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Impacts of Band Structures and Scattering Processes on High-field Carrier Transport in Wide Bandgap Semiconductors

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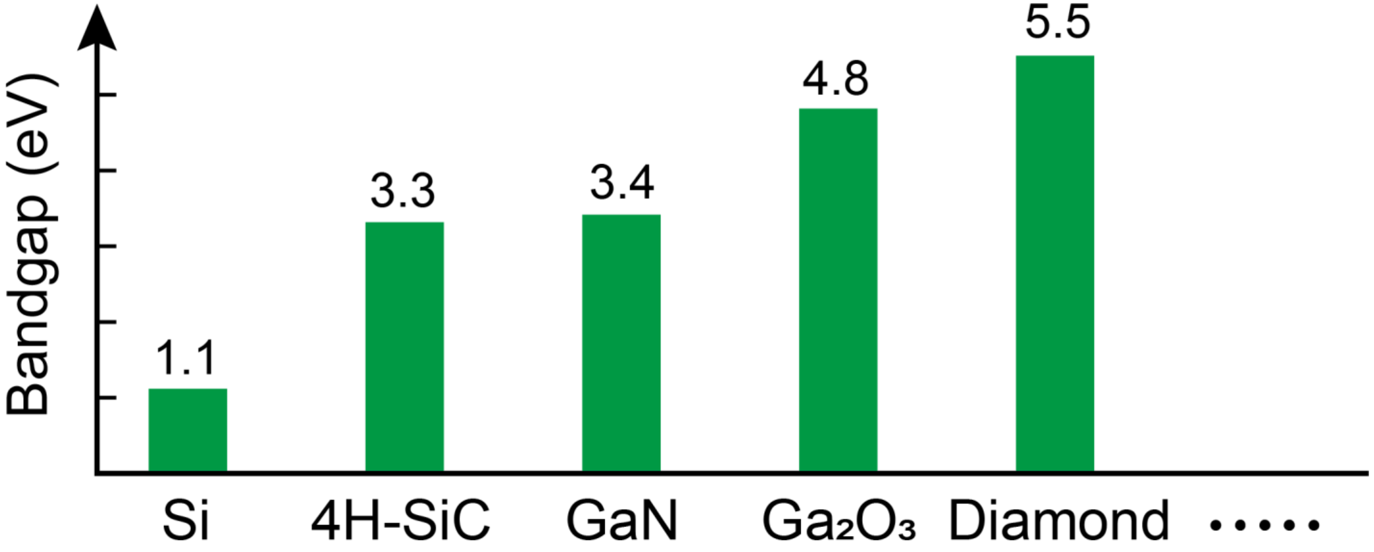
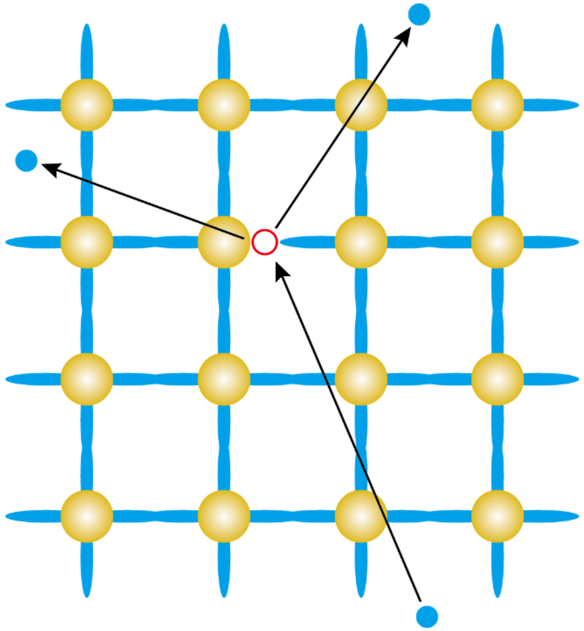
Wide Bandgap Semiconductors

- Wide bandgap semiconductors have attracted great attention for power device applications owing to the high breakdown electric field

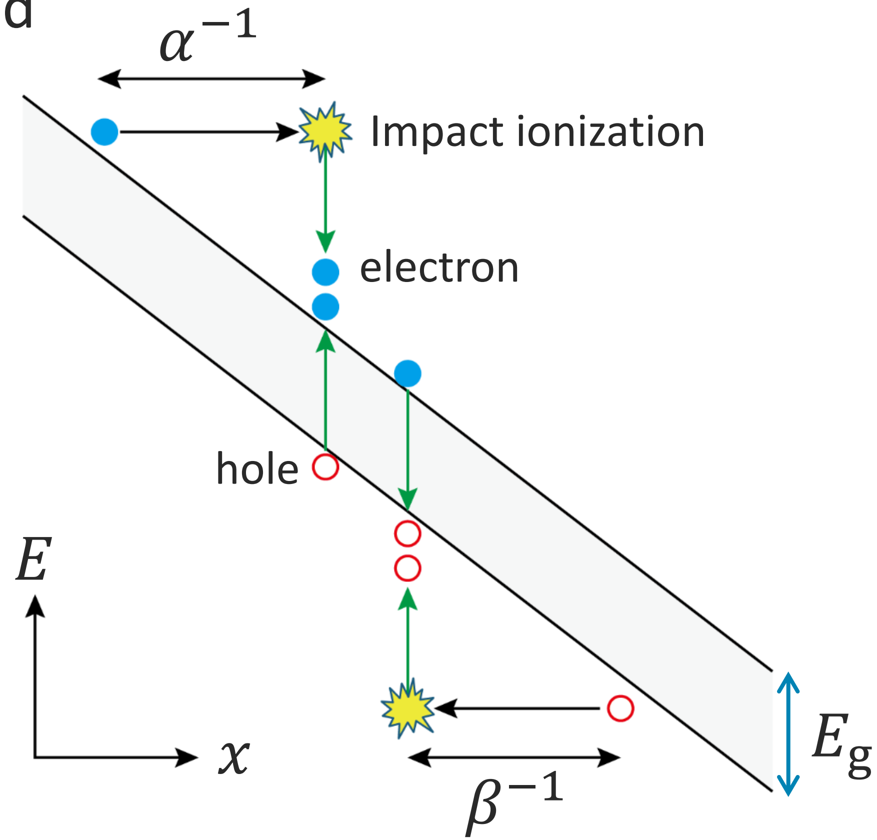


Impact Ionization and Ionization Coefficients

- Breakdown in most cases results from **impact ionization**
- **Ionization coefficients**, α for electrons and β for holes, are defined as the number of e-h pairs generated per unit distance traveled



