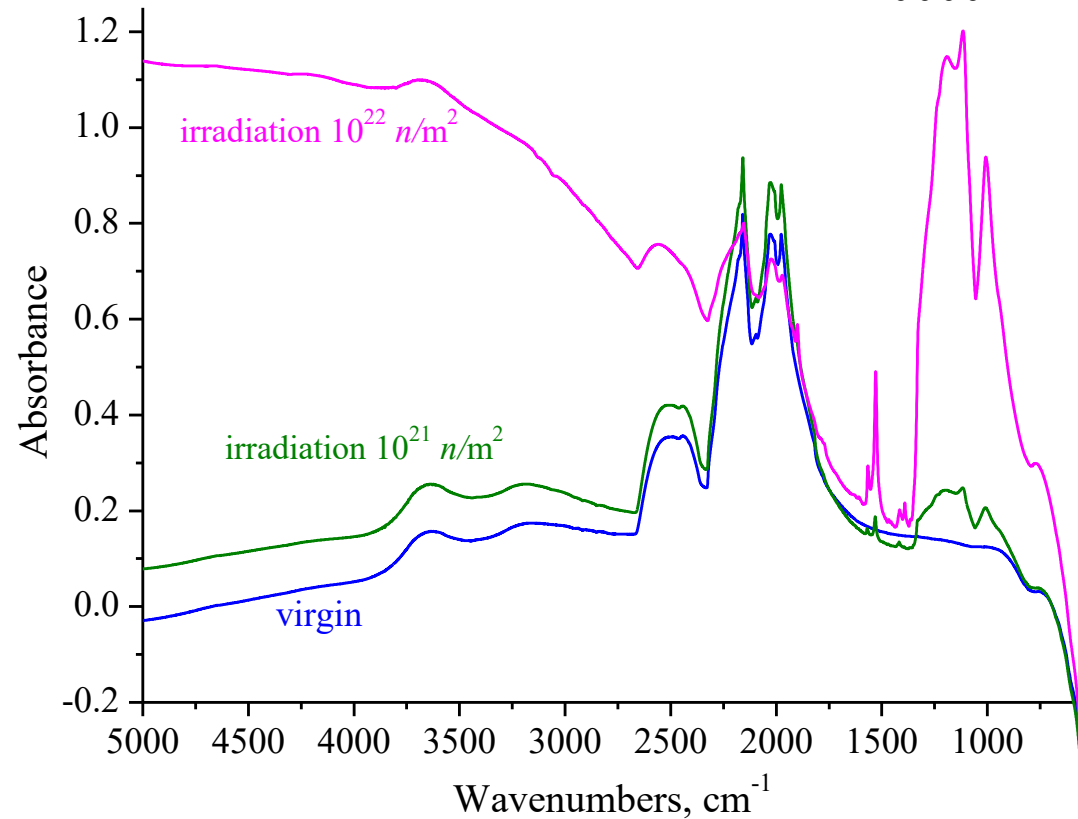
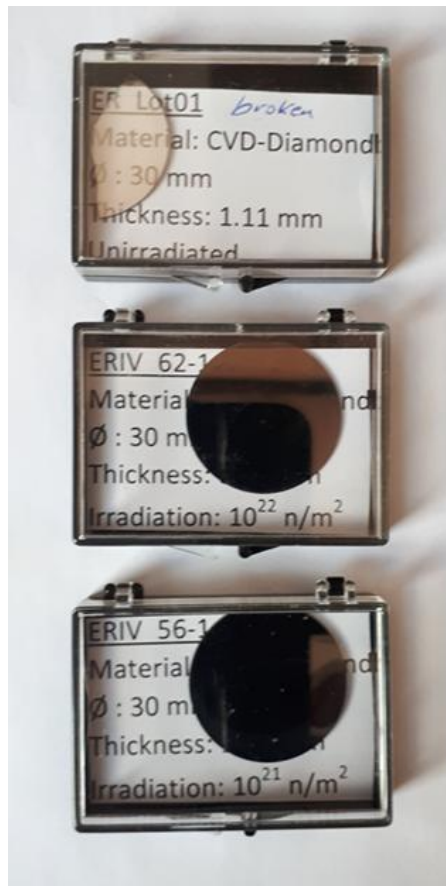
IR spectroscopy of neutron irradiated diamond

Spectrometer Vertex 80v (Bruker)

