Observation of the Random-to-Correlated Transition of the Ionized Impurity Distribution in Compensated Semiconductors

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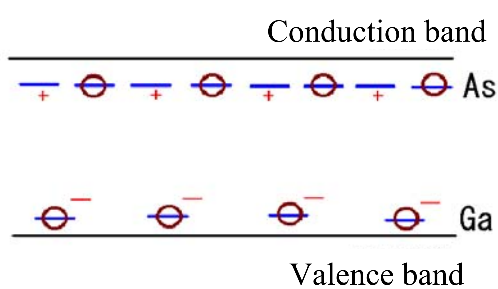
1. Introduction

Compensated Semiconductor

Ge:(As;Ga)

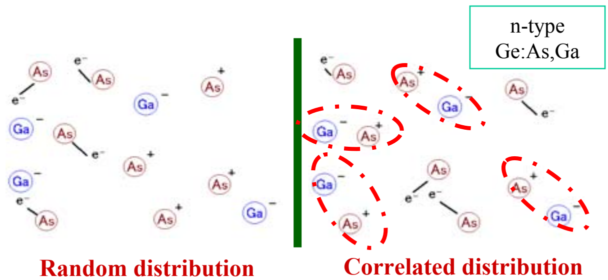
major impurity is As
minor impurity is Ga



Ionized impurity concentration: $N_I = 2[Ga]$
Neutral impurity concentration: $N_0 = [As] - [Ga]$
Compensation ratio: $K = [Ga]/[As]$

(our samples are K=0.6)

Distributions of Ionized Impurities



Random Theory :

D. M. Larsen, Phys. Rev B 13, 1681 (1976)

Correlated Theory :

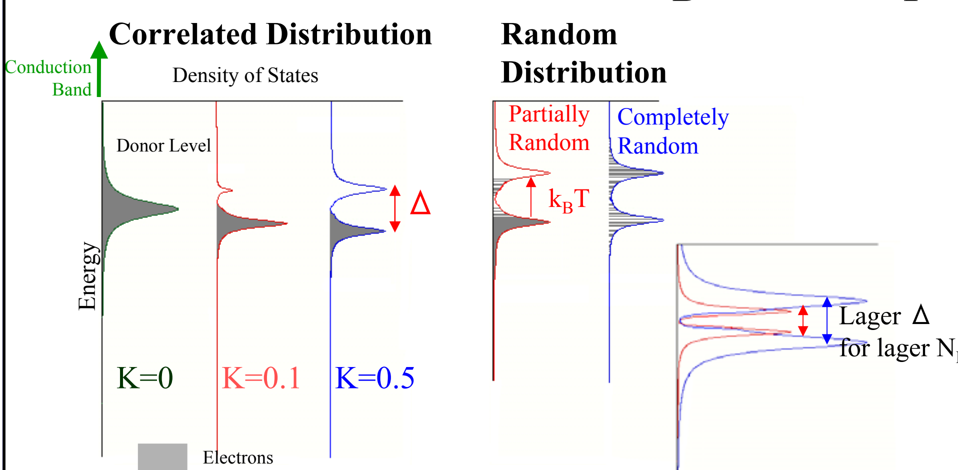
S. M. Kogan and N. Van Lien, Sov. Phys. Semicond. 15, 26 (1981)

Ionized Impurity Concentration (Coulombic Energy)

Temperature (Thermal Energy)

Can we change distribution of ionized impurities by changing T and N_I?

