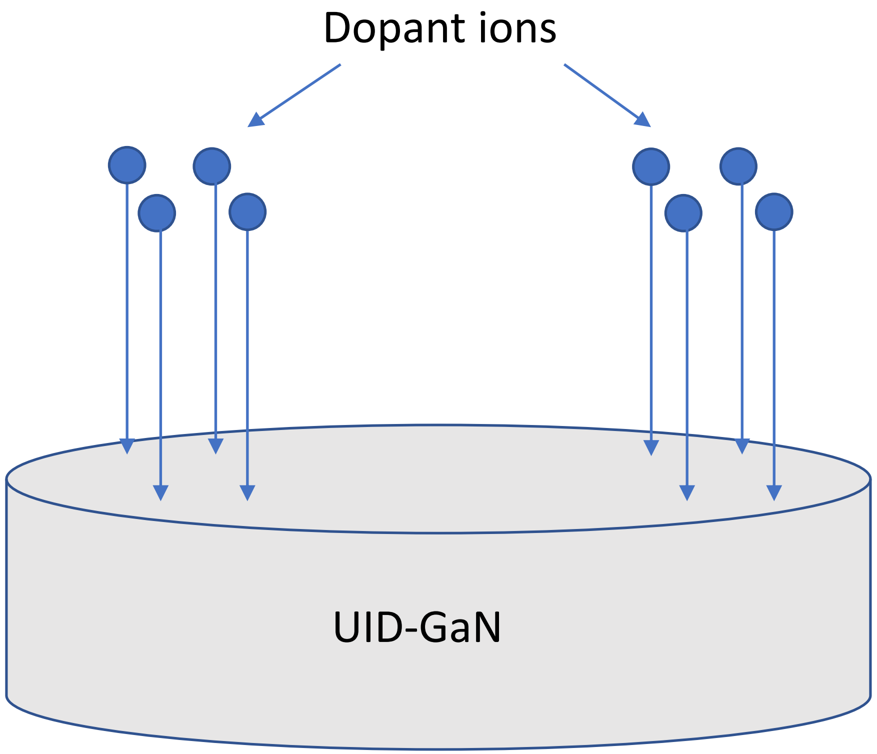
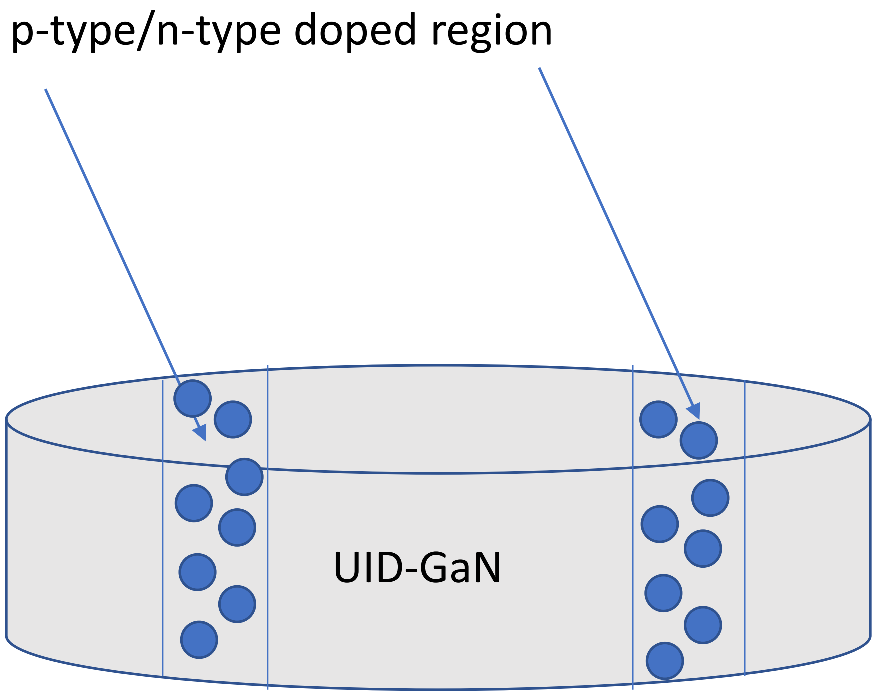
Investigation of Diffusion Mechanism of Beryllium in GaN

Ion Implantation (I/I)





I/I difficulties

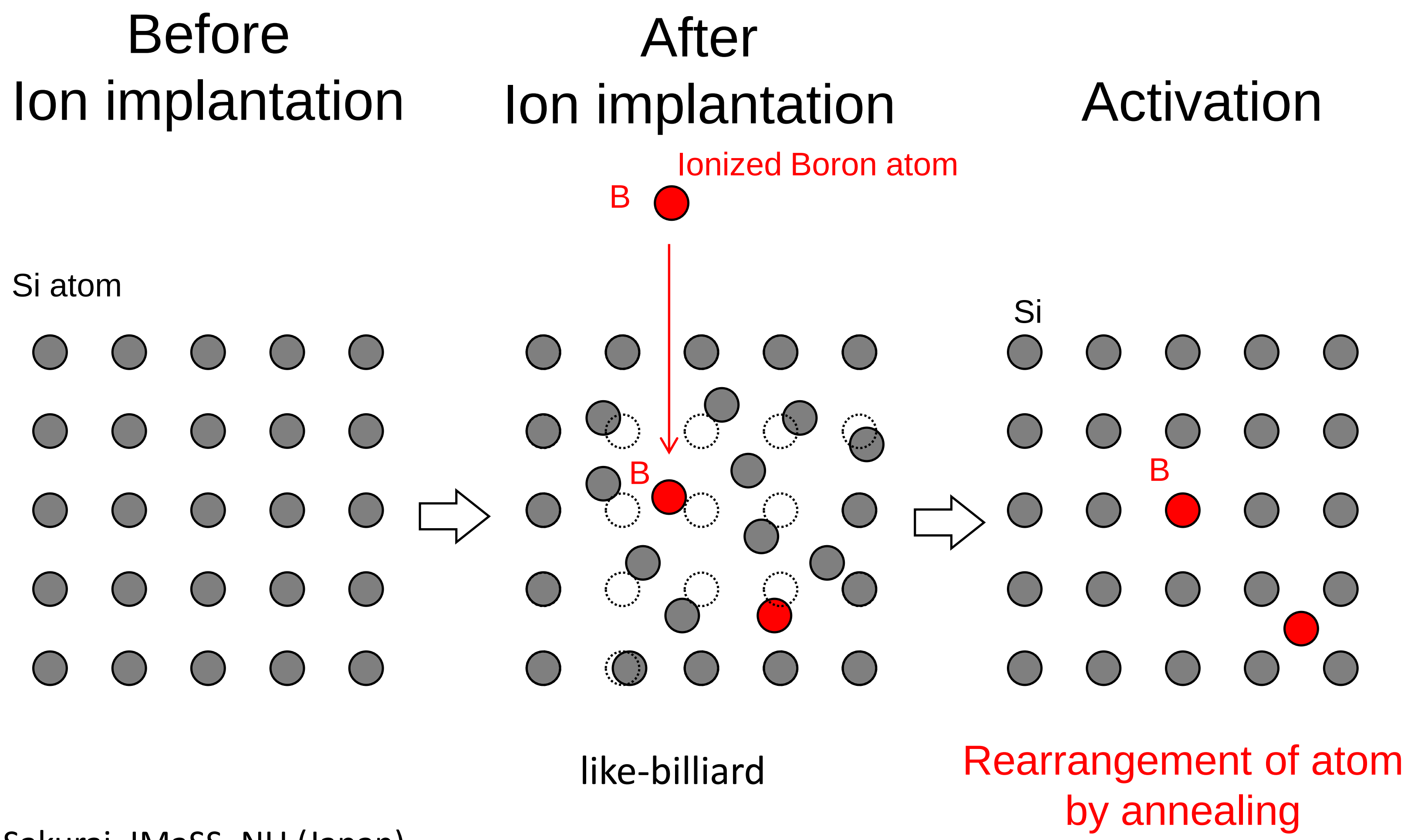
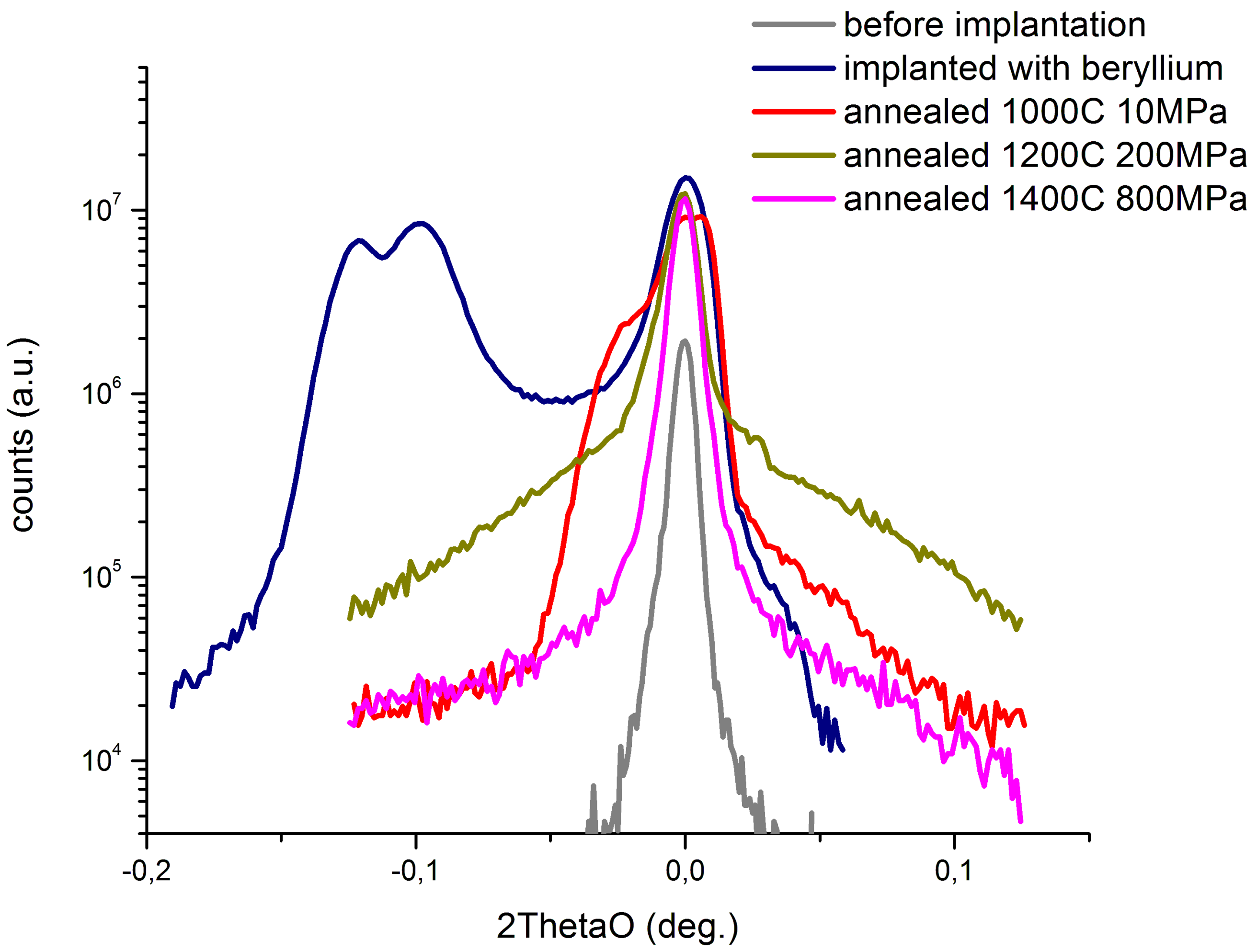