Resolution = 2 cm^{-1}

rich radiation-induced
vibrational structure

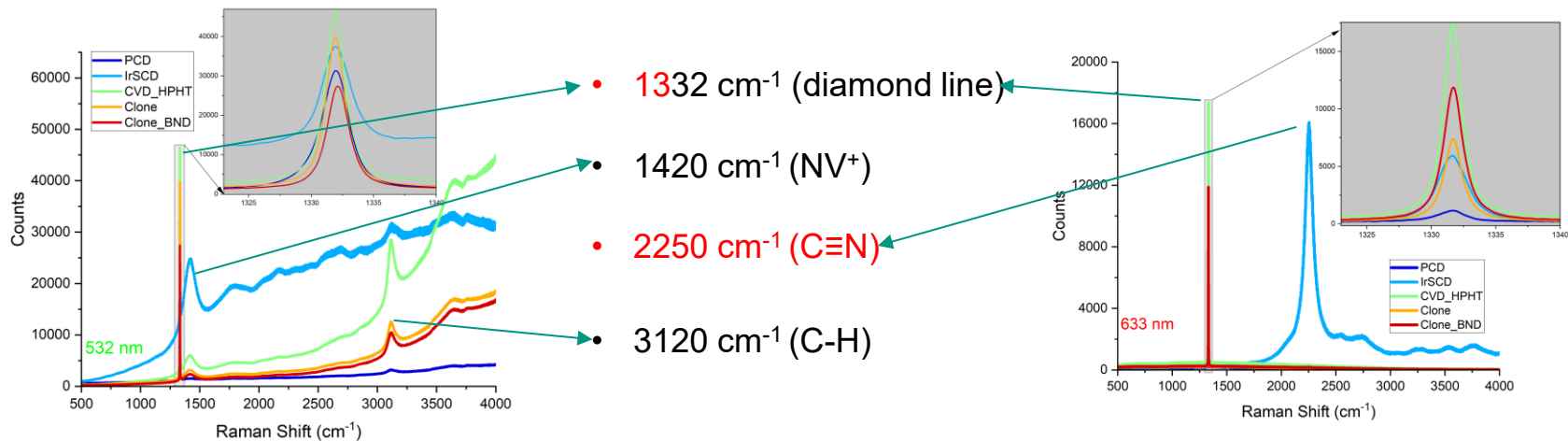
$5000 \text{ cm}^{-1} = 0.62 \text{ eV}$
 $1000 \quad 0.124$
 $10000 \quad 1.24 \text{ eV}$



New RAMAN spectrometer at IAM-AWP: HORIBA Jobin Yvon Odyssey LabRAM – UV-VIS-NIR

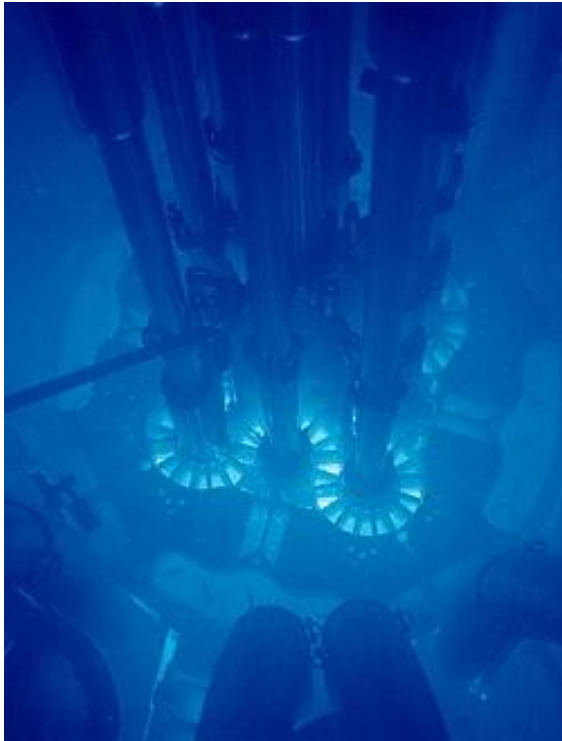


Experimental Results – Raman spectroscopy



- 1332 diamond line overlaps with very close NV^0 line $\rightarrow$ peak height influenced by nitrogen content
- IrSCD $\rightarrow$ $\text{C}\equiv\text{N}$ line (2250 cm^{-1}) + C-N vibrations (2250 – 2730 cm^{-1}) $\rightarrow$ growth incorporates N strongly inside the lattice.
- O-H and C-H stretching (hydroxyl and hydrocarbons) (> 3000 cm^{-1}) $\rightarrow$ surface contamination
- NV^- zero phonon line sidebands (3500 – 3700 cm^{-1})
- Luminescence background under green light, intensity $\propto$ N-content / TLS losses