Coulomb gap width vs. k_BT and N_I



Width of the Coulomb gap $\Delta = \frac{e^2}{2\kappa}\cdot\left(\frac{3\pi \cdot N_I{}^4}{K}\right)^{\frac{1}{6}} = k_BT$ ⟶ $N_I = 7.5\text{x}10^{13}\ cm^{-3}$ at T=4 K

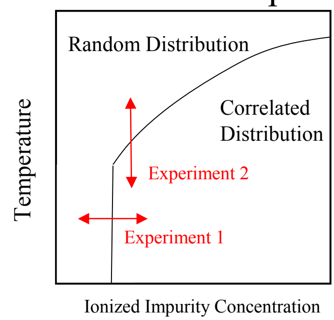
Objectives

Experimental observation of

the correlated to random ionized impurity distribution

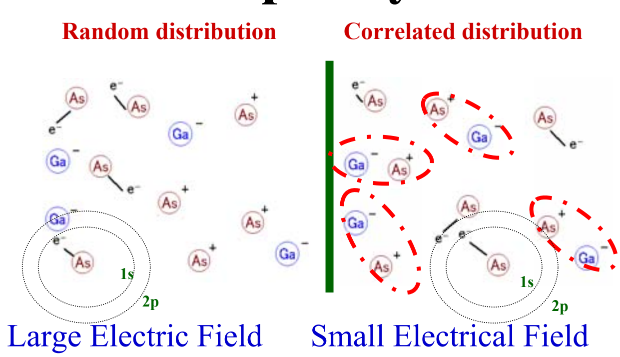
as ionized impurity concentration (Experiment 1)

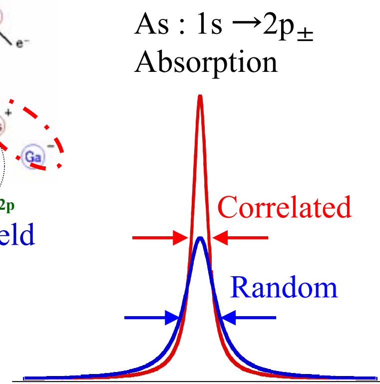
and functions of the temperature (Experiment 2)