Image by H. Sakurai, IMaSS, NU (Japan)

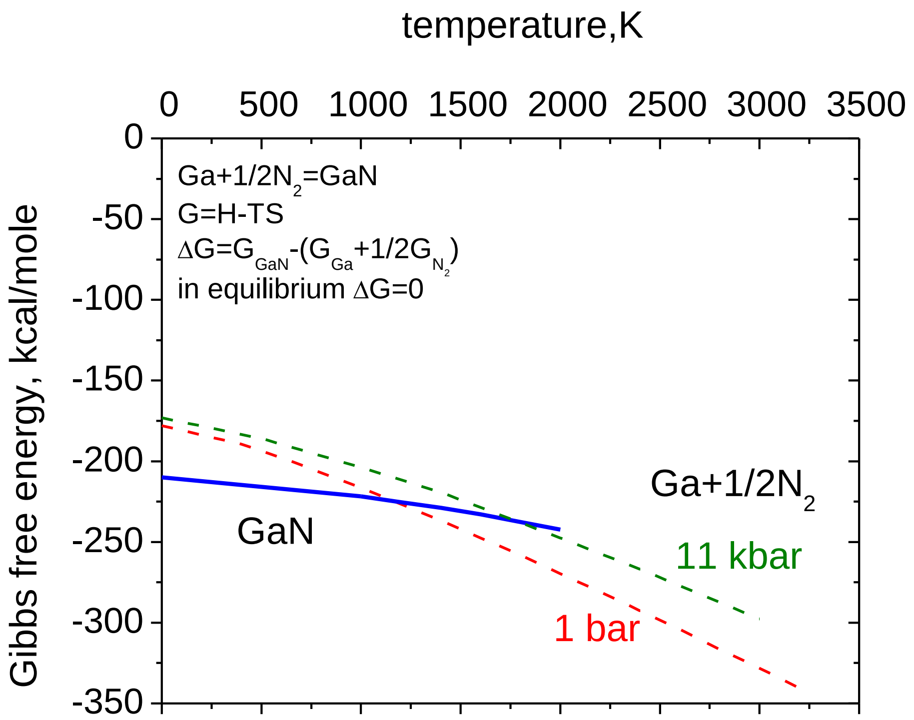
Post implantation treatment for GaN



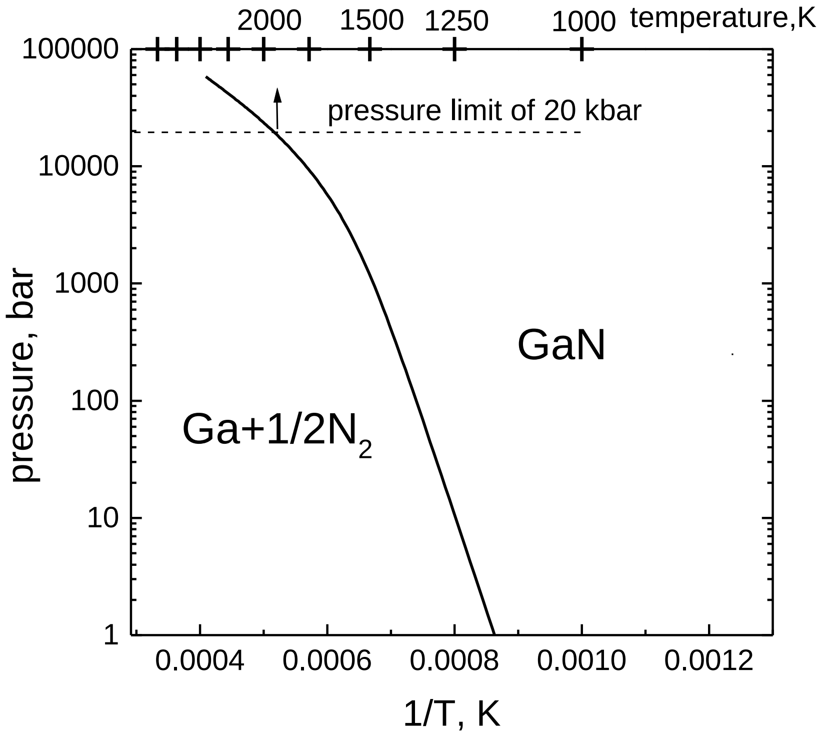
High temperature is needed to fully recover from implantation damage in case of gallium nitride

Anneling in high temperature is possible in high pressure only due to GaN thermodynamics