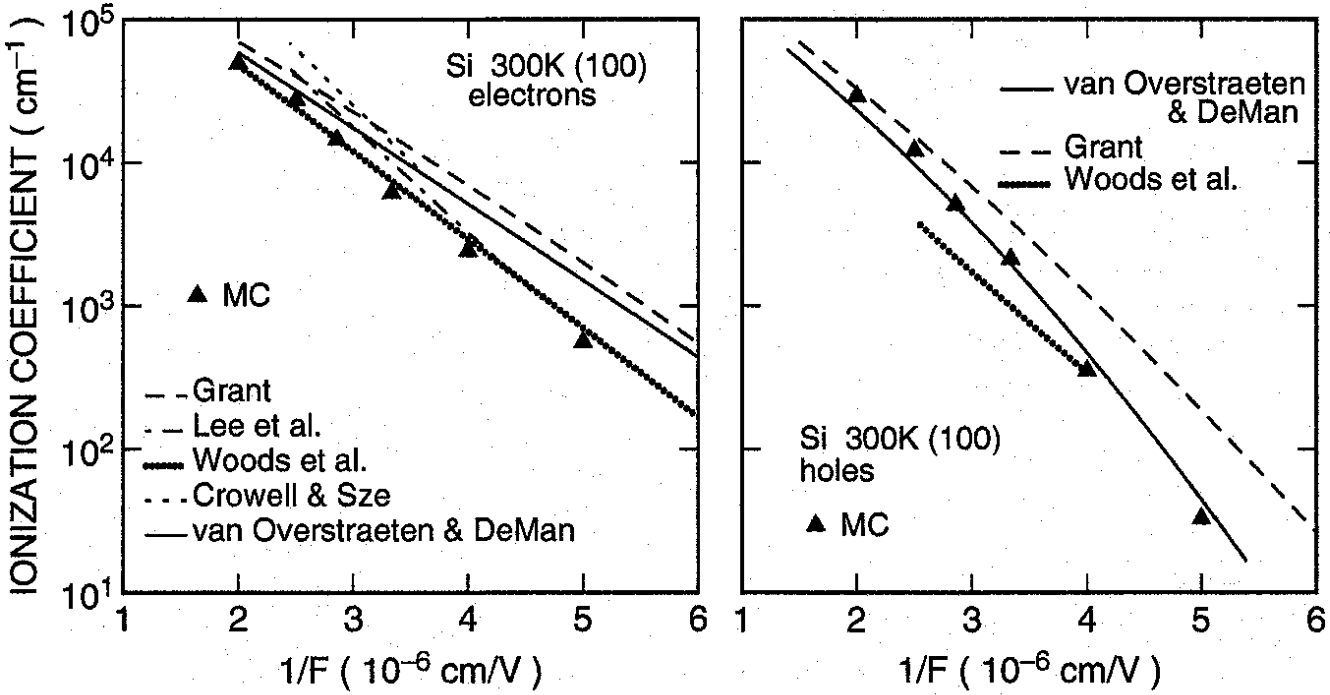
Impact ionization



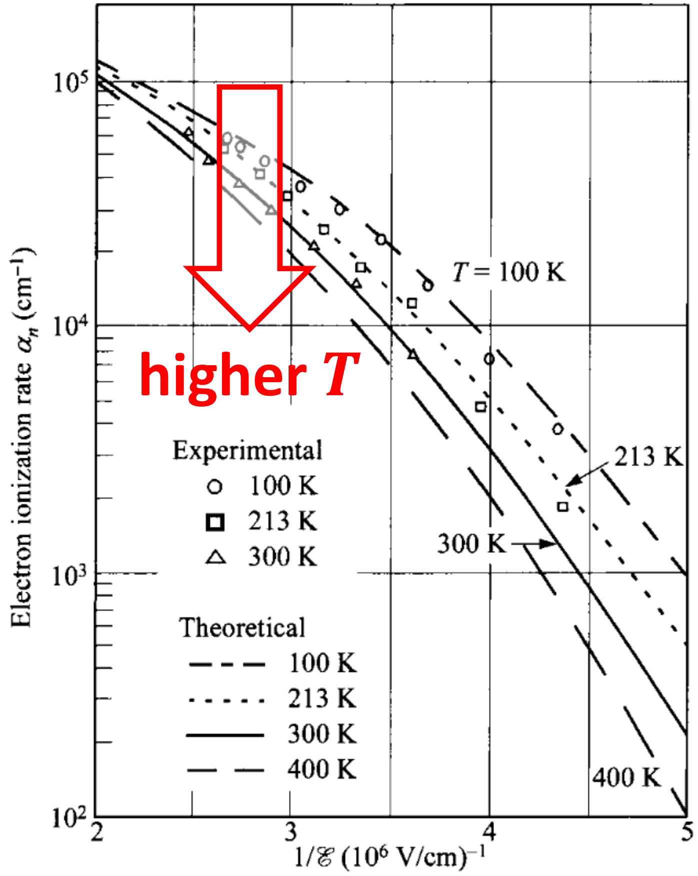
Ionization coefficients

Ionization Coefficients in Si

α (electron) β (hole)



α (electron)



$\alpha \approx \beta$

$\alpha \downarrow$ as $T \uparrow$

M.V. Fischetti and W.G. Vandenberghe, “Advanced Physics of Electron Transport in Semiconductors and Nanostructures”