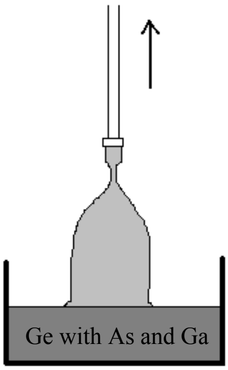
2: Experiment

Determination of the ionized impurity distribution

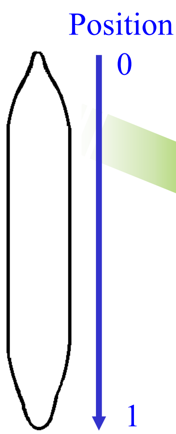




Samples



CZ-grown Ge



Ge Ingot

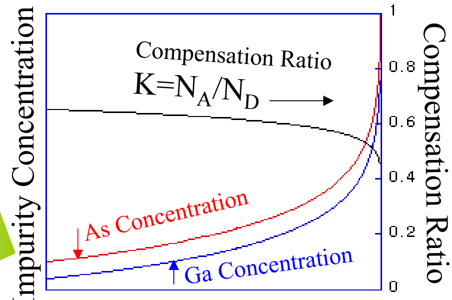


Fig.1 Impurity concentration vs. position of the ingot

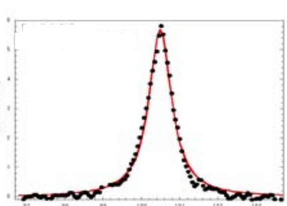
Samples were cut from several points

Theoretically expected linewidth for the two distributions at fixed T

Far infrared absorption
of As:1s →2p$_\pm$ line

BOMEM DA-8

Si:B Bolometer



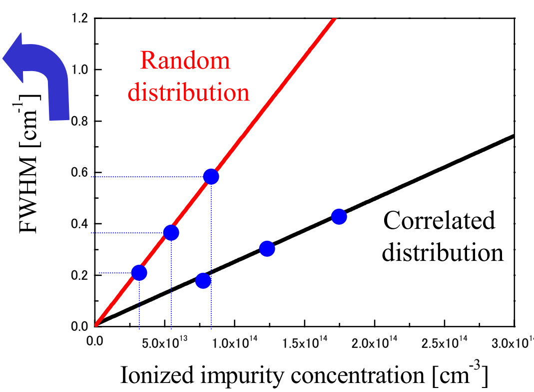


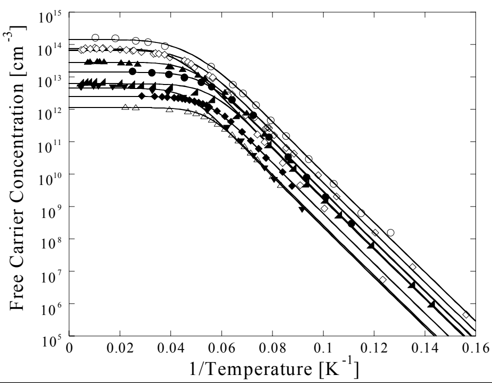
Fig.2 Theoretical predictions

Hall effect
300K～10K

Determination of the horizontal axis of Fig.2

$$n = \frac{2(N_D - N_A)}{1 + \frac{\beta N_A}{N_C}\exp\left(\frac{E_D}{k_B T}\right) + \sqrt{\left\{1 + \frac{\beta N_A}{N_C}\exp\left(\frac{E_D}{k_B T}\right)\right\}^2 + \frac{4\beta(N_D - N_A)}{N_C}\exp\left(\frac{E_D}{k_B T}\right)}}$$

N : Carrier concentration
N_D : Donor concentration
N_A : Acceptor concentration
E_D : Ionize energy of donors
k_B : Boltzmann constant
T : Temperature
$\beta = 2$



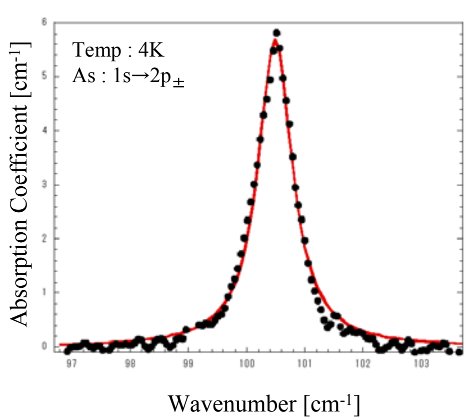
Find N_D, N_A, and K for each sample

(Compensation ratio : $K = N_D/N_A$)

N_I (Ionized Impurity Concentration)

$N_I = 2 \times N_A$

Determination of the vertical axis of Fig.2

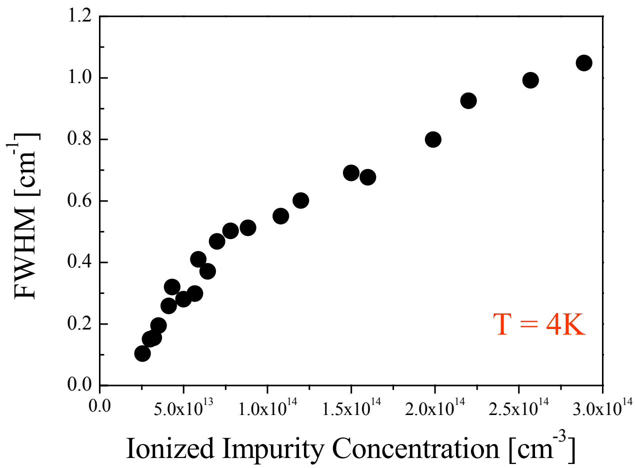


Lorenztian Fitting

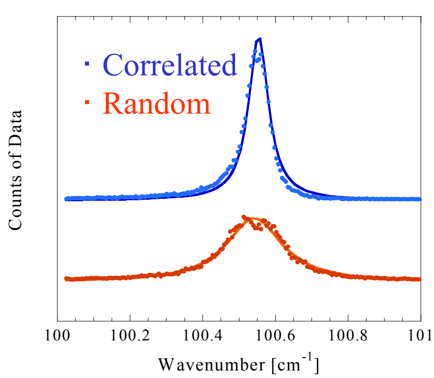
$$A\frac{FWHM/2}{(k - k_0)^2 + (FWHM/2)^2}.$$