Irradiation



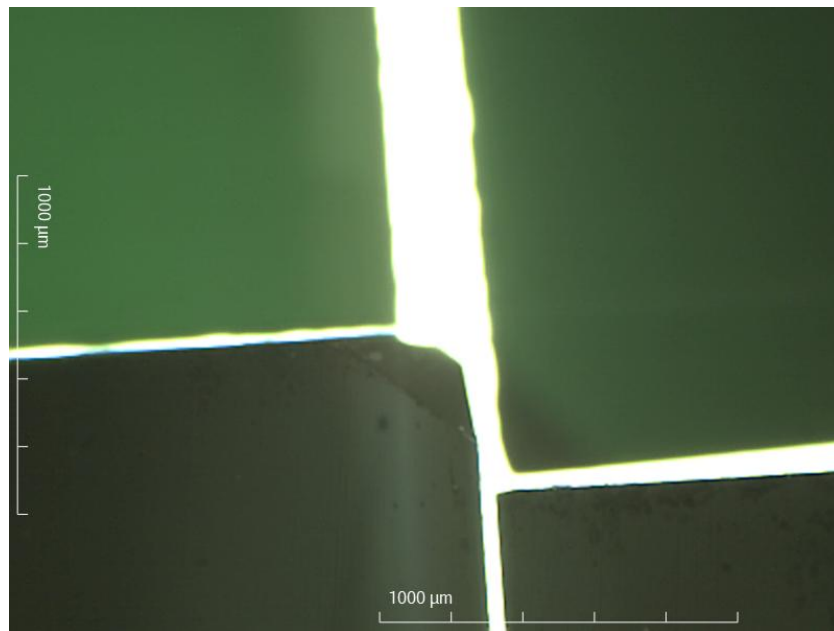
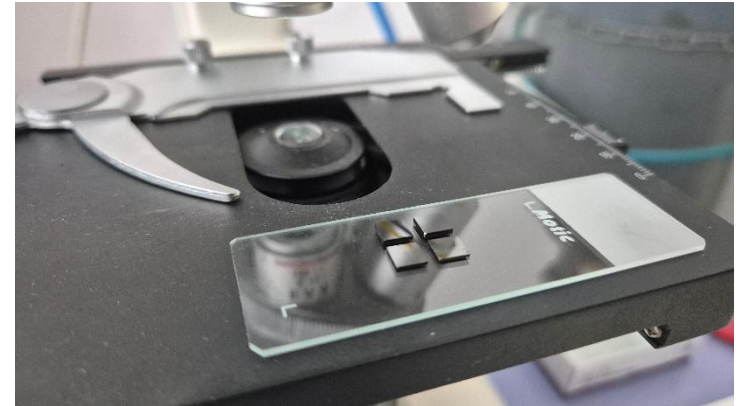
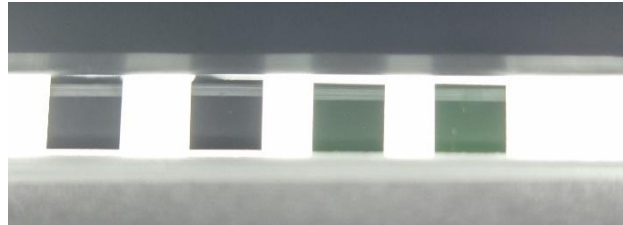
- **Fast neutron fluence**
 $1.76 \times 10^{18} \text{ cm}^{-2} \pm 20 \%$
- **Displacements per atom**
 $\sim 1.25 \times 10^{-3} \text{ DPA (1.25 mDPA)}$
- **Thermal neutron fluence**
 $2.36 \times 10^{19} \text{ cm}^{-2}$
- **Total dose (mainly γ)**
 $\sim 140 \text{ MGy} \pm 30 \%$
- **Sample temperature:**
 $35\text{--}40^\circ \text{C}$ no annealing



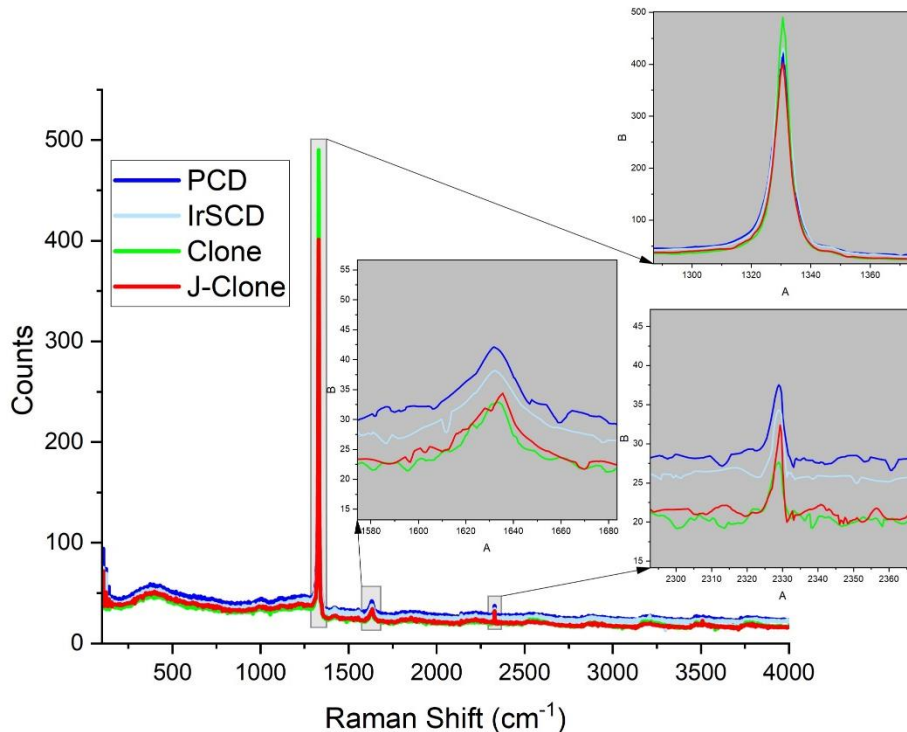
• Radionuclides

- Sc-47 – 35 Bq
- Cr-51 – 300 Bq
- Co-60 – 30 Bq
- Zn-65 – 150 Bq
- Sb-122 – 150 Bq
- Sb-124 – 350 Bq
- Ta-182 – 40 Bq
- Au-198 – 150 Bq