S.M. Sze *et al.*, “Physics of Semiconductor Devices”

Models

- **Lucky electron model (Shockley)**

$$\alpha(F) = \frac{eF}{E_{\mathrm{I}}} \exp\left(-\frac{E_{\mathrm{I}}}{eF\lambda}\right)$$

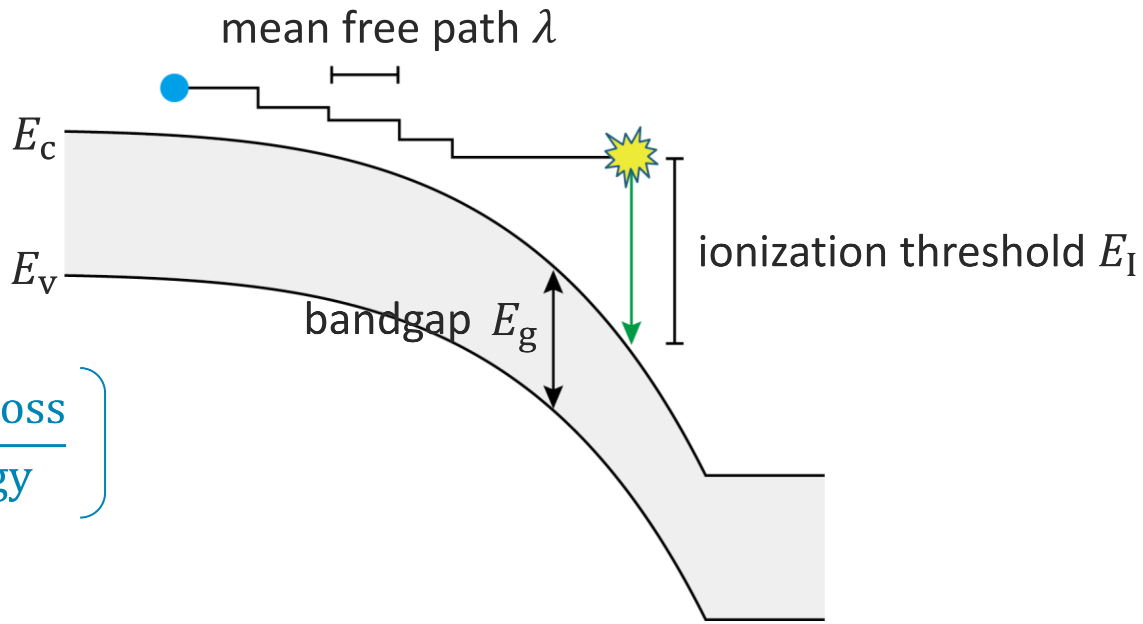
- **Lucky drift model (Ridley)**

$$\alpha(F) = \frac{eF}{E_{\mathrm{I}}} P\left[\frac{E_{\mathrm{I}}}{eF\lambda}, r\right]$$

$$\left(r = \frac{\text{effective energy loss}}{\text{threshold energy}} \right)$$

- **Scaling theory (Thornber)**

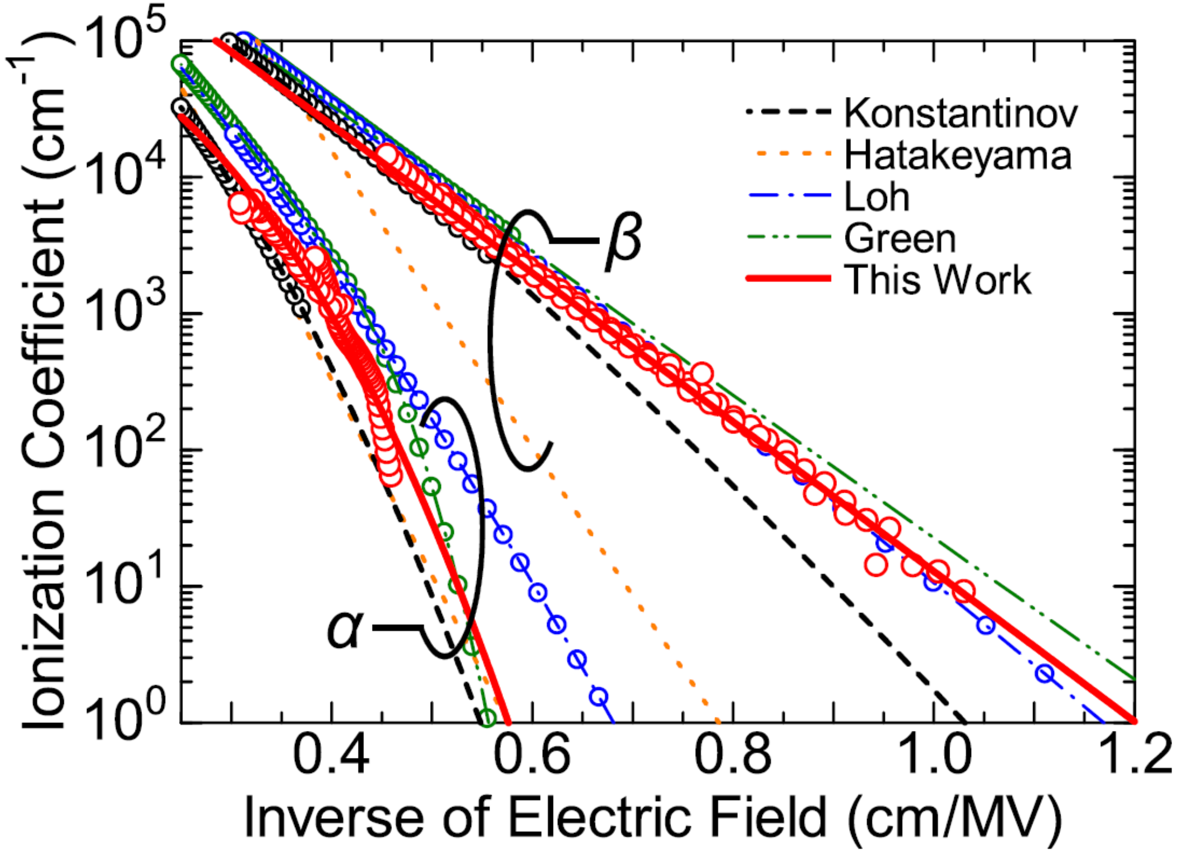
$$\alpha(F) = \frac{eF}{E_{\mathrm{I}}} \exp\left(-\frac{F_{\mathrm{I}}}{F_{kT} + F + F^2/F_{\mathrm{ph}}}\right)$$