GaN thermodynamics

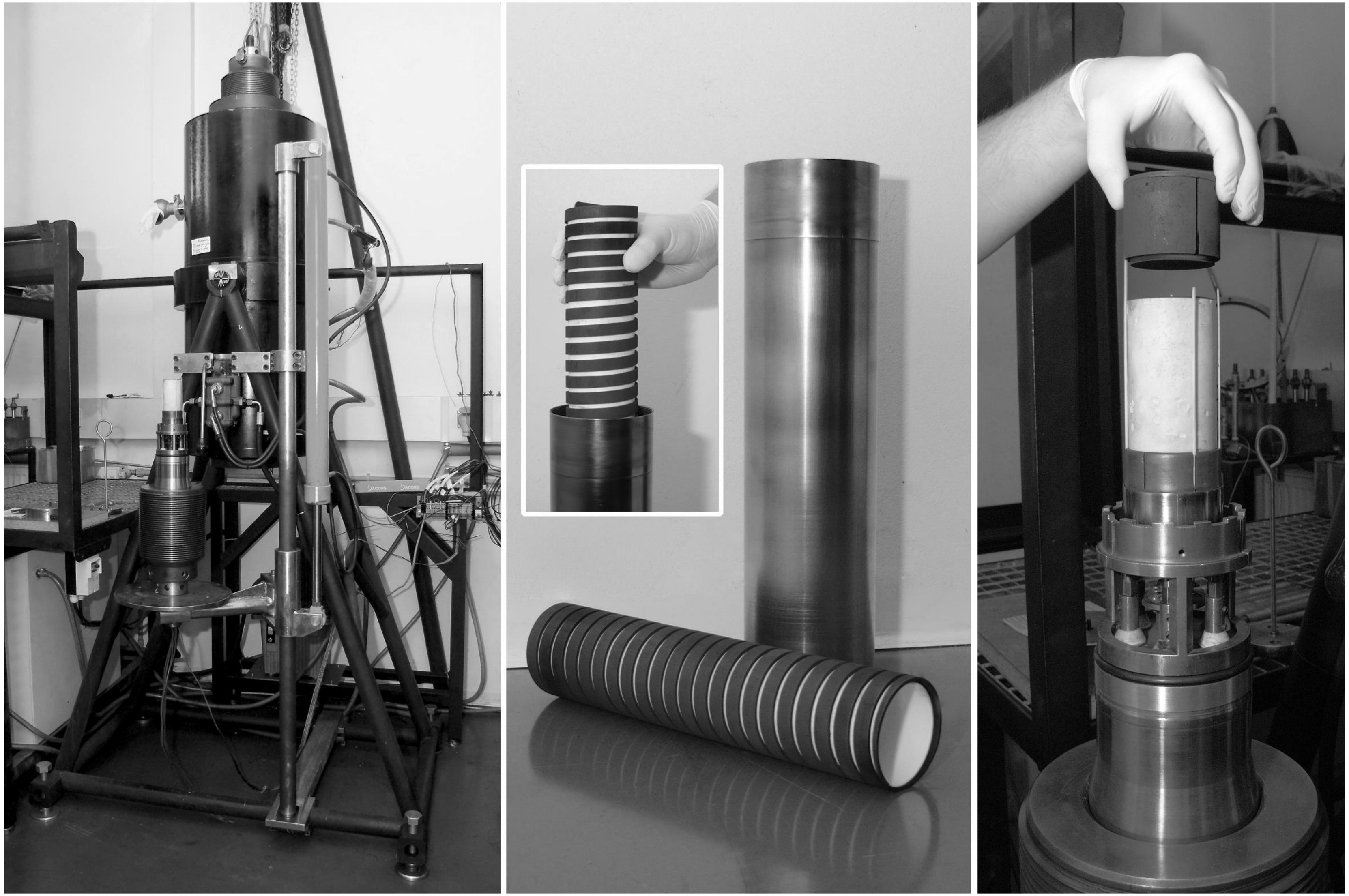


I. Grzegory et al. in Bulk Crystal Growth of Electronic, Optical and Optoelectronic Materials, ed. by P. Capper, Wiley&Sons, (2005), 173

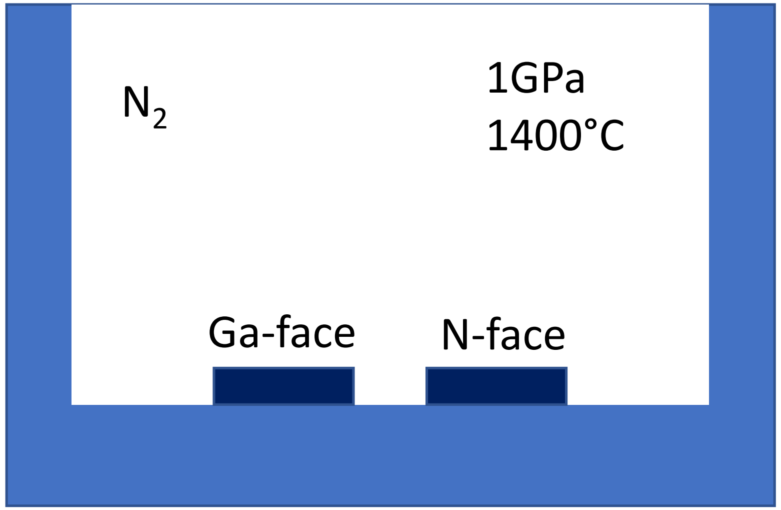


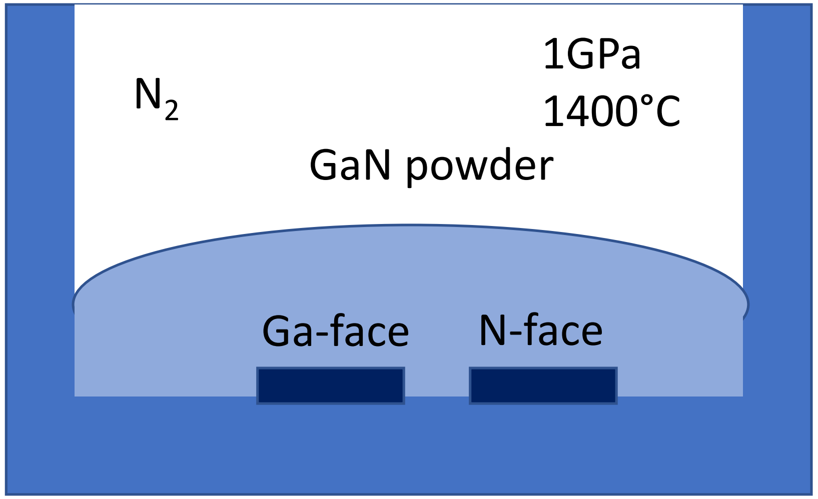
J. Karpinski, J. Jun, S. Porowski, Journal of Crystal Growth, 66, 1984, Pages 1-10