1E-4 dpa neutrons at MARIA/Poland



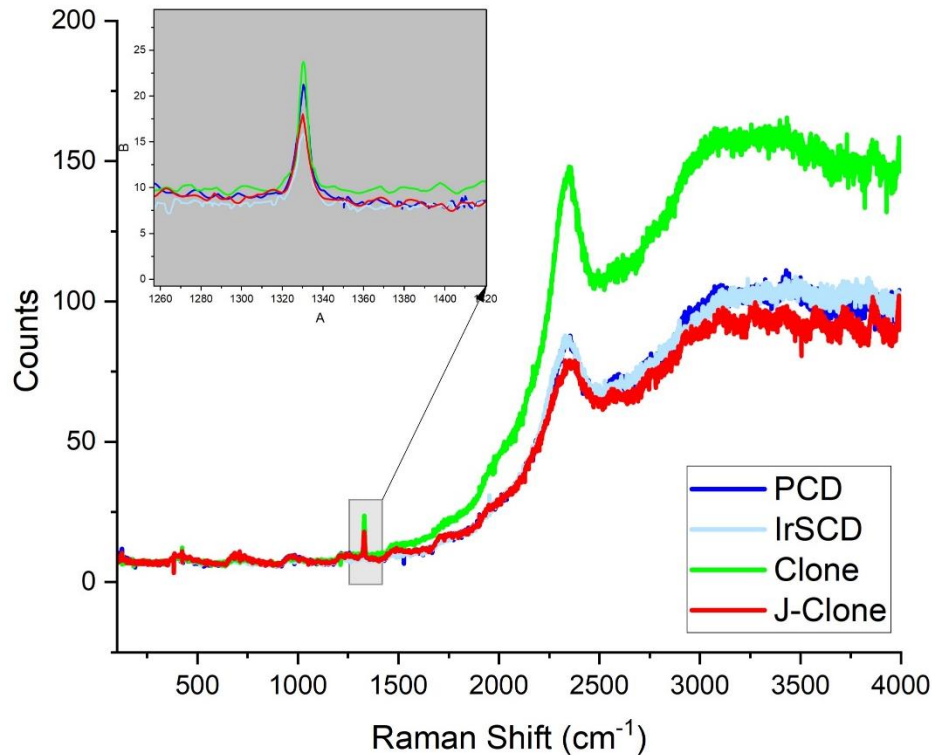
Raman spectroscopy (532 nm) – After Irradiation



- The samples appear completely black, having lost most spectral features observed before irradiation. Raman signal intensity dropped by over 98% due to strong self-absorption in the damaged lattice.

- **Diamond lattice severely damaged but partially preserved:** the faint 1332 cm^{-1} Raman line indicates residual crystalline sp^3 regions.
- **Disordered carbon signature ($\sim 1630 \text{ cm}^{-1}$):** broad feature reveals formation of sp^2 -bonded clusters and amorphous carbon from neutron-induced bond rearrangement.
- **N_2 vibration at $\sim 2328 \text{ cm}^{-1}$:** trapped molecular nitrogen formed by migration and aggregation of displaced nitrogen atoms in radiation-induced voids.

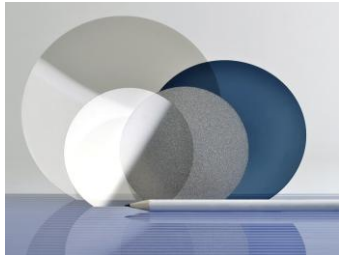
Raman spectroscopy (633 nm) – After Irradiation



- **Raman signal nearly extinguished under 633 nm excitation:** very faint 1332 cm^{-1} diamond line confirming extreme optical opacity and deep lattice disorder.
- **$\text{C}\equiv\text{N}$ bond signature at 2250 cm^{-1} disappears:** Neutron damage breaks $\text{C}-\text{N}$ bonds; nitrogen migrates and aggregates.
- **New broad band at 2345 cm^{-1} appears:** associated to the $\text{N}\equiv\text{N}$ stretching mode of molecular nitrogen trapped within radiation-induced nanovoids.
- **Broad continuum above 3000 cm^{-1} :** Weak defect-related luminescence and multi-phonon background from heavily disordered carbon–nitrogen regions.

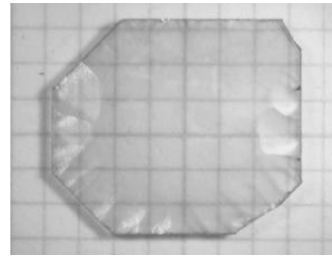
Diamond samples

Polycrystalline CVD diamond



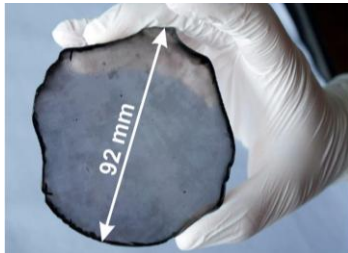
- Reference sample
- ECRH standard
- $\tan\delta < 10^{-5}$ (100-200 GHz)

Single crystal CVD over HPHT seed



- HPHT growth template
- High degree of cristallinity
- Very low dislocation density