α is determined mainly by Ionization threshold E_{I} ($\sim E_{\mathrm{g}}$) and scattering strength

W. Shockley, SSE **2**, 35 (1961); B.K. Ridely, JPC **16**, 3373 (1983); K.K. Thornber, JAP **52**, 279 (1981)

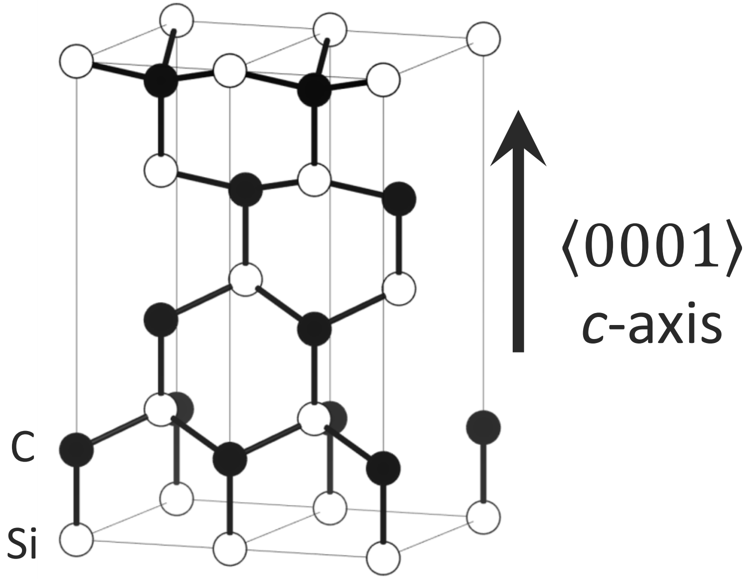
Ionization Coefficients in 4H-SiC



H. Niwa *et al.*, IEEE TED **62**, 3326 (2015)

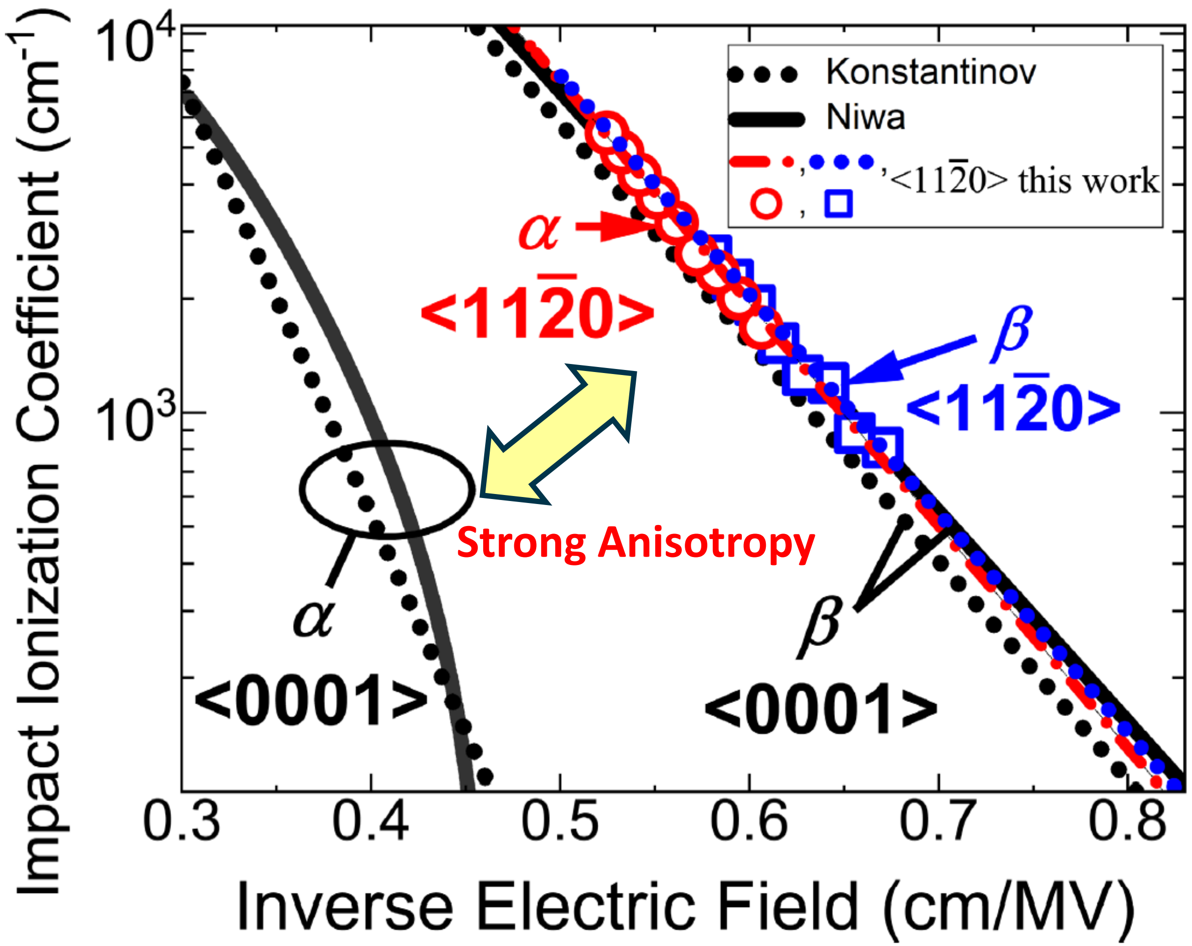
1. Large $k = \beta/\alpha$ for $\langle 0001 \rangle$

