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Modeling Mechanical Deformation and Optical Waveguiding Properties of Ion-Implanted Diamond with COMSOL Multiphysics

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ABSTRACT

Ion implantation in insulating materials leads to local variations in mechanical and optical properties that can be exploited for the fabrication of micro-structures. In particular, ion irradiation of diamond causes the formation of buried amorphised layers, with correspondent mass density and refractive index variations that depend on the level of "damage" of the crystal structure, i.e. on the employed ion fluence. For low damage levels, the damaged layer retains its optical transparency and wave guiding structures can be fabricated. In this study, we perform COMSOL Multiphysics FEM simulations to verify the number and type of propagating modes in such a waveguide, as a function of geometry and refractive index variation. At the same time, surface deformation ("swelling") and internal strains due to the buried damaged layer expansion are analyzed, to evaluate the deformation of the waveguide and account for stress-optic effects, respectively. Hence the need for a "multiphysics" approach. Numerical results are compared to preliminary experimental measurements and used as "in silico" tests to derive the desired wave guiding properties..

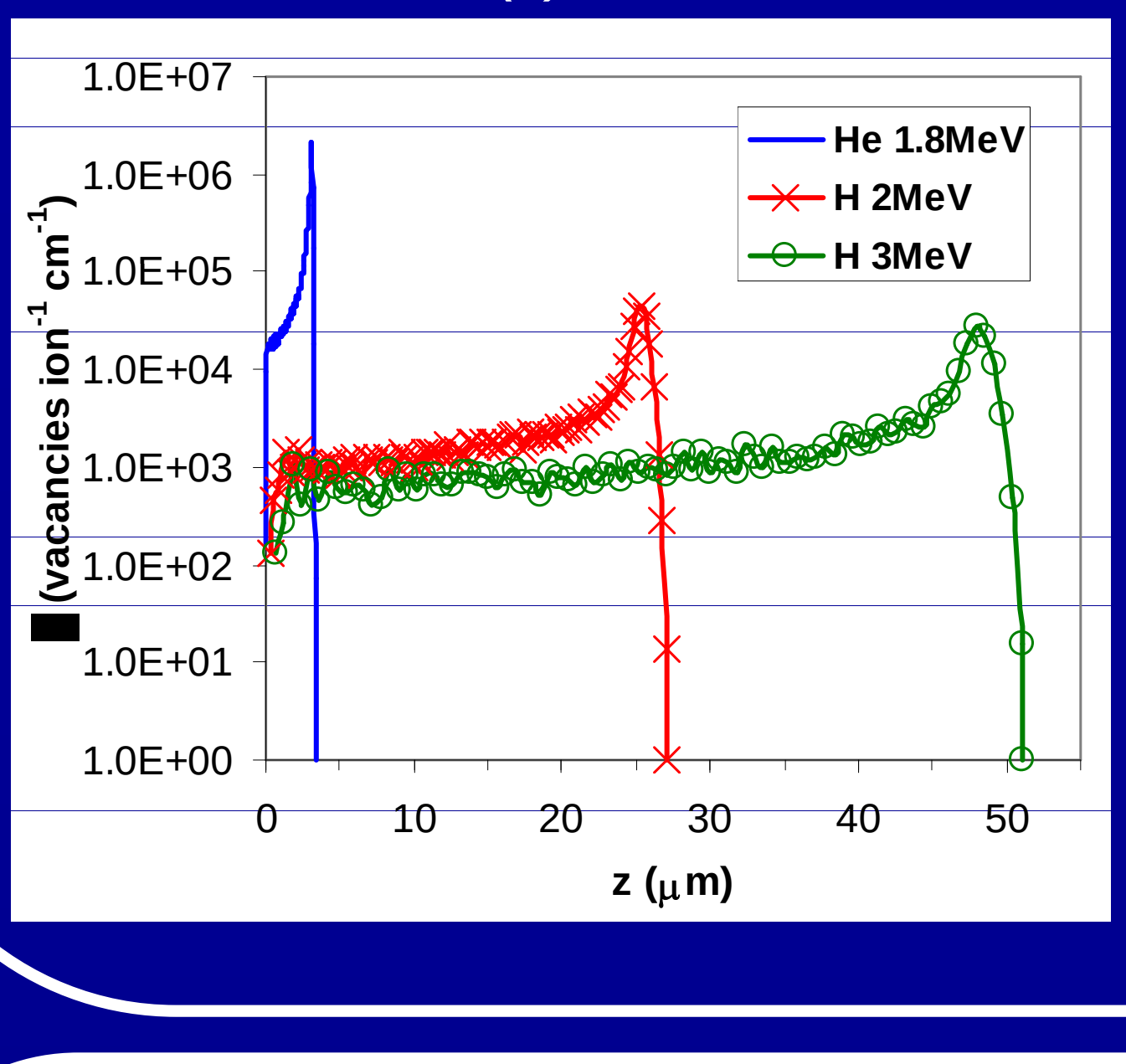
1 MODEL FOR DENSITY VARIATION

- ✓ Ion implantation induces density change ("amorphisation")
- ✓ Surface swelling due to significant difference in density between diamond and amorphous carbon
- ✓ Swelling localized at the implanted areas
- ✓ Model accounts for a **saturation in density** variation for heavily damaged diamond (high ion fluences):
- ✓ Density of damaged diamond vs. implantation fluence *F* and depth *z*:

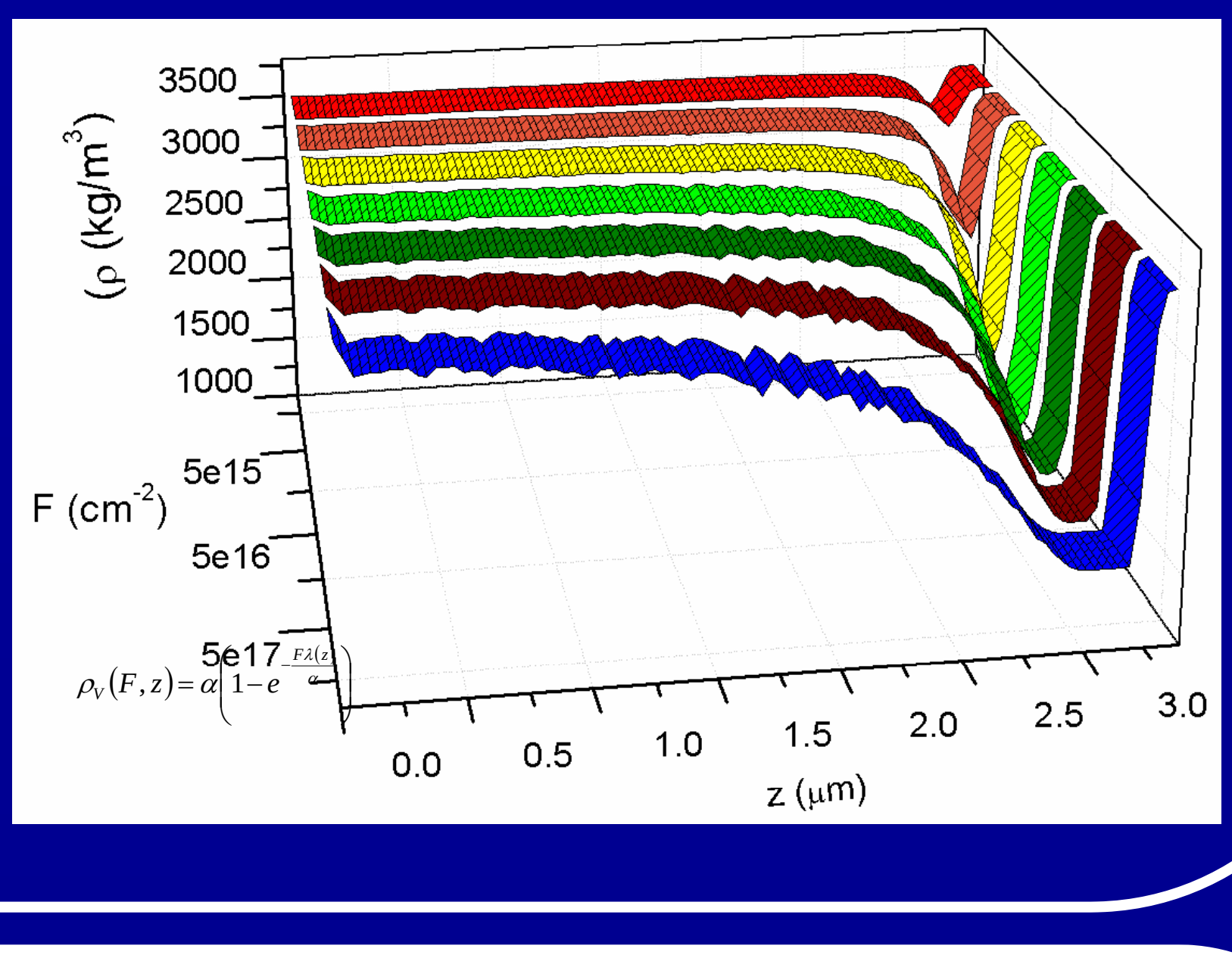
$$\rho(F,z)=\rho_d-\beta\cdot\rho_V(F,z)=\ldots=\rho_d-(\rho_d-\rho_{aC})\left(1-e^{-\frac{F\lambda(z)}{\alpha}}\right) \qquad (1)$$