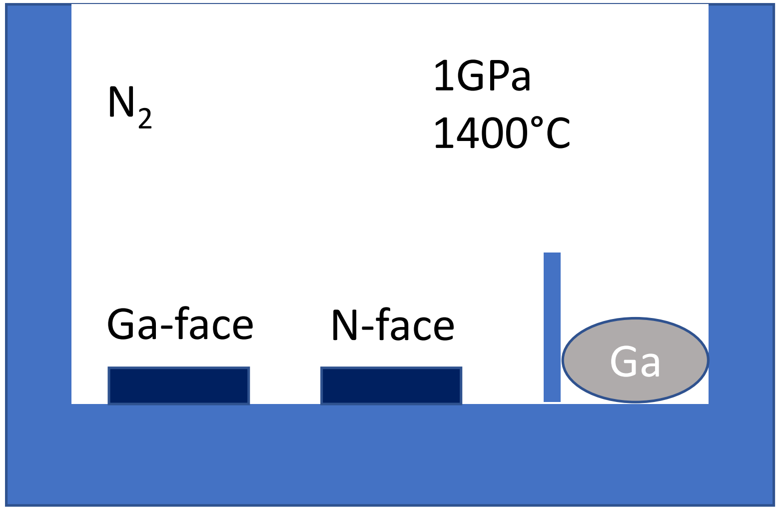
Ultra High Pressure Reactors



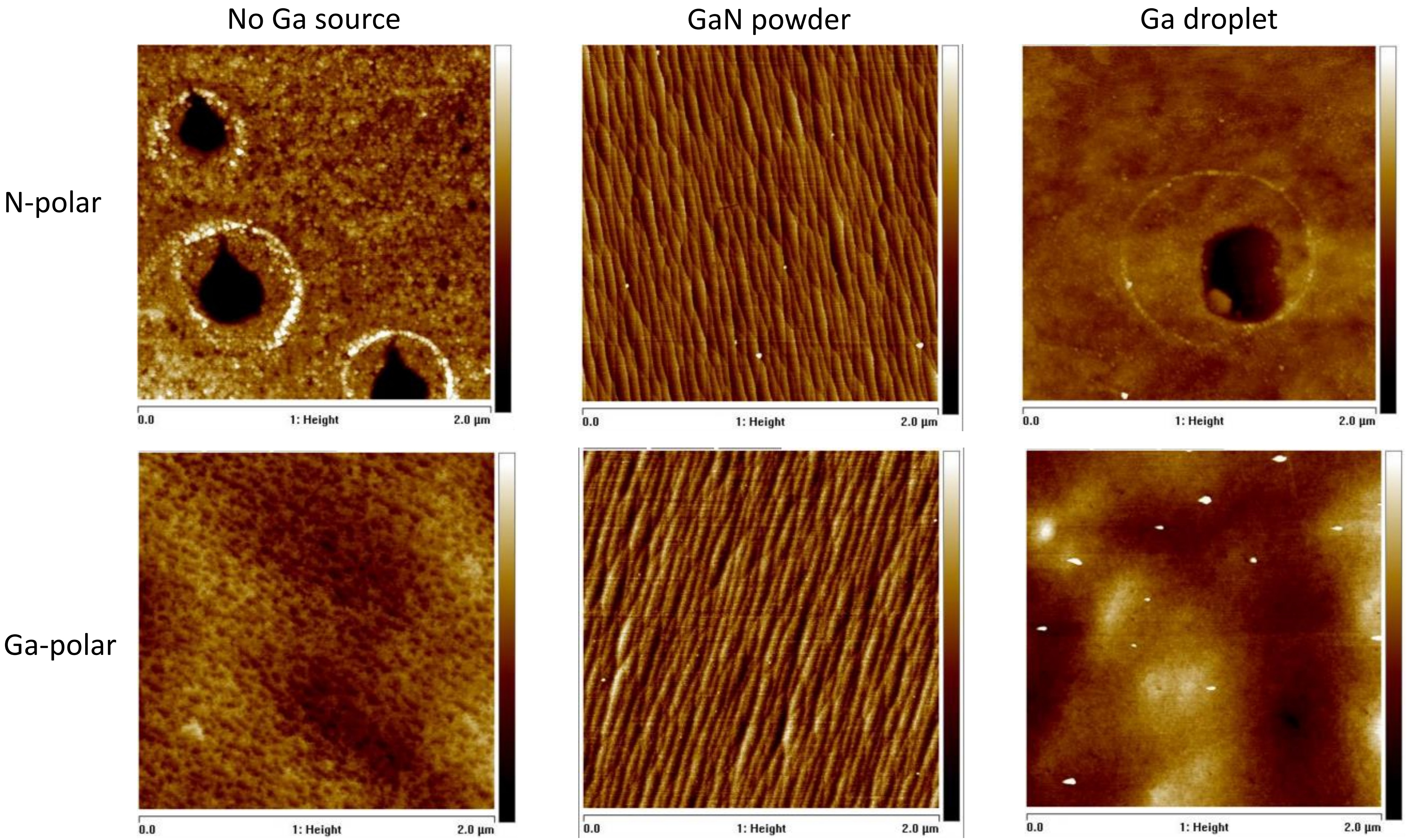
Ultra high pressure annealing (UHPA)







K. Sierakowski et al. High Pressure Processing of Ion Implanted GaN, Electronics 2020, 9(9), 1380



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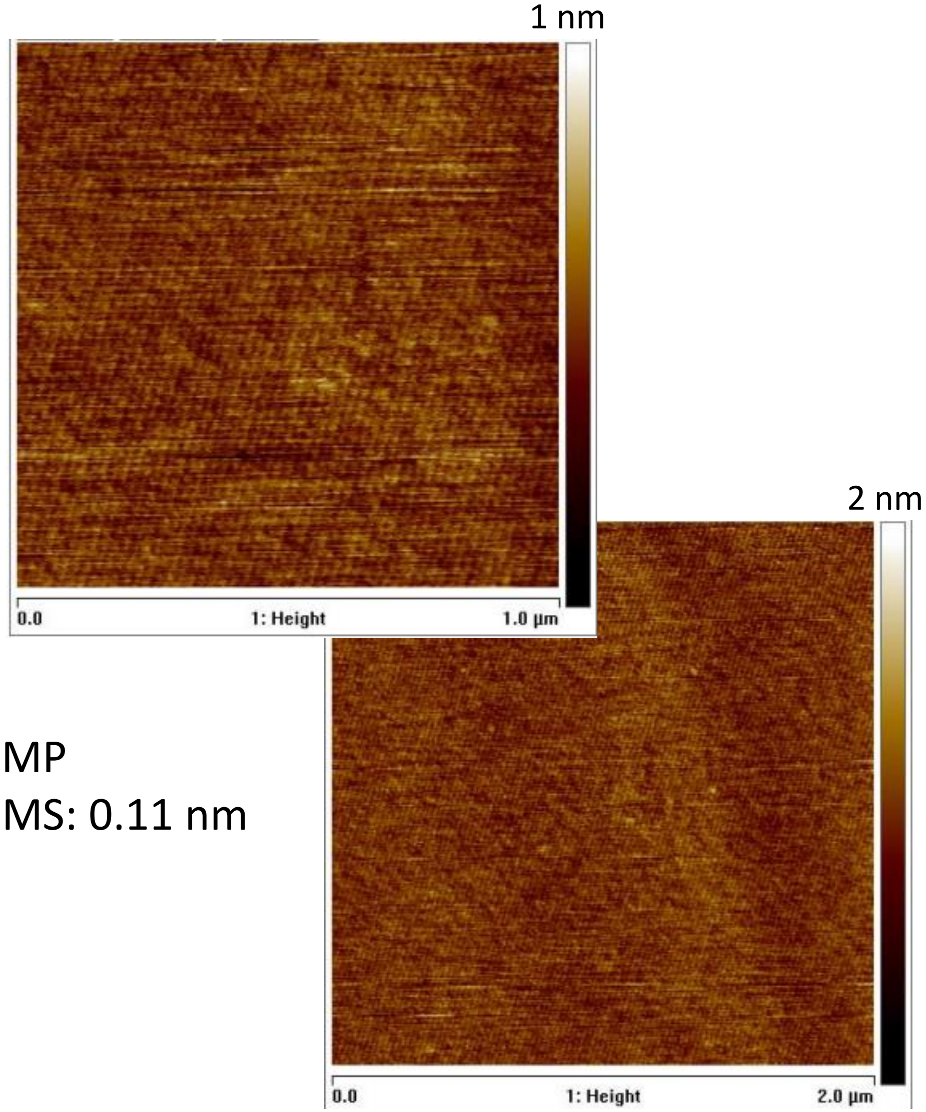
AFM after and before UHPA