α: electron coefficient
β: hole coefficient



Lattice structure of 4H-SiC

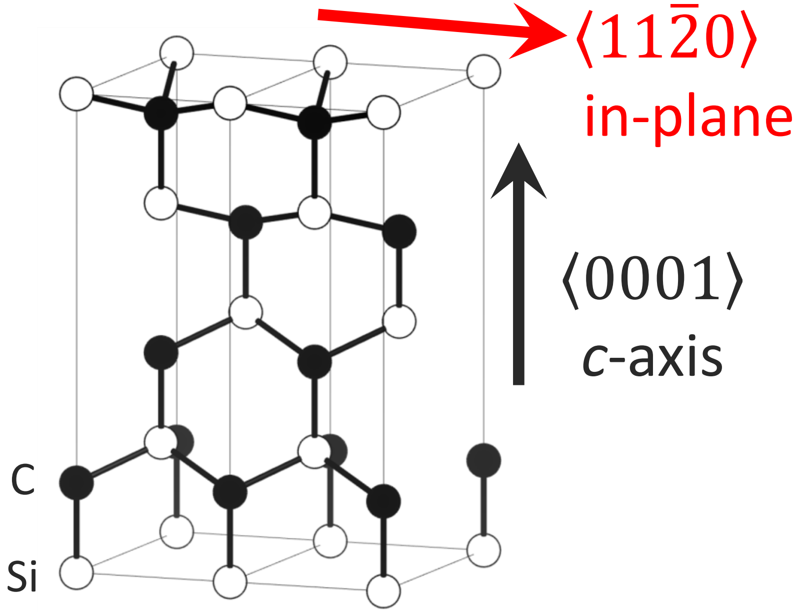
Ionization Coefficients in 4H-SiC



D. Stefanakis *et al.*, IEEE TED **67**, 3740 (2020)

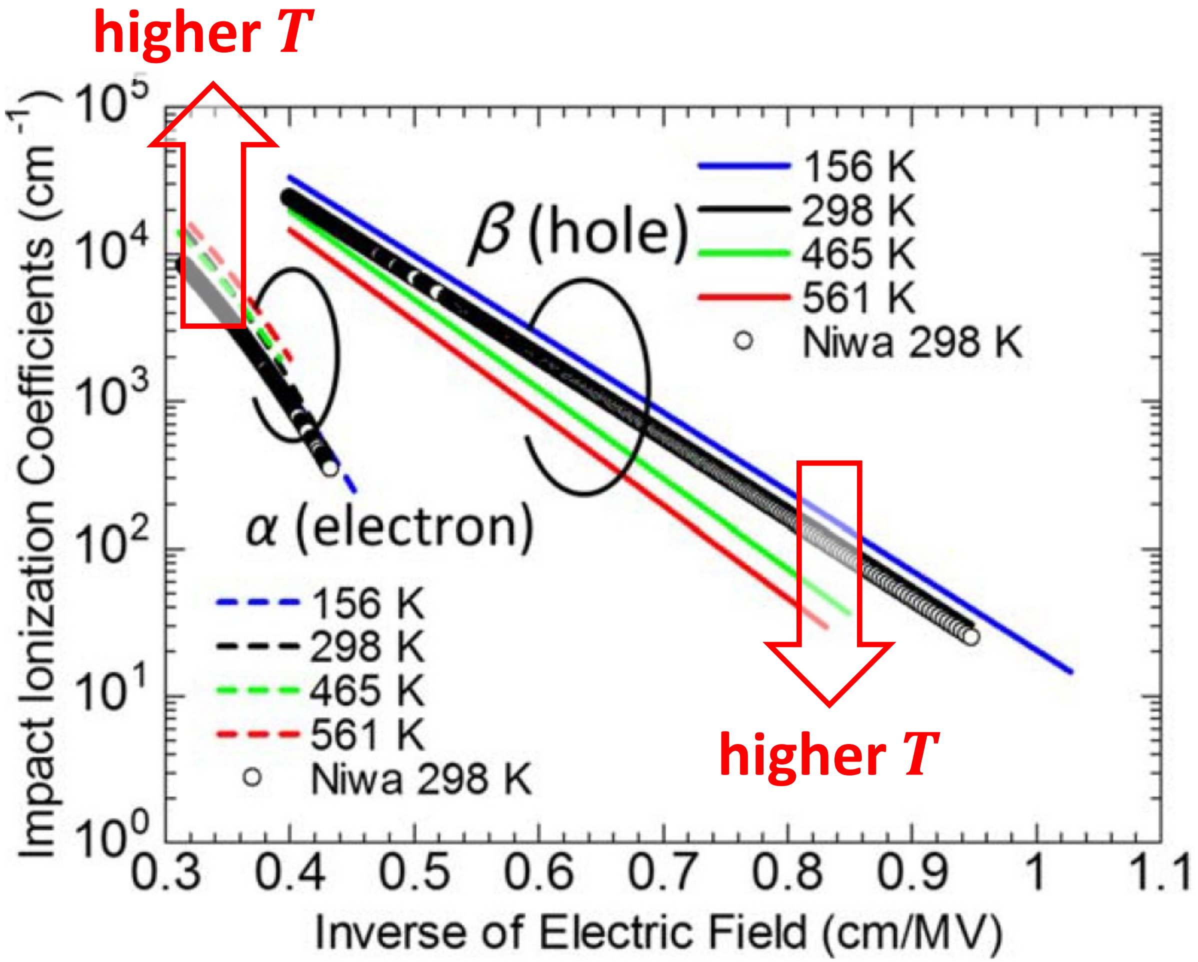
1. Large $k = \beta / \alpha$ for $\langle 0001 \rangle$
2. Strong anisotropy