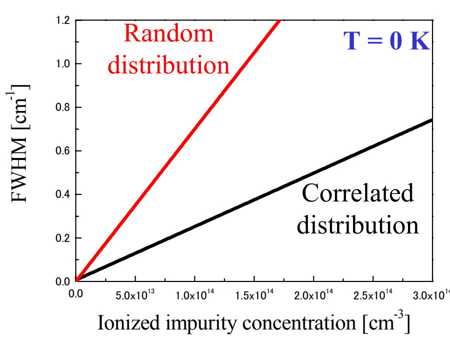
Full Width at Half Maximum of As:1s→$2p_{\pm}$ line

Experimental Results



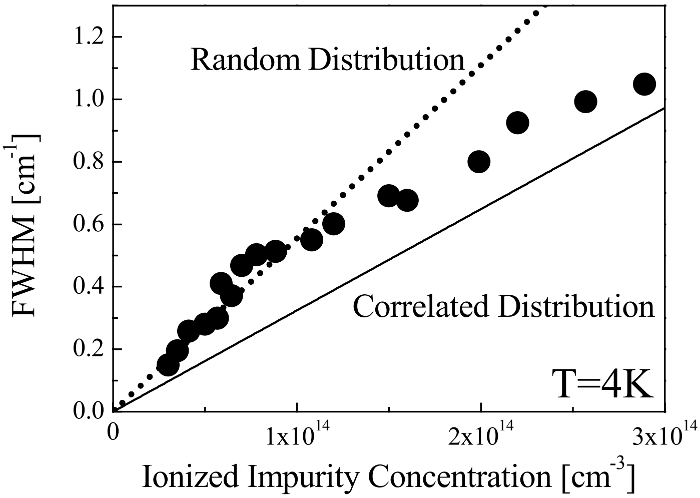
3. Monte Carlo simulation of the linewidth for correlated and random distributions



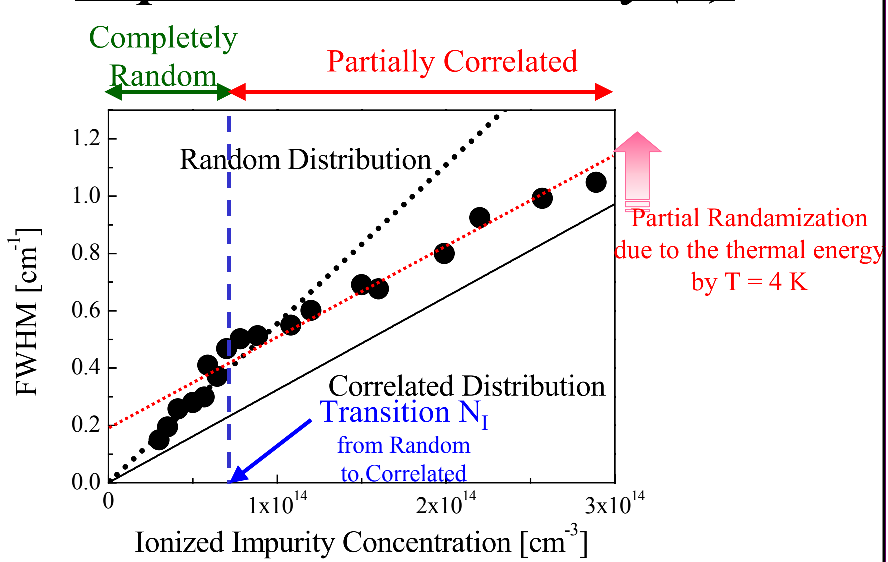


$N_I = 3.50 \times 10^{13} cm^{-3}$
K = 0.6
Number of Donors = 200
Number of Acceptors = 120