CMP
RMS: 0.11 nm

Annealed under GaN powder
RMS: 0.46 nm

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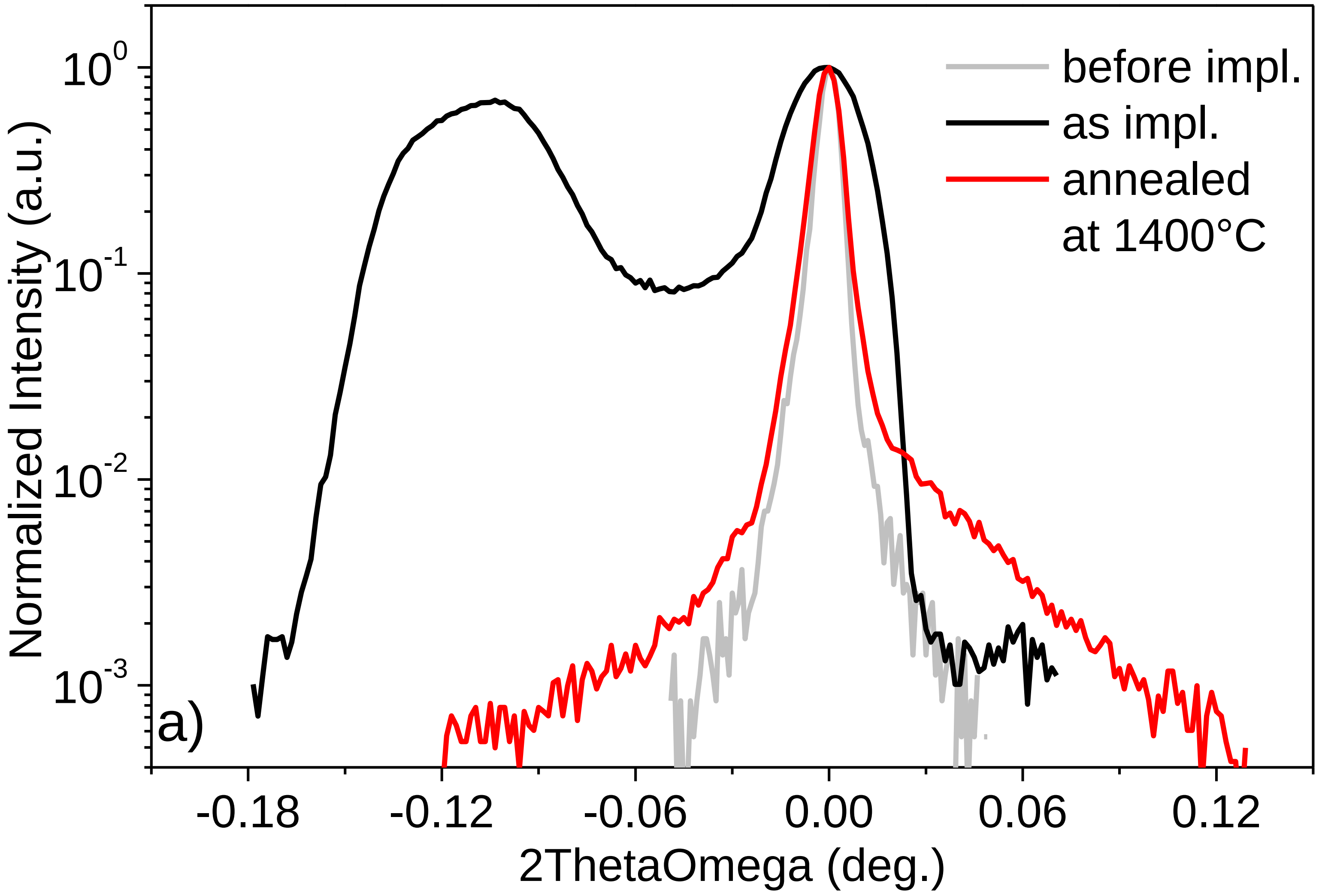
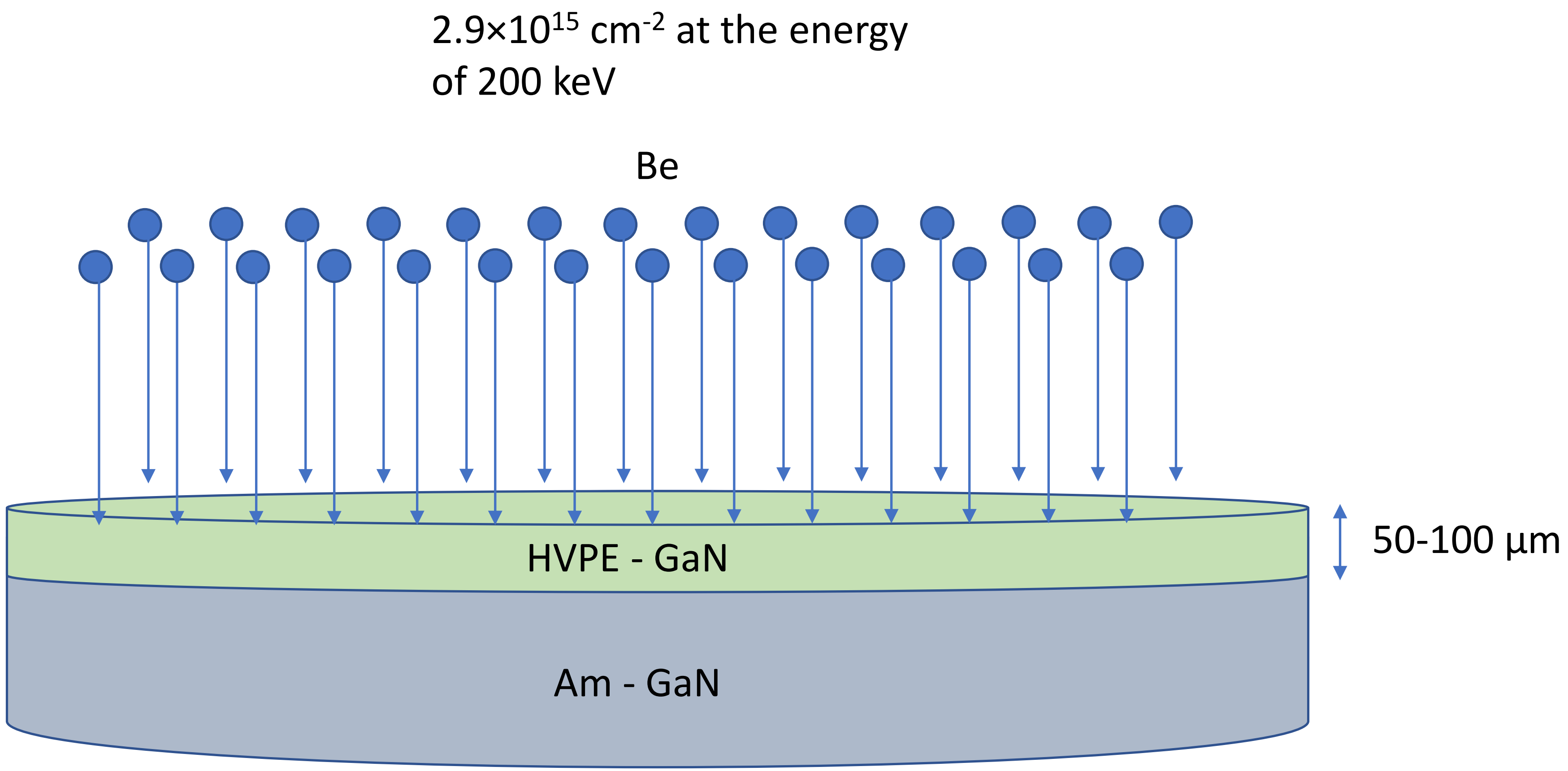
XRD rocking curves after UHPA