$$\alpha_{\langle 0001 \rangle} \ll \alpha_{\langle 11\bar{2}0 \rangle}$$



Lattice structure of 4H-SiC

Ionization Coefficients in 4H-SiC



Y. Zhao *et al.*, JJAP **58**, 018001 (2019)

1. Large $k = \beta/\alpha$ for $\langle 0001 \rangle$
2. Strong anisotropy

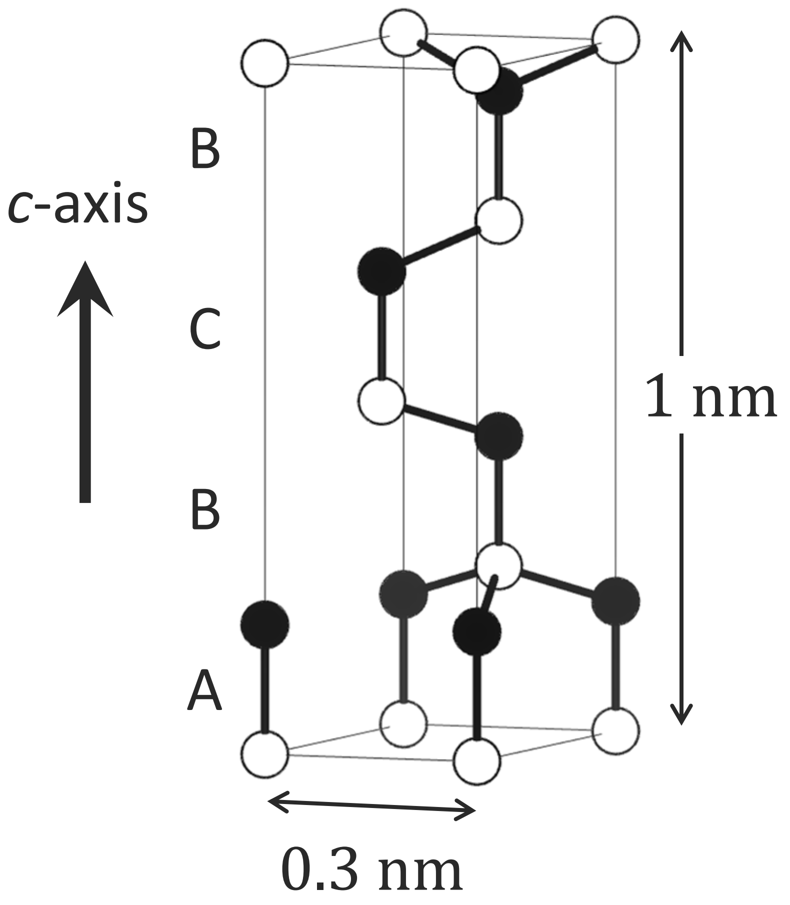
$$\alpha_{\langle 0001 \rangle} \ll \alpha_{\langle 11\bar{2}0 \rangle}$$

3. Positive T dependence of α

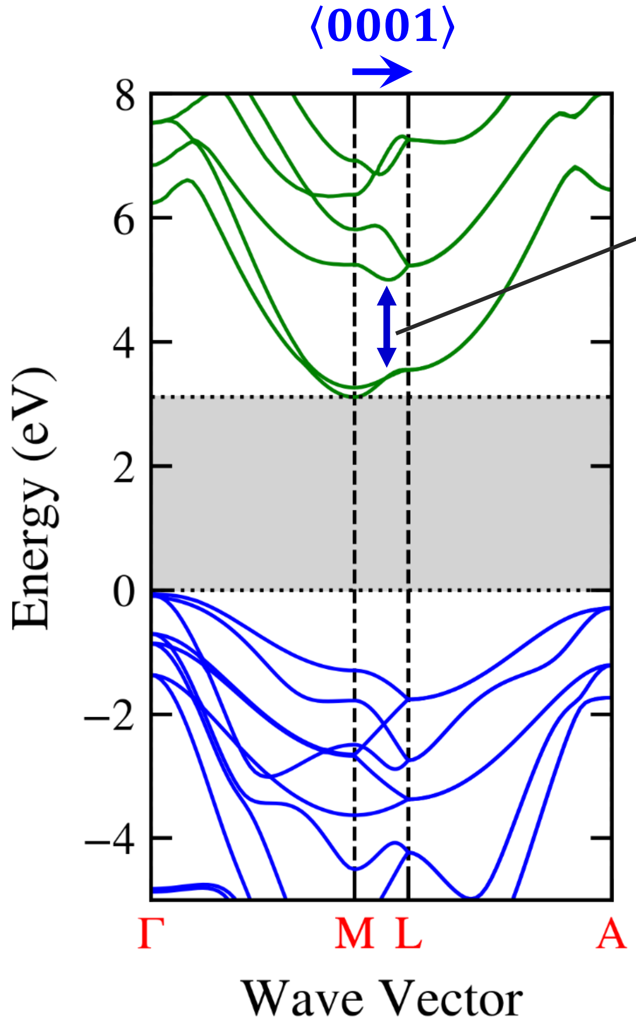
$$\left(\begin{array}{c} \alpha \uparrow \text{as } T \uparrow \\ \beta \downarrow \text{as } T \uparrow \end{array} \right)$$