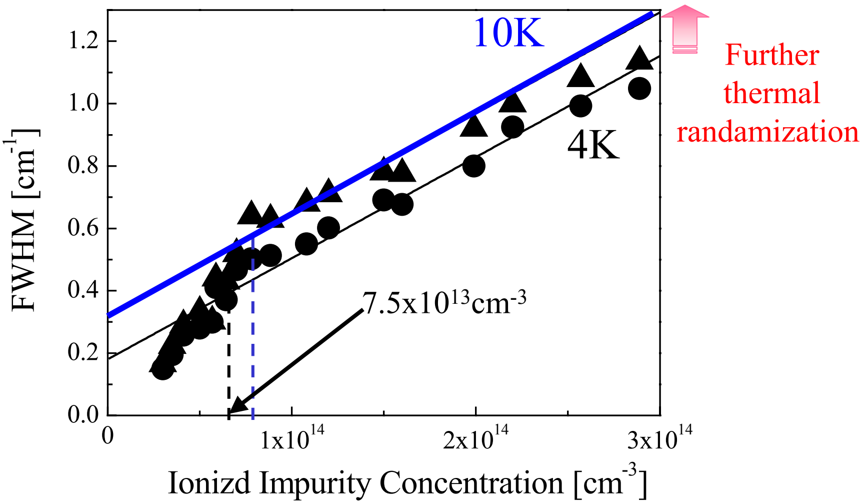
4: Comparison:
Experiment and Theory (1)



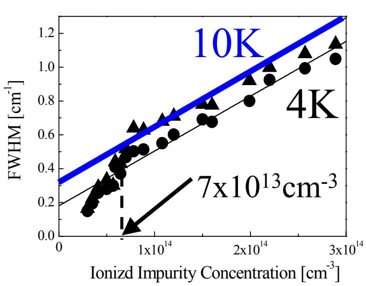
Comparison:
Experiment and Theory (2)



Effect of raising Temperature



Relation between critical T and N_I



For N_I=7.5x10^{13}cm^{-3}

Coulomb Gap linewidth

$$\Delta = \frac{e^2}{2\kappa} \cdot \left(\frac{3\pi \cdot N_I{}^4}{K} \right)^{\frac{1}{6}} = 0.33\ \text{meV} \quad \begin{pmatrix} \kappa = 16.1 \\ K = 0.66 \end{pmatrix}$$

Thermal Energy k_BT= 0.34 meV

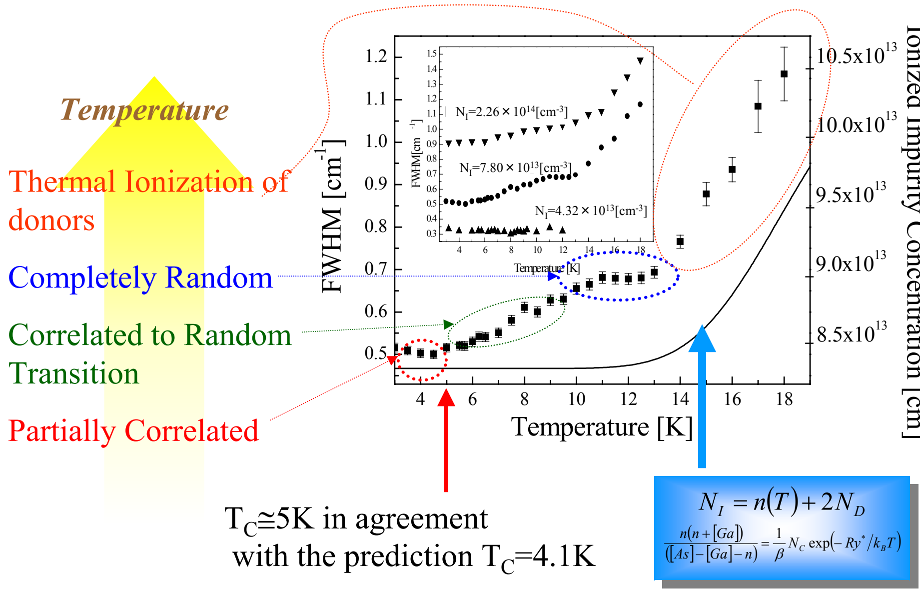
(T＝4K)