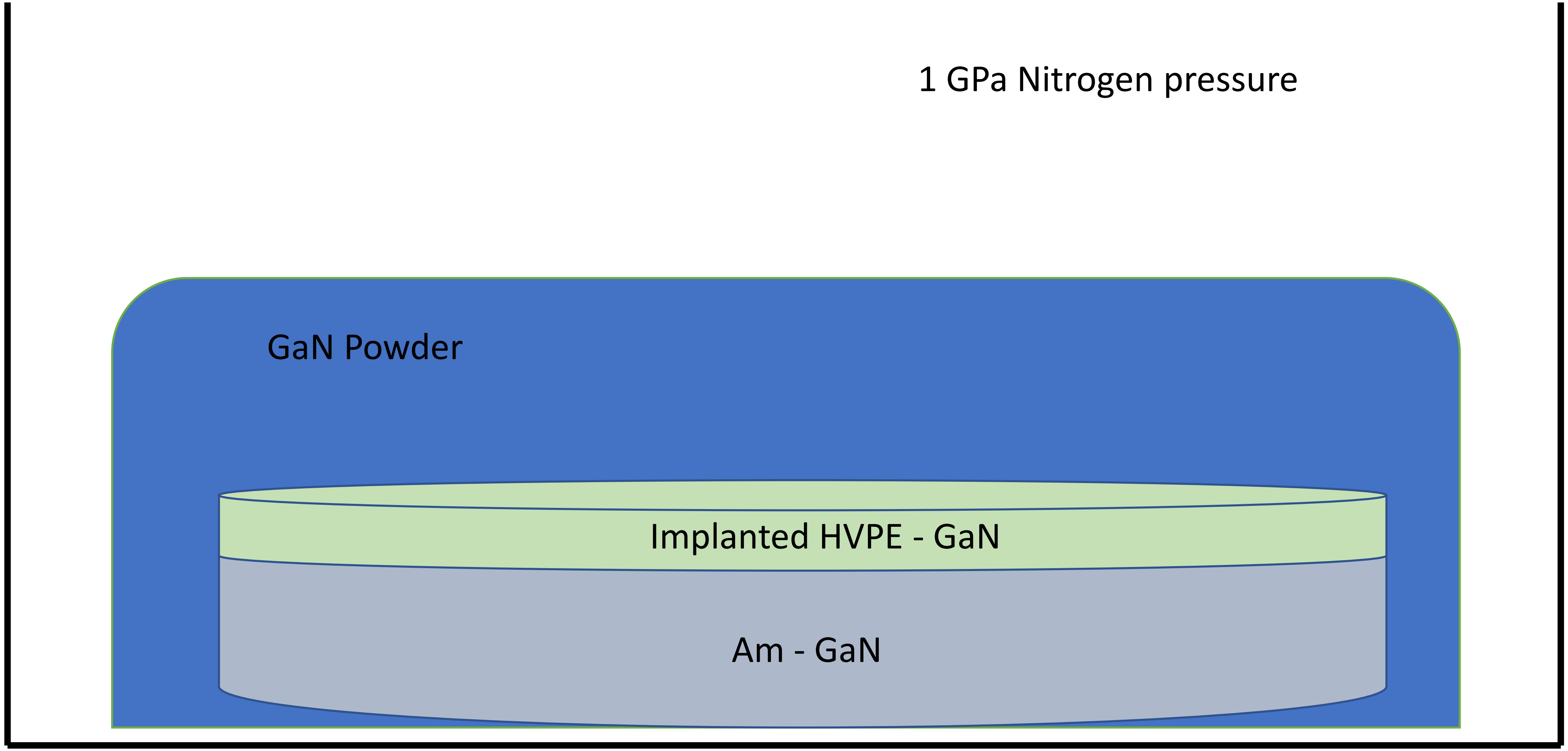


Implantation configuration

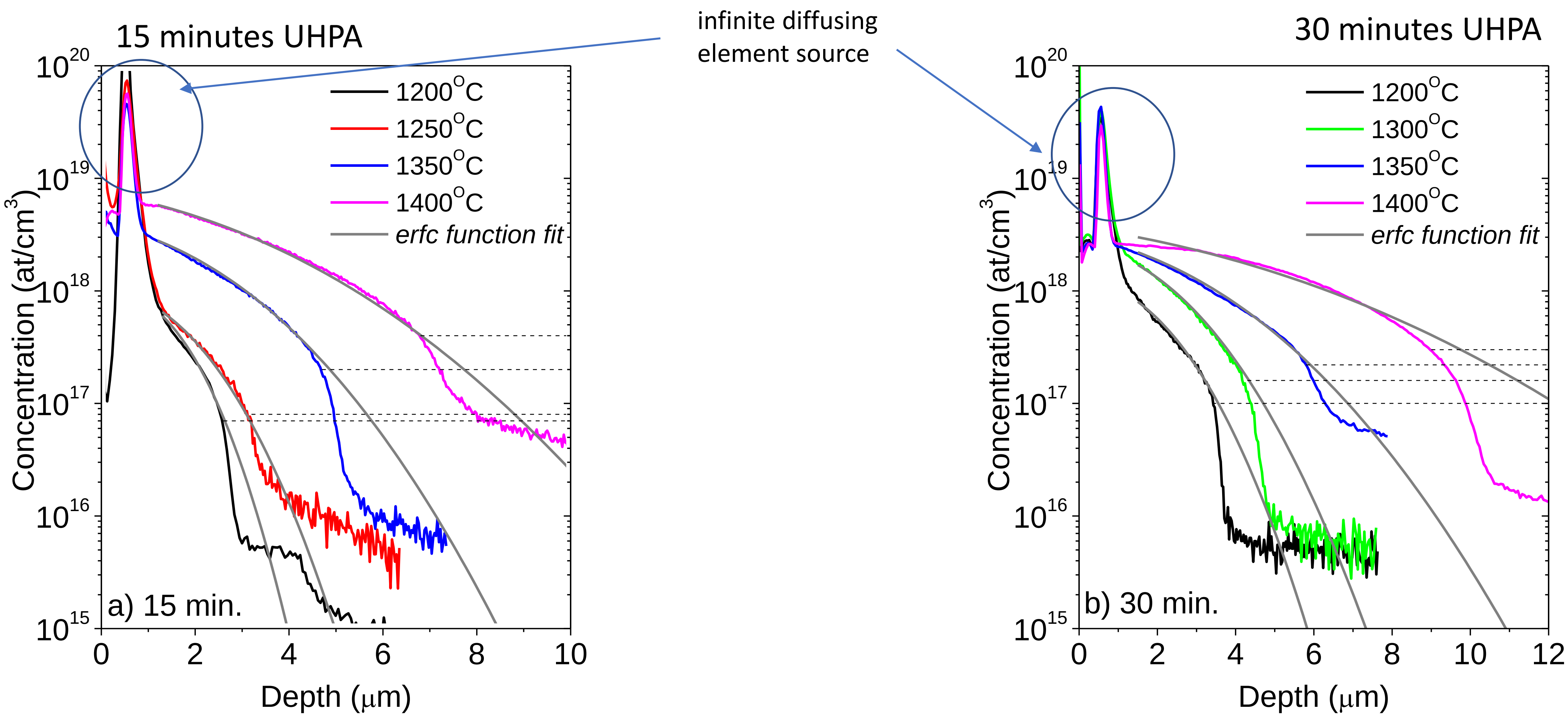


Implantation by M. Turek, UMCS, Lublin, Poland

UHPA configuration



SIMS profiles

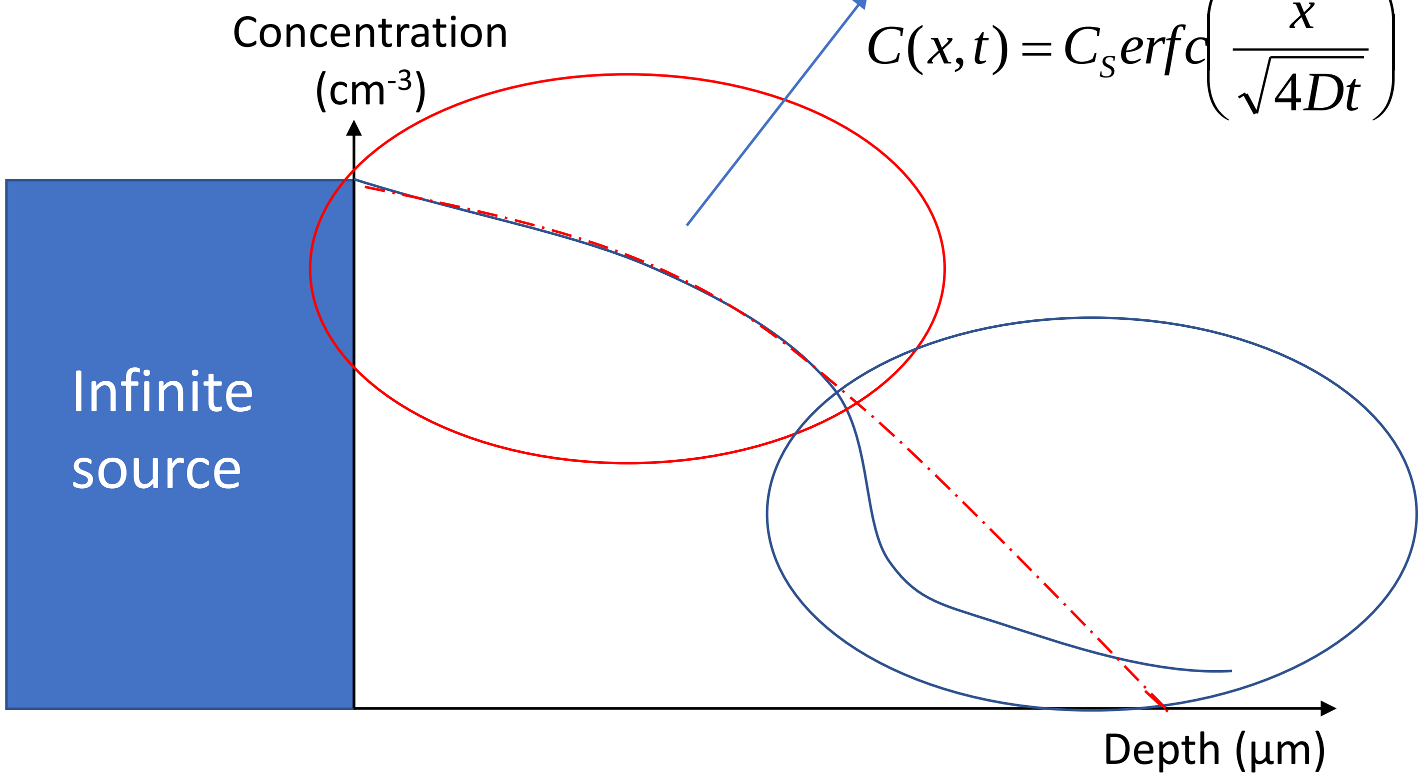


R. Jakiela et al. Investigation of diffusion mechanism of beryllium in GaN. Physica B Condens. Matter 2020, 594, 412316

SIMS profiles vs diffusion

complementary error function – *erfc*

$$C(x,t) = C_S erfc\left(\frac{x}{\sqrt{4Dt}}\right)$$



Boltzmann-Matano method for cases with concentration dependent diffusion coefficient:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} D\left(\frac{\partial C}{\partial x}\right) \longrightarrow D(C^1) = -\frac{1}{2t}\left(\frac{dx}{dC}\right)\bigg|_{C^1} \int_0^{C_1} x dC$$