Single crystal diamond on iridium



- Hetero-epitaxial growth
- Ir low tendency to form carbides
- Middle dislocation density

Single crystal cloned

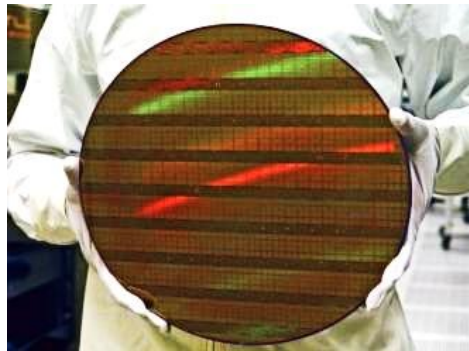


- Each tile is a “clone” of the original substrate
- Tiles are joined by additional growths

Nitrogen is added to the growth processes to control the growth speed and grain size

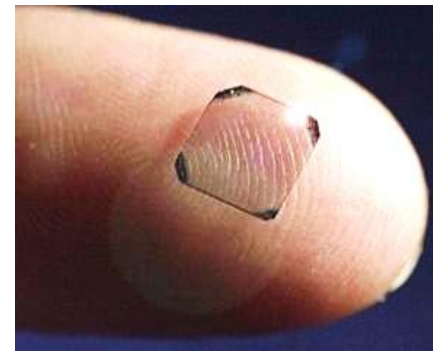
Did we say Electronic materials?

Silicon



Impurities $< 10^{10} / \text{cm}^3$

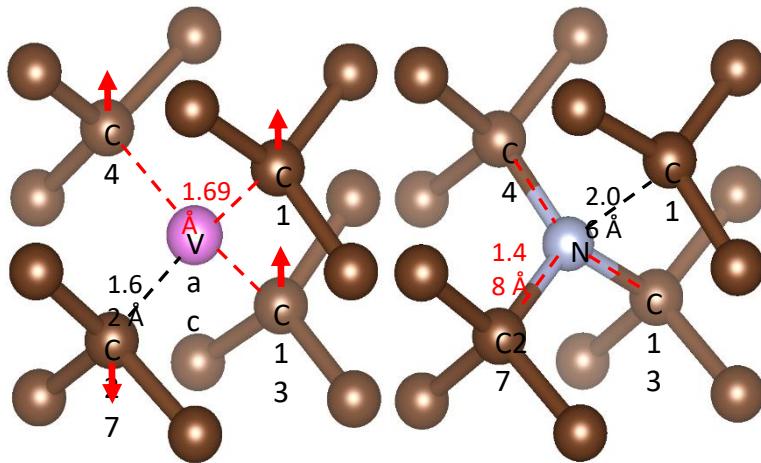
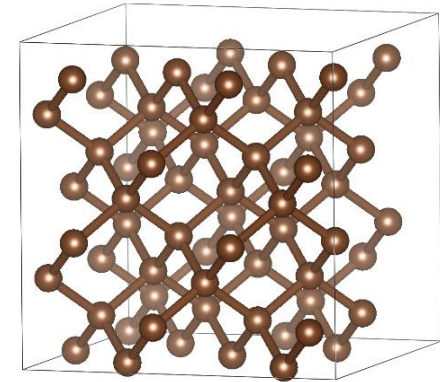
Diamond



Impurities $< 10^{15} / \text{cm}^3$

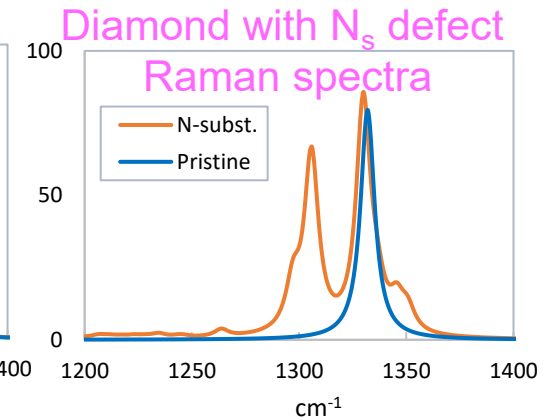
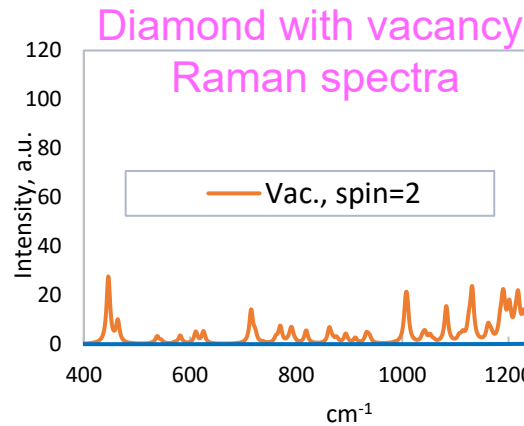
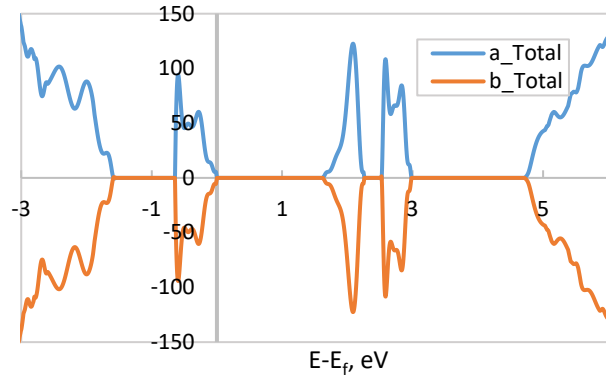
In 2021, theoretical activities included the first principles calculations of the atomic, electronic, vibrational properties and dielectric properties of basic defects in diamond, corundum, as well as interfaces between corundum and thin films of AlN and SiO₂. The state of the art first principles methods using the CRYSTAL17 computer code within the linear combination of atomic orbitals (LCAO) approximation and VASP plane wave code have been used.