Excellent agreement between Δ and k_BT

Thermal Energy > Coulomb Gap : complete random distribution

Thermal Energy < **Coulomb Gap** : correlated distribution

Temperature - Induced Transition



Conclusion

- Experimentally observed Random-Correlated transition for the first time
- The transition occurs around $N_I = 7.5 \times 10^{13}\ cm^{-3}$ at 4K in excellent agreement with the theoretical prediction
- thermal energy > coulomb gap : completely random distribution
  thermal energy < coulomb gap : correlated distribution

Appendix 1 :

Monte Carlo calculation of the linewidth for the correlated and random distributions

Monte Carlo Method

Distribute more than 100 donors and acceptors in the cell randomly

↓

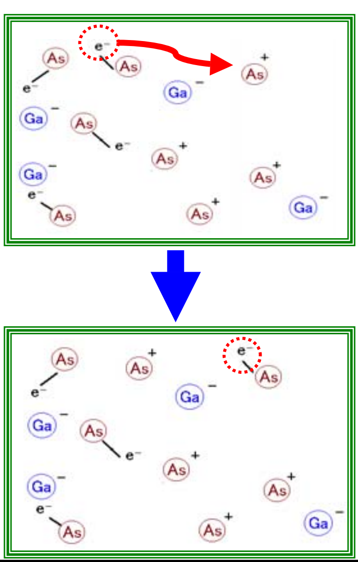
Create distribution of neutral and ionized impurities randomly

Random distribution → Calculate electric field for the neutral donor at the center of the cell

Correlated distribution → Create correlated distribution → Calculate electric field for the neutral donor at the center of the cell

Repeat for 8000 central donors to calculate the inhomogeneous broadening

Creation of the Correlated Distribution (1)