Band Splitting along ⟨0001⟩ Direction

4H-SiC



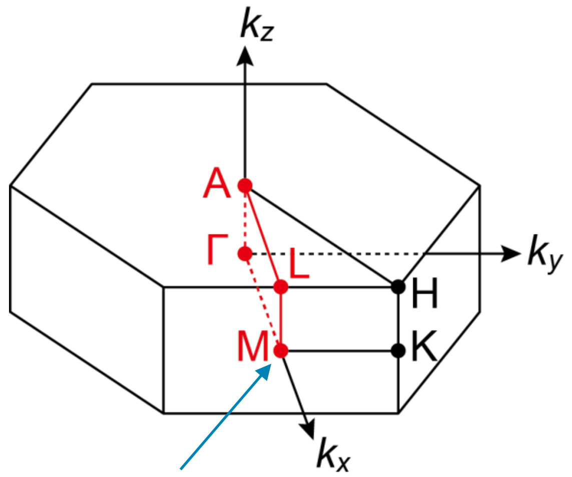
Primitive unit cell



⟨0001⟩ direction

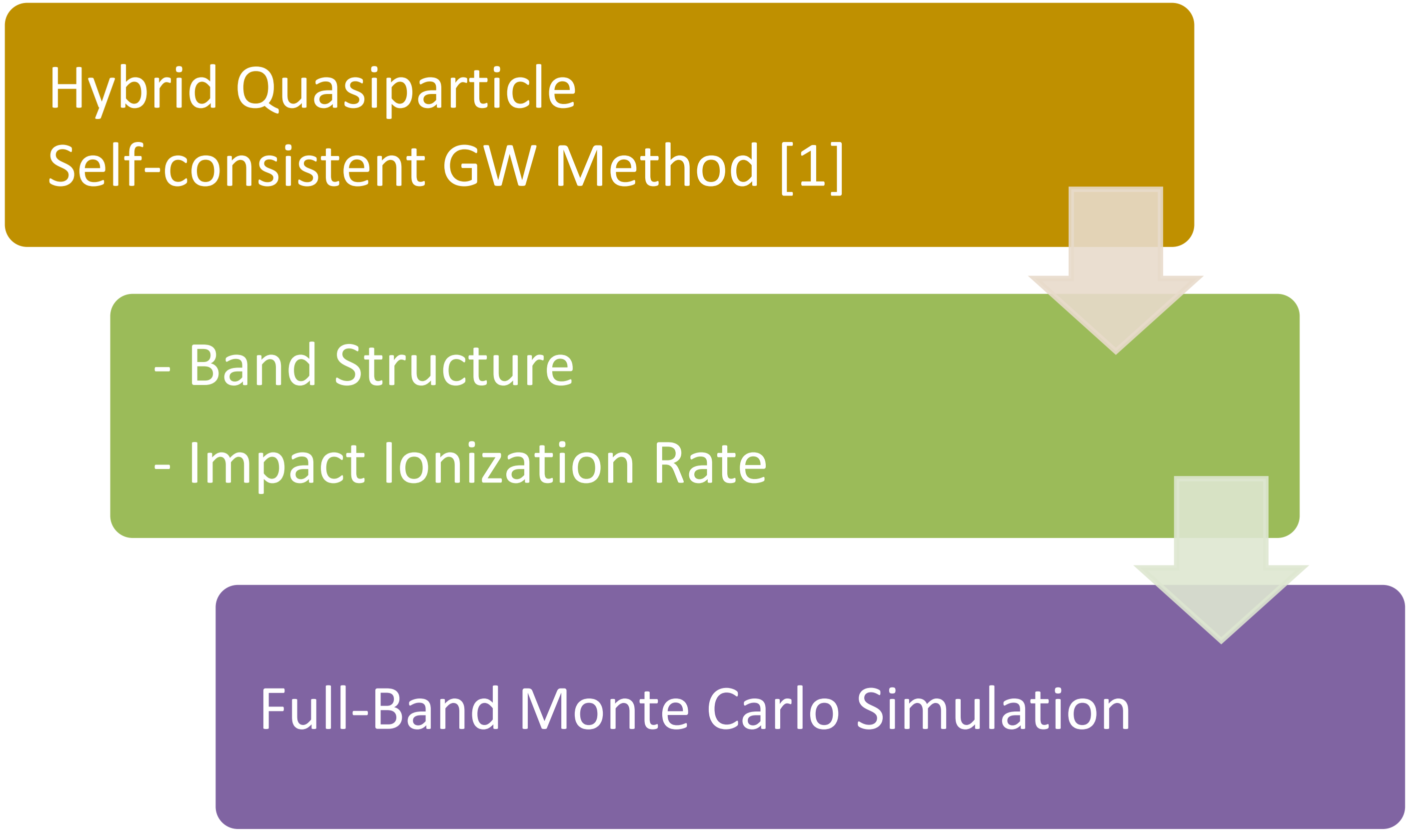
Band splitting suppresses electron transition to upper bands