For defects in diamond – the **supercells** containing 64 C atoms each and periodically repeated defects; a few basis sets for C, unrestricted DFT with B1WC as well as B3LYP advanced hybrid DFT with exchange-correlation functionals.



Results of our computational simulation of **a neutral vacancy** (V_a, left) and **a nitrogen substitutional atom** (N_s defect, right) in diamond.

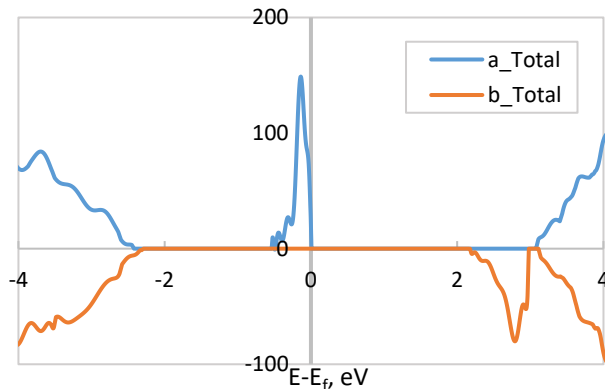
The calculations of harmonic phonon frequencies at the Γ point, IR and Raman spectra, dielectric functions (loss tangent) have been performed for **defective diamond**. DOS, diamond with neutral vacancy, spin = 0



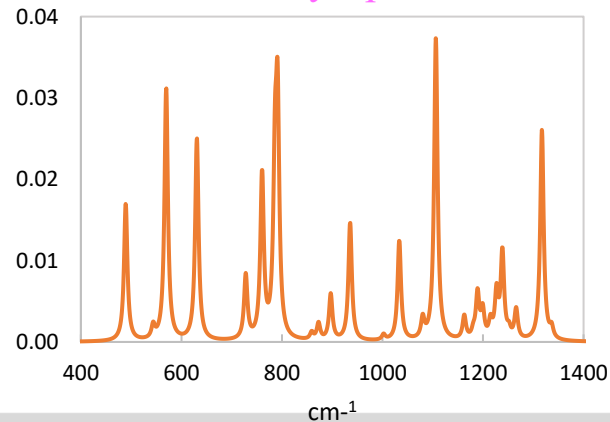
For pristine diamond,
 $E_g = 5.7$ eV.

Calculated Raman peak for pristine diamond is at 1332 cm^{-1} (coincides with the experimental value). Calculated loss tangent for defective diamond in range 140-206 GHz used in monitoring is about 2×10^{-7} .

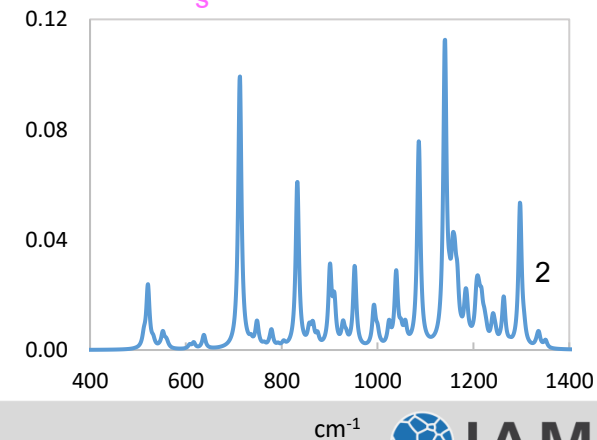
DOS, diamond with N_s defect



Loss tangent for diamond
with vacancy, spin=4



Loss tangent for diamond
with N_s defect



The main conclusion on diamond

Both defects (Va, Ns) produce negligible (10^{-7}) loss tangent in the operational frequency range 140-206 GHz.

Other defects such as B or larger pores/surfaces have to be checked.