Change the position of 1 electron

↓

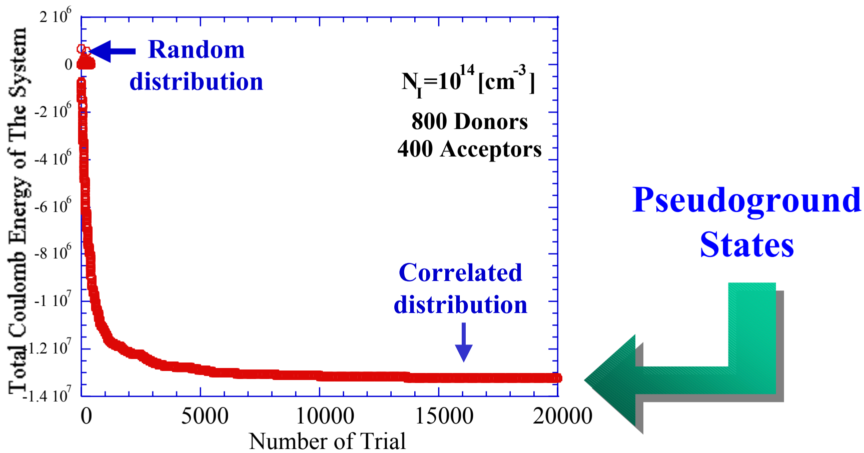
Compare the total coulombic energy

Reduced → Accept the new distribution

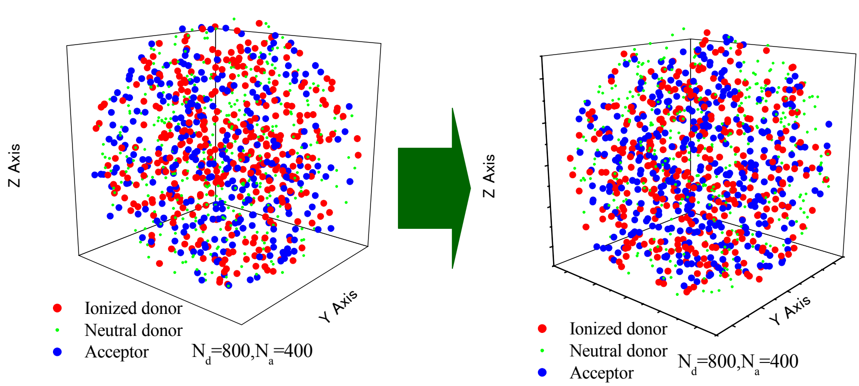
Increased → Reject the new distribution

Repeat for more than 20,000 times

Creation of the Correlated Distribution (2)



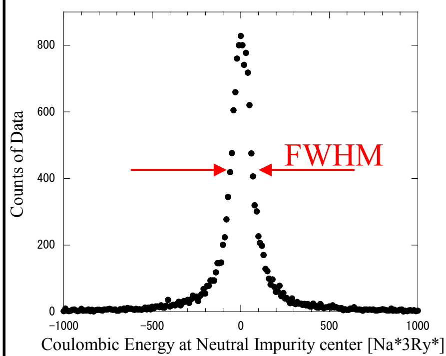
Distribution in a unit cell

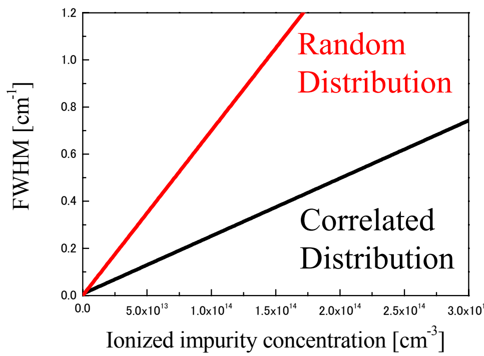


Random Distribution

Correlated Distribution

Calculational Results





Distribution of the Stark Energies
in case of the Random distribution

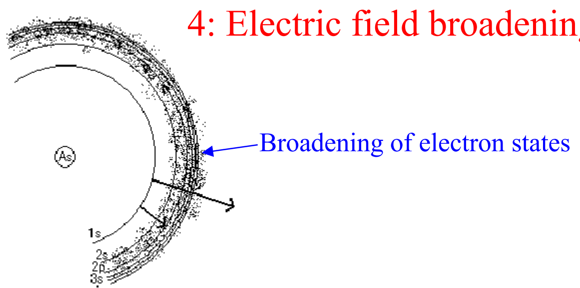
Appendix 2 :
Other broadening mechanism

1: Phonon life broadening・・・ 0.066 cm^{-1}

2: Concentration broadening・・・ 0.04 cm^{-1}

3: Dislocation broadening・・・ 0 cm^{-1}

4: Electric field broadening



Electric field broadening

(1) Linear Stark effect ($\propto E$)

$\Delta\varepsilon \propto N_I^{2/3}$

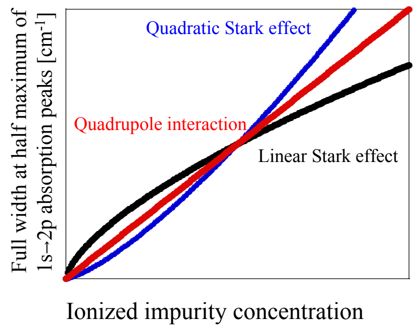
(2) Quadratic Stark effect ($\propto E^2$)

$\Delta\varepsilon \propto N_I^{4/3}$

(3) Quadrupole interaction ($\propto dE/dz$)

$\Delta\varepsilon \propto N_I$

⟶ Important for low N_I



$1s \rightarrow 2p_{\pm}$: Linear Stark effect does not occur

E : electric field strength
$\Delta\varepsilon$: The increase of linewidth
N_I : Ionized impurity concentration