S. Nakamura *et al.*, APL **80**, 3355 (2002)



CBM @ M-point

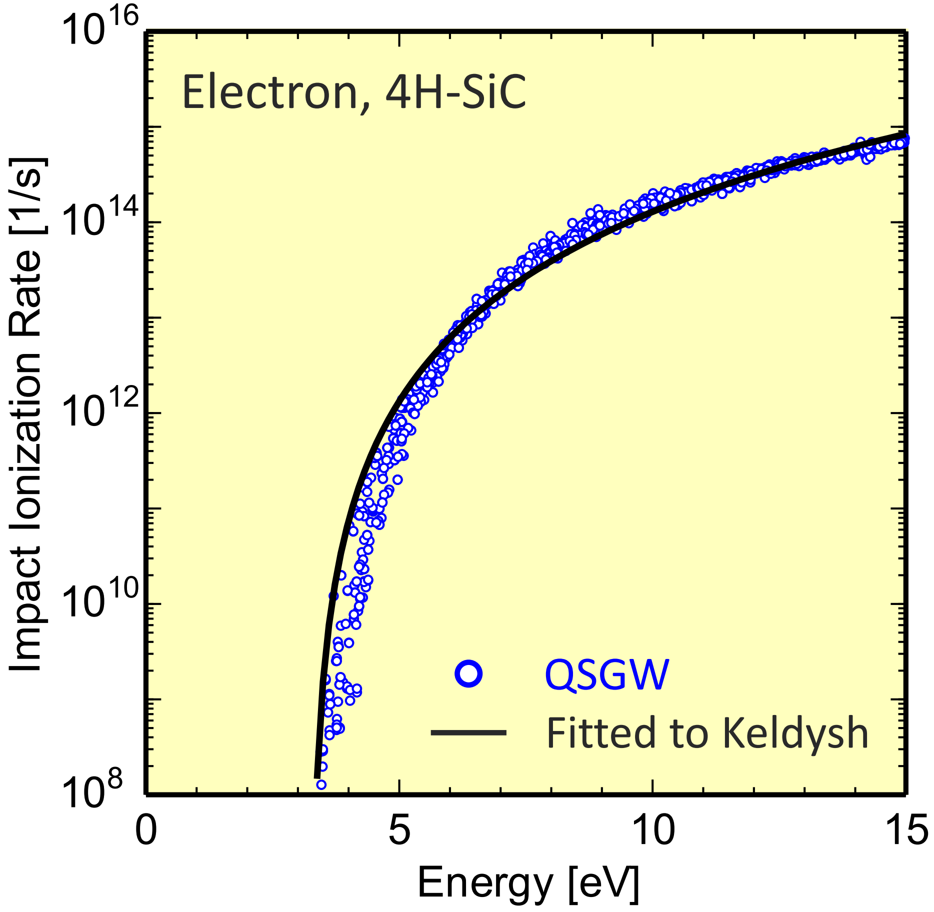
Full-Band Monte Carlo Simulation



Hybrid Quasiparticle
Self-consistent GW Method [1]

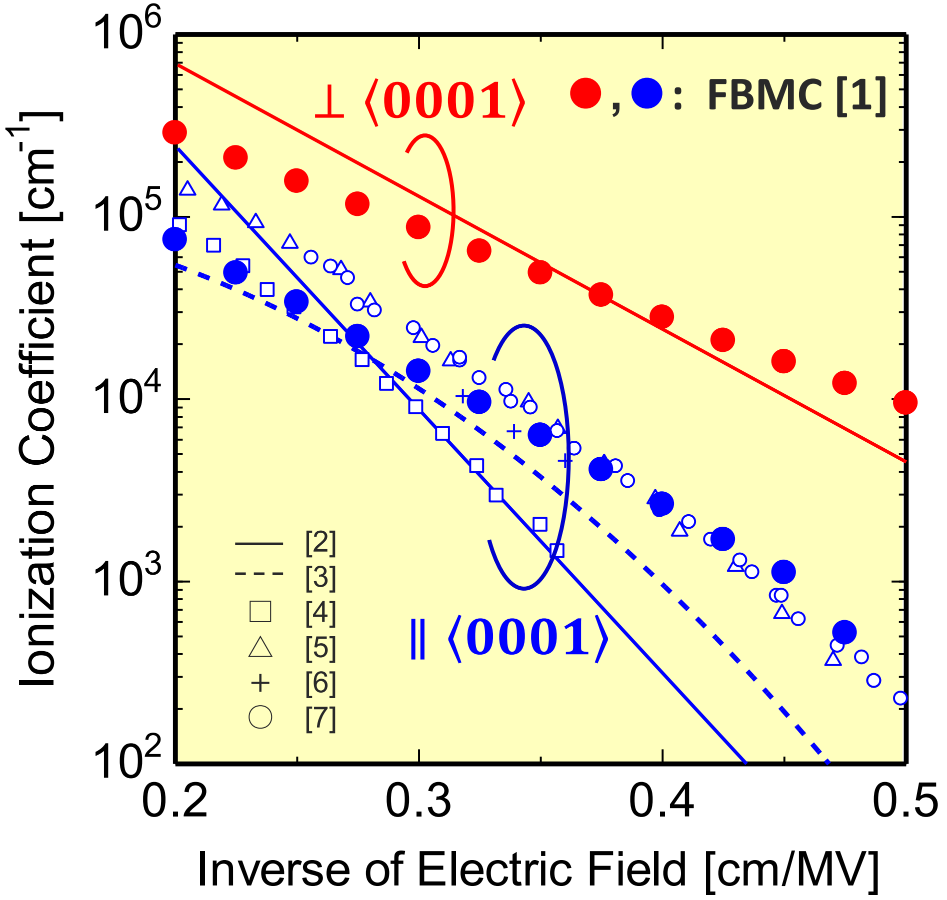
- Band Structure
- Impact Ionization Rate

Full-Band Monte Carlo Simulation

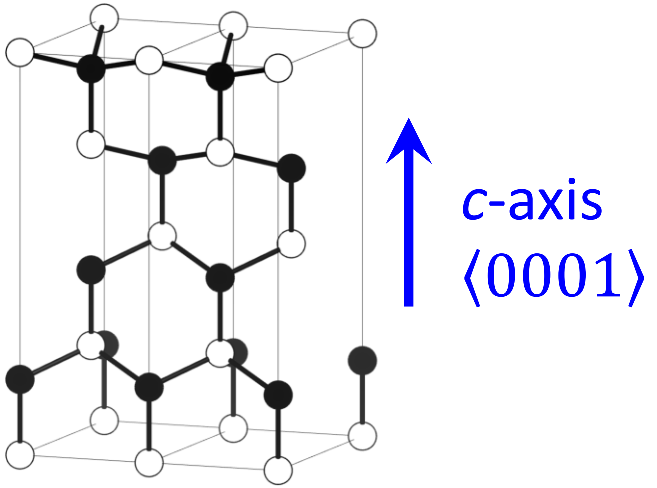


[1] T. Kotani, JPSJ **83**, 094711 (2014)

Ionization Coefficient α



- Adjust D_{op} to fit the experimental data of Niwa *et al.* [3] under high field along *c*-axis
- Larger α was obtained for in-plane direction, $\perp \langle 0001 \rangle$ compared to along *c*-axis, $\parallel \langle 0001 \rangle$