Crystal substrate - LaAlO₃

Raman measurements

Excitation wavelength: 532nm

LaAlO₃

Orientation:

110

Dimension:

∅ 25.4 x 0.5

LaAlO₃

Orientation:

111

Dimension:

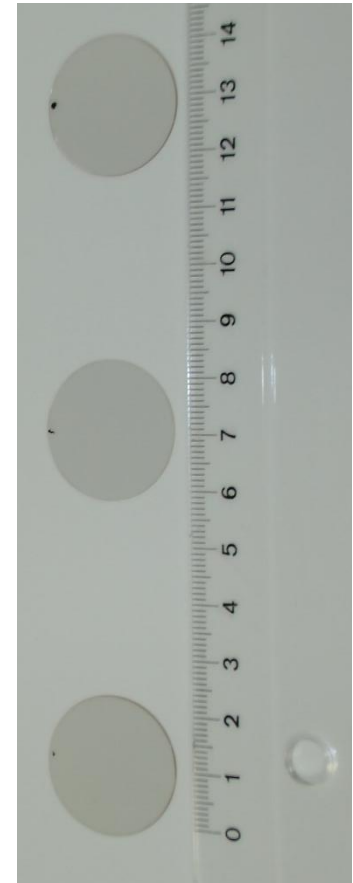
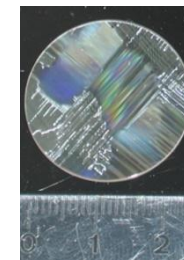
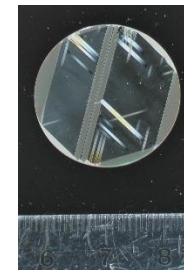
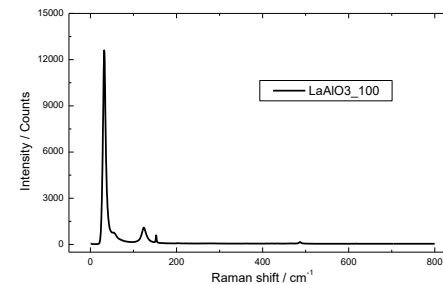
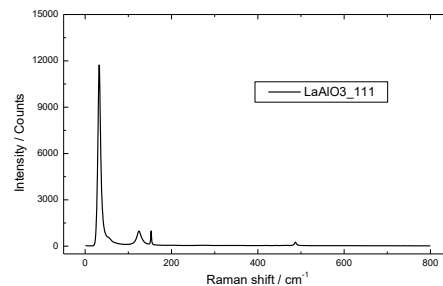
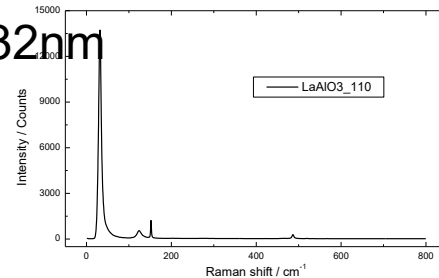
∅ 25.4 x 0.5

LaAlO₃

Orientation: 100

Dimension:

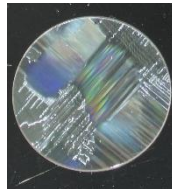
∅ 25.4 x 0.5 mm



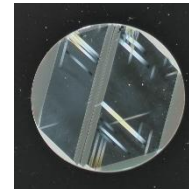
Crystal substrate - LaAlO₃

Dielectric measurements

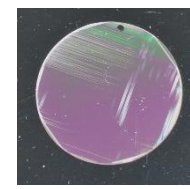
LaAlO₃_100



LaAlO₃_111



LaAlO₃_110



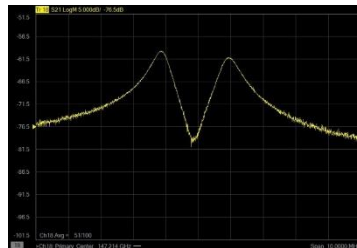
Birefringence 90°

Double peak of
the
rhombohedral
distorted
perovskite
structure

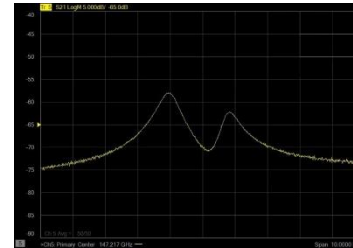
Resonance frequency

ϵ_e / ϵ_o

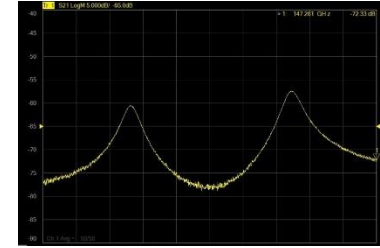
$\tan \delta$



LA100:
24.1 and
23.9
 $4 \cdot 10^{-4}$



LA111:
24.4 and 23.8
 $8 \cdot 10^{-4} / 2 \cdot 10^{-4}$



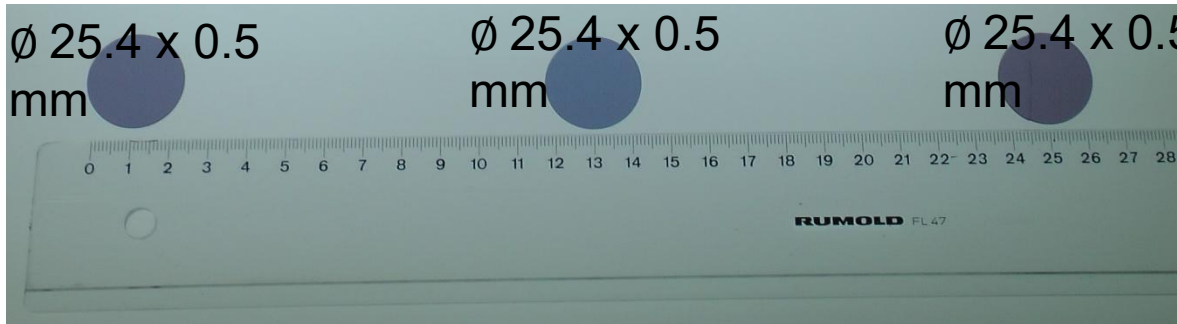
LA110:
24.0 and 23.5
 $2 \cdot 10^{-4} / 3 \cdot 10^{-4}$