C. Matano, Japan. J. Phys. 8 (1933) 109

Boltzman-Matano method

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} D\left(\frac{\partial C}{\partial x}\right)$$

$$\eta \equiv \frac{x - x_M}{2\sqrt{t}}$$

$$-2\eta \frac{\mathrm{d}C}{\mathrm{d}\eta} = \frac{\mathrm{d}}{\mathrm{d}\eta}\left[\tilde{D}(C)\frac{\mathrm{d}C}{\mathrm{d}\eta}\right]$$

$$\int_{C_L}^{C_R} \eta \mathrm{d}C = 0$$

$$-2\int_{C_L}^{C^*} \eta \mathrm{d}C = \tilde{D}\left(\frac{\mathrm{d}C}{\mathrm{d}\eta}\right)_{C^*} - \tilde{D}\left(\frac{\mathrm{d}C}{\mathrm{d}\eta}\right)_{C_L}$$

$$\underbrace{\int_{-\infty}^{x_M} [C(x) - C_L]\,\mathrm{d}x}_{gain} = \underbrace{\int_{x_M}^{\infty} [C_R - C(x)]\,\mathrm{d}x}_{loss}$$

$$\tilde{D}(C^*) = -2\frac{\int_{C_L}^{C^*} \eta \mathrm{d}C}{(\mathrm{d}C/\mathrm{d}\eta)_{C=C^*}}$$

$$\tilde{D}(C^*) = -\frac{1}{2t}\frac{\int_{C_L}^{C^*} (x - x_M)\mathrm{d}C}{(\mathrm{d}C/\mathrm{d}x)_{C^*}}$$

H. Mehrer „Diffusion in Solids", Springer series in solid state science 155

Boltzman-Matano method

1. Determine the position of the Matano plane from Eq. and use this position as the origin of the x-axis.

2. Choose $C*$ and determine the integral $A^* = \int_{C_L}^{C*} xdC$ from the experimental concentration-distance data.

3. Determine the concentration gradient $S = (\frac{dC}{dx})_{C*}$. S corresponds to the slope of the concentration-distance curve at the position $x*$.

4. Determine the interdiffusion coefficient $\tilde{D}$ for $C = C*$ from the Boltzmann-Metano equation as: $\tilde{D}(C*) = \frac{-A*}{2tS}$.

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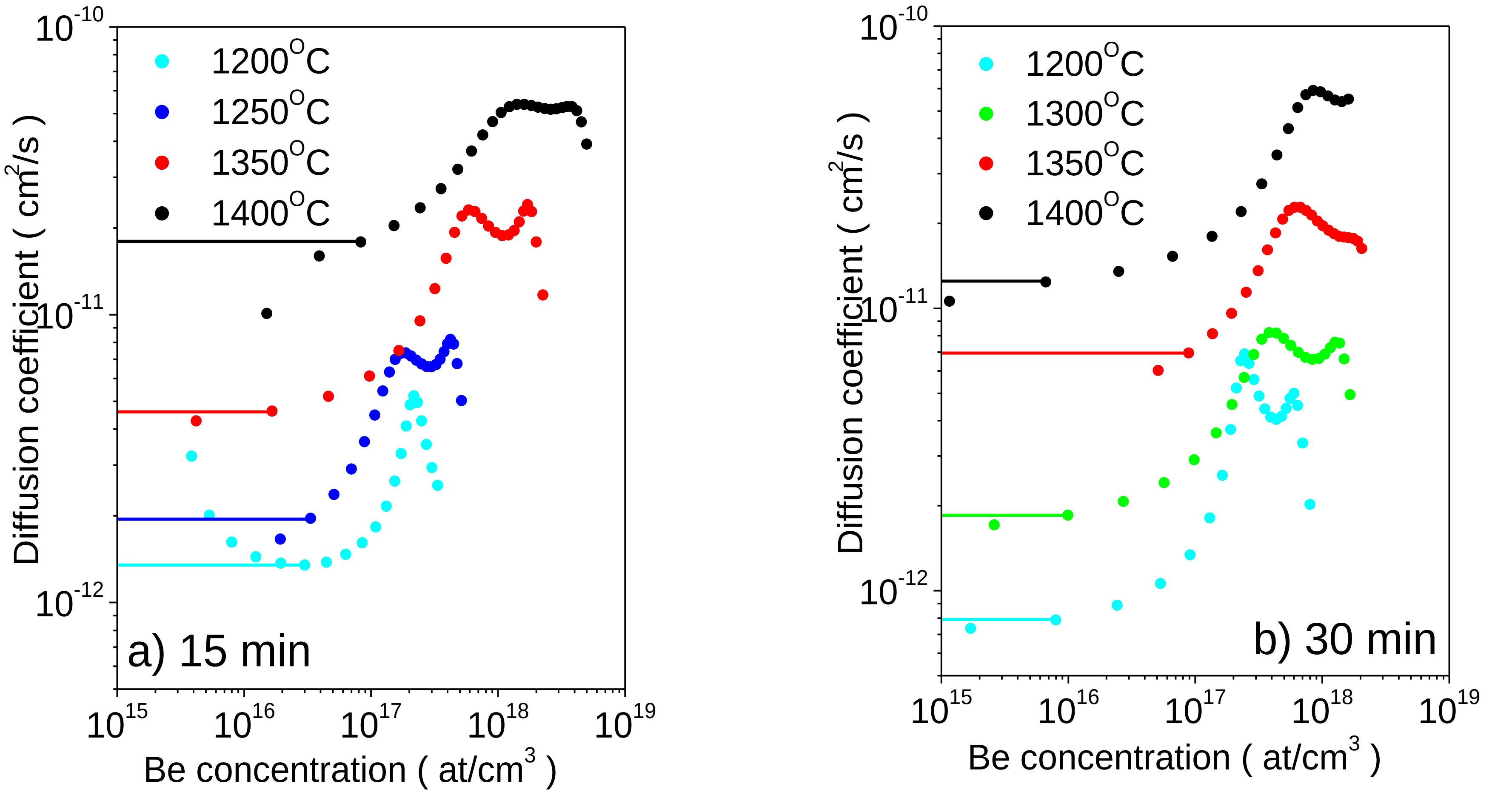
Boltzmann-Matano analysis of Be depth profiles



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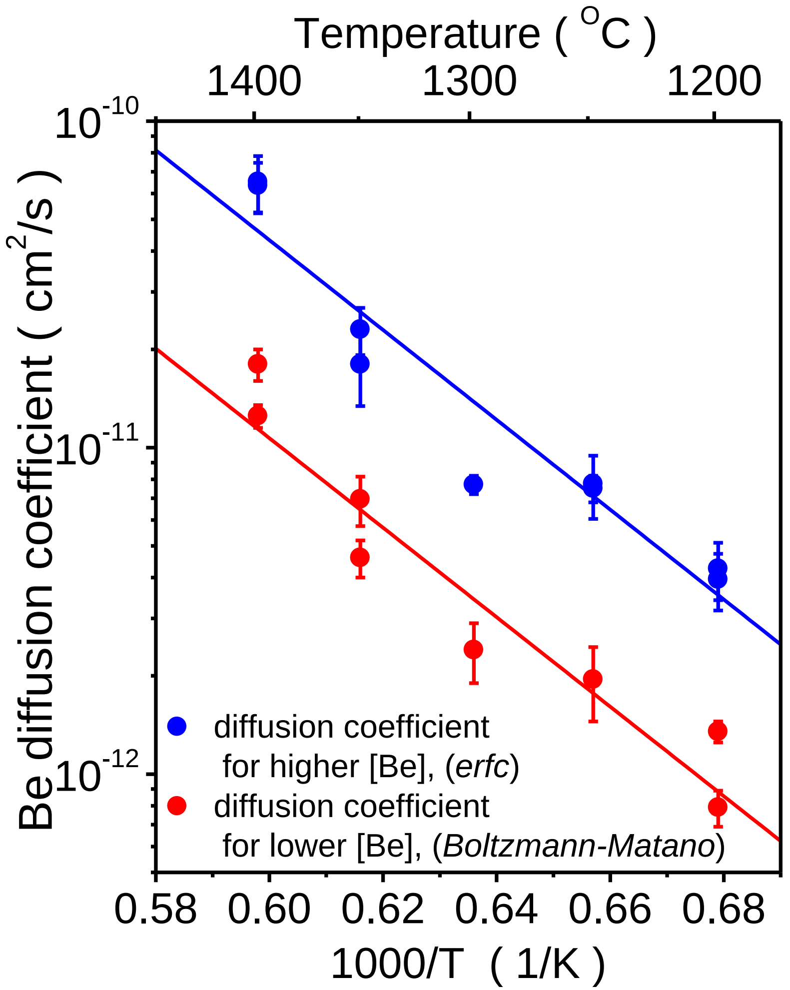
Diffusion coefficients of Be atoms in GaN as a function of inverse temperature

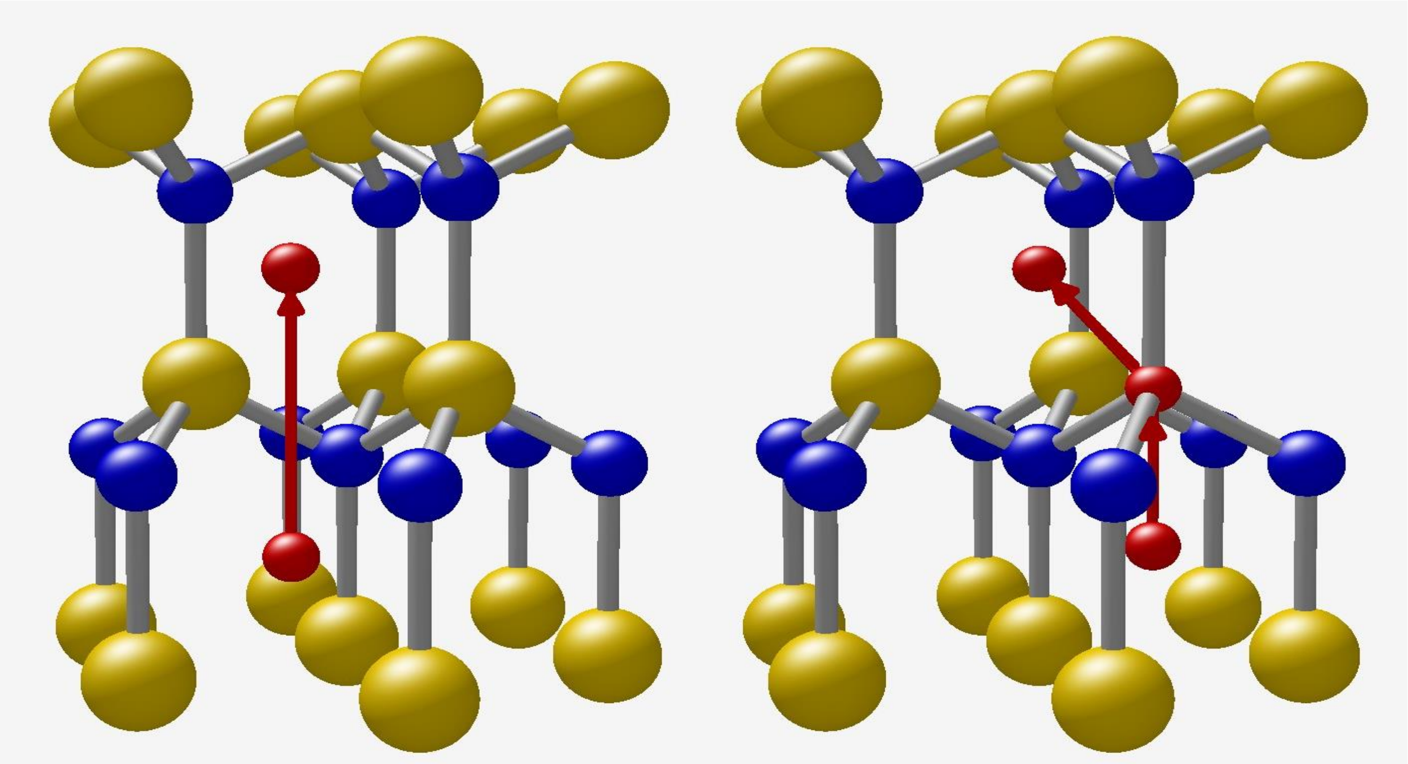


$$D = D_O \exp\left(\frac{-E_A}{kT}\right)$$

Temperature-independent pre-exponent factor D_0 and the activation energy for the Be diffusion

	Pre-exponent factor D_0 (cm^2/s)	**Activation energy (eV)**
Higher Be concentration (erfc fitting)	$7.8 \pm 1 \times 10^{-3}$	2.73 ± 0.05
Lower Be concentration (Boltzmann-Matano analysis)	$1.8 \pm 1 \times 10^{-3}$	2.72 ± 0.05

Two different diffusion mechanisms



Pure interstitial diffusion via octahedral lattice sites

Interstitial-substitutional diffusion via tetrahedral lattice sites and Ga vacancies

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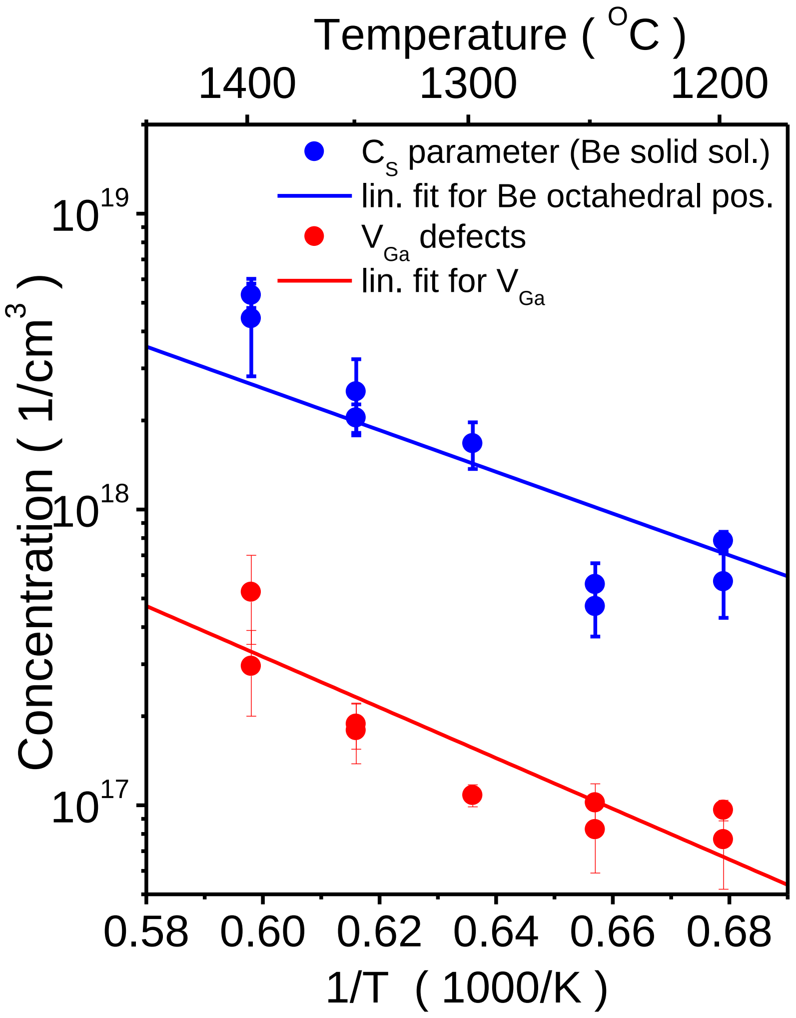
Gallium vacancy V_{Ga} concentration



$$C_d = N \exp\left(\frac{-E_f}{kT}\right)$$

Gallium vacancy

E_a = 1.7 eV

In agreement with JL Lyons and CG Van de Walle, npj Computational Materials (2017) 12

Be impurity in octahedral site

E_a = 1.4 eV

Summary

- UHPA is proven to be efective method for post implantation treatment of GaN
- Be diffusion coefficients were calculated for different conditions
- Two mechanisms of diffusion were proposed for Be

Next step:

- N-rich UHPA conditions for faster Be diffusion
- Analysis of Be diffusion in other crystal directions

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