λ Linear damage profile, calculated with SRIM
ρ_V vacancy density,
ρ_d diamond density
ρ_{aC} amorphous carbon density
α "critical density"= fitting parameter

$\lambda(z)$



$\rho(F,z)$

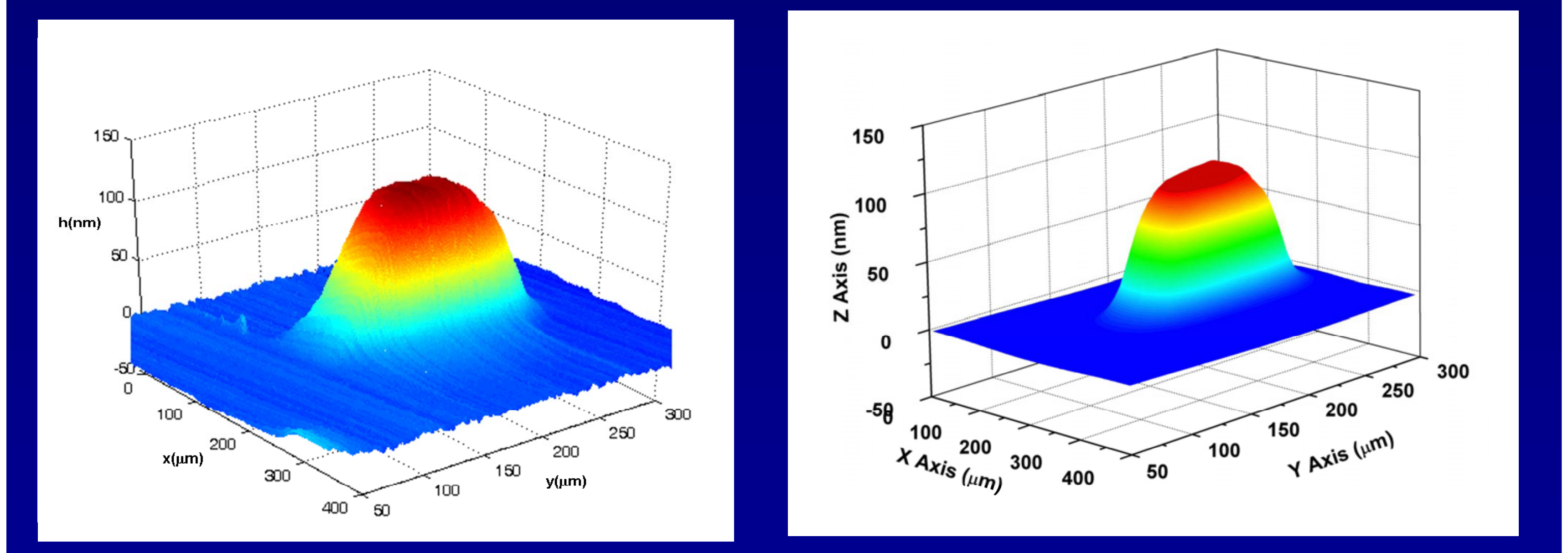


2 SURFACE DEFORMATION AND INTERNAL STRAINS

- ✓ Through-the-thickness variation of material properties:

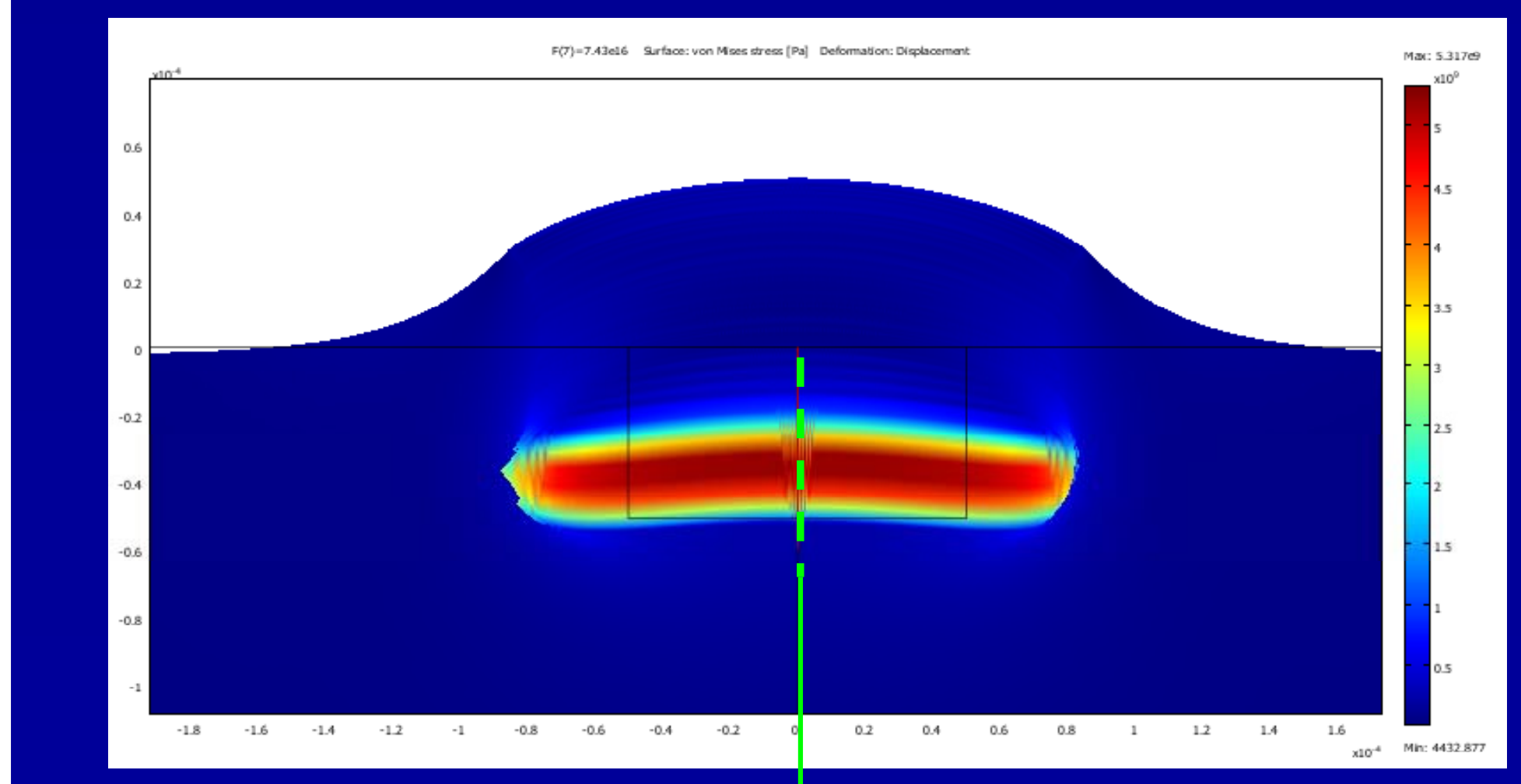
$$E(F,z)=E_d-(E_d-E_{aC})\left(1-e^{-\frac{F\lambda(z)}{\alpha}}\right) \qquad \nu(F,z)=\nu_d-(\nu_d-\nu_{aC})\left(1-e^{-\frac{F\lambda(z)}{\alpha}}\right)$$

ρ_d = 3.515 g·cm^{-3}, E_d =1144.6 GPa, $\nu_d = 0.2$
ρ_{aC} =1.557 g·cm^{-3} E_{aC} = 21.38 GPa, $\nu_{aC}= 0.184$



Swelling effect over implanted area for 1.8 MeV He (F=3.67 10^{16} cm^{-2}) : comparison between experimental (white light interferometry profilometry) measurements and simulations.

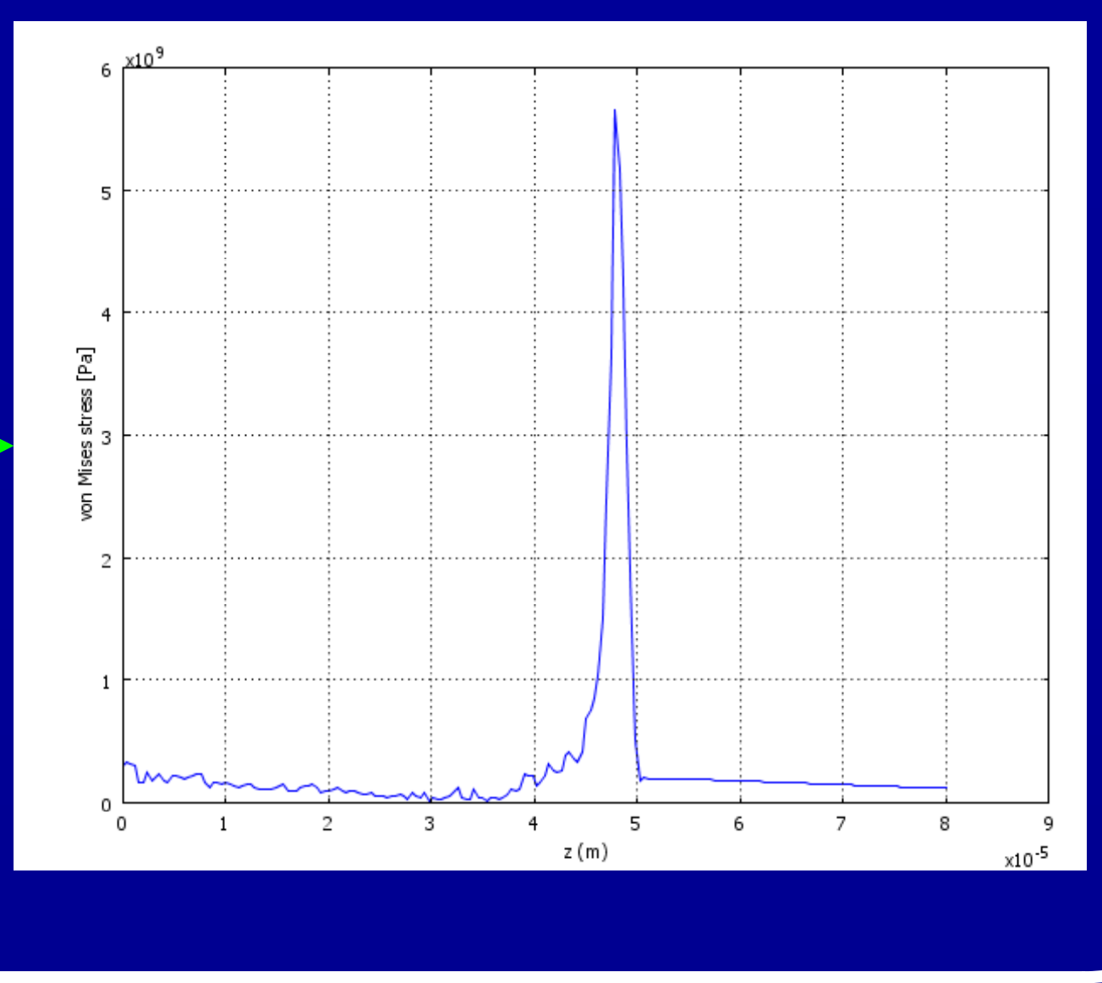
- ✓ Swelling effects typically below 100nm: waveguide deformation can be neglected



Internal Von Mises Stress relative to 3 MeV H

Stress-optic effect

Through-the thickness stress profile

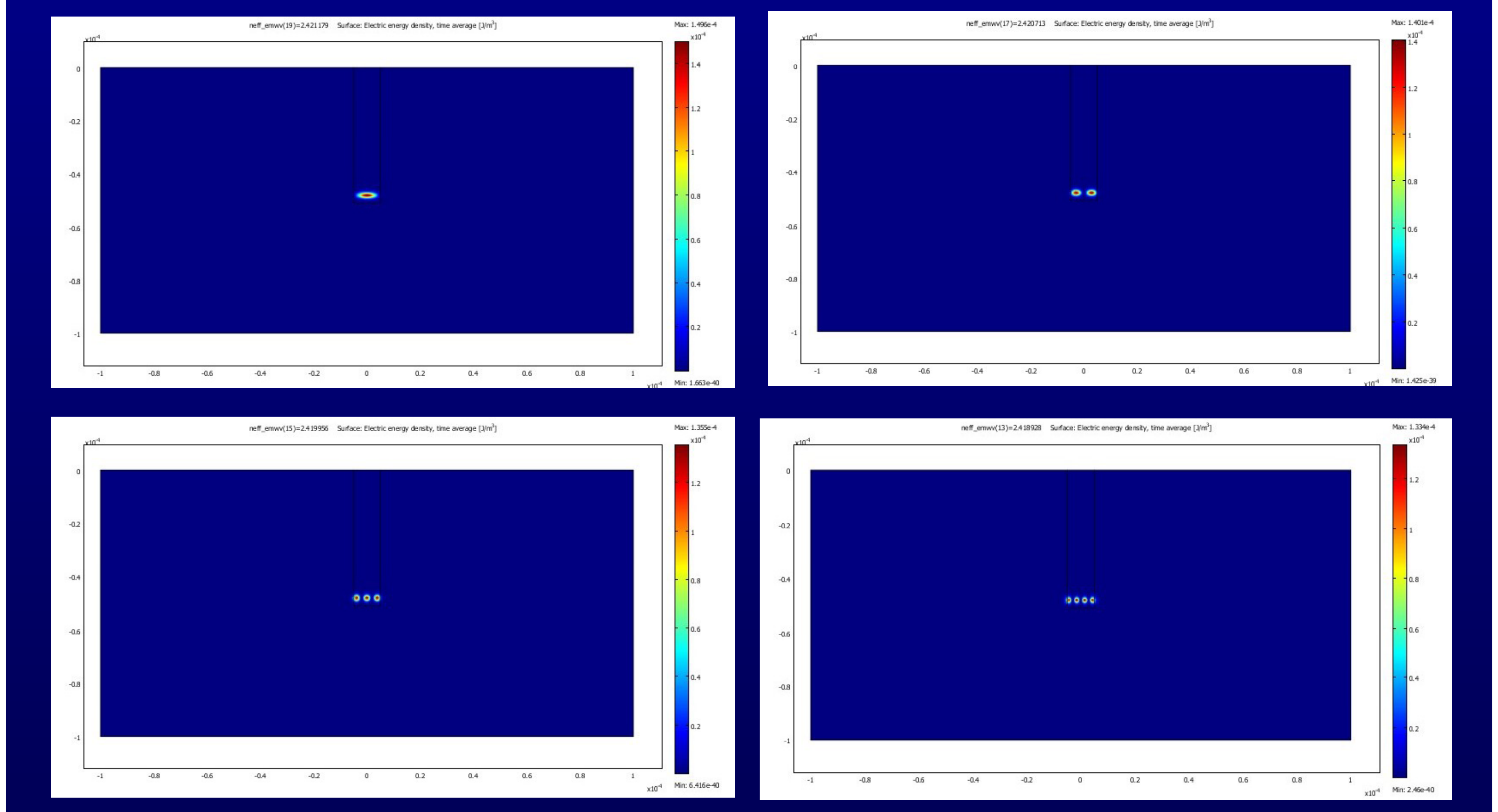


- ✓ 2 effects contribute to refractive index variation_
  - **- Stress-optic effect**
  - **- Density variation**
- ✓ Overall dependency:

$$n(z)=n_0+c_1F\lambda(z)$$

3 OPTICAL WAVEGUIDE MODES

- ✓ Eigenmode analysis n_0 = 2.41, λ = 633nm, c_1 = 4.26·10^{-23} cm^3 F = 5·10^{15} #/cm^2



- ✓ Number of guided modes increases with fluence
- ✓ Minimum fluence for which waveguiding occurrs: F = 10^{14} #/cm^2

4 CONCLUSIONS

- ✓ Numerical modelling of surface swelling in ion-implanted diamond, carried out using COMSOL Multiphysics, yields good accordance between experimental and numerical data and provides encouraging insight in the structural damage mechanisms
- ✓ Surface swelling values for low fluence implantations (typical for optical waveguide applications, in order to avoid high optical absorption) are limited to below ~100nm. Waveguide deformation can thus be neglected.
- ✓ Stress-optical effect due to internal strains can be evaluated, leading to a refractive index variation.
- ✓ Through-the thickness refractive index variation due to density variation and stress-optic effect leads to the possibility of creating buried waveguides situated various micrometres below the surface in diamond substrates.
- ✓ The number and type of guided modes depends on the entity of refractive index variation: the number increases with increasing fluence

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