Crystal substrate - NdGaO₃

NdGaO₃
Orientation:
110
Dimension:
Ø 25.4 x 0.5
mm

NdGaO₃
Orientation:
001
Dimension:
Ø 25.4 x 0.5
mm

NdGaO₃
Orientation:
100
Dimension:
Ø 25.4 x 0.5
mm



Results @ 95GHz
 ϵ
 $\tan\delta$

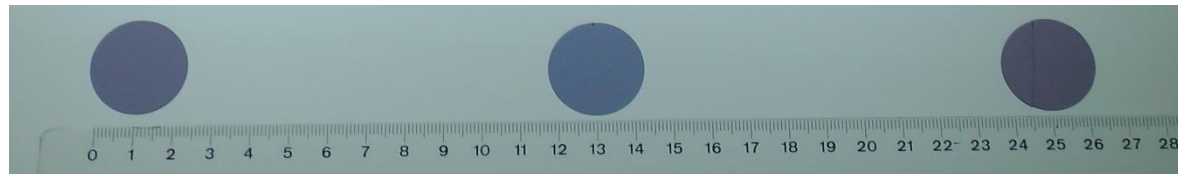
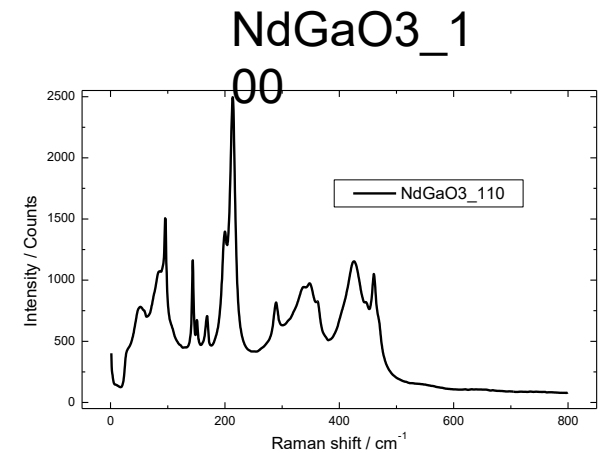
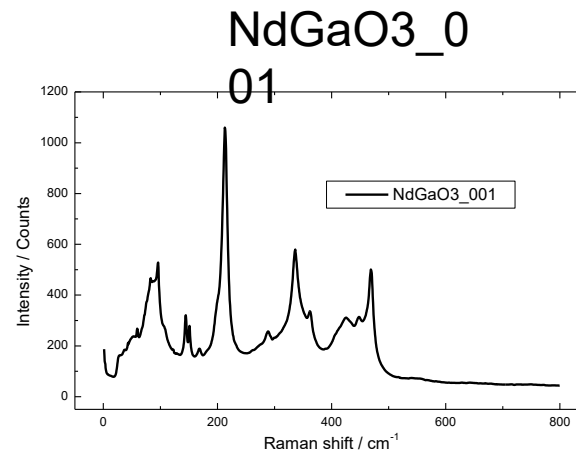
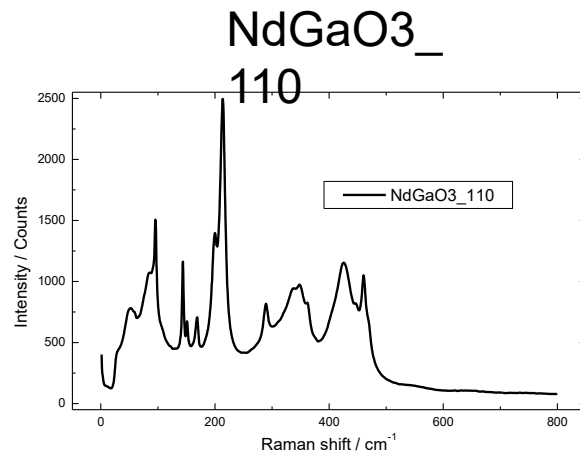
NdGaO₃_11
0
22.5
 $1.1 \cdot 10^{-3}$

Not determined

Not determined

Crystal substrate - NdGaO₃

Raman measurements - Excitation wavelength: 532nm



Crystal substrate - NdGaO₃

Dielectric measurement

NdGaO₃

Orientation:

110

Dimension:

Ø 25.4 x 0.5
mm

NdGaO₃

Orientation:

001

Dimension:

Ø 25.4 x 0.5
mm

NdGaO₃

Orientation:

100

Dimension:

Ø 25.4 x 0.5
mm



ϵ_r
 $\tan\delta$

22.5
 $1.1 \cdot 10^{-3}$

Not determined

Not determined

Tanks to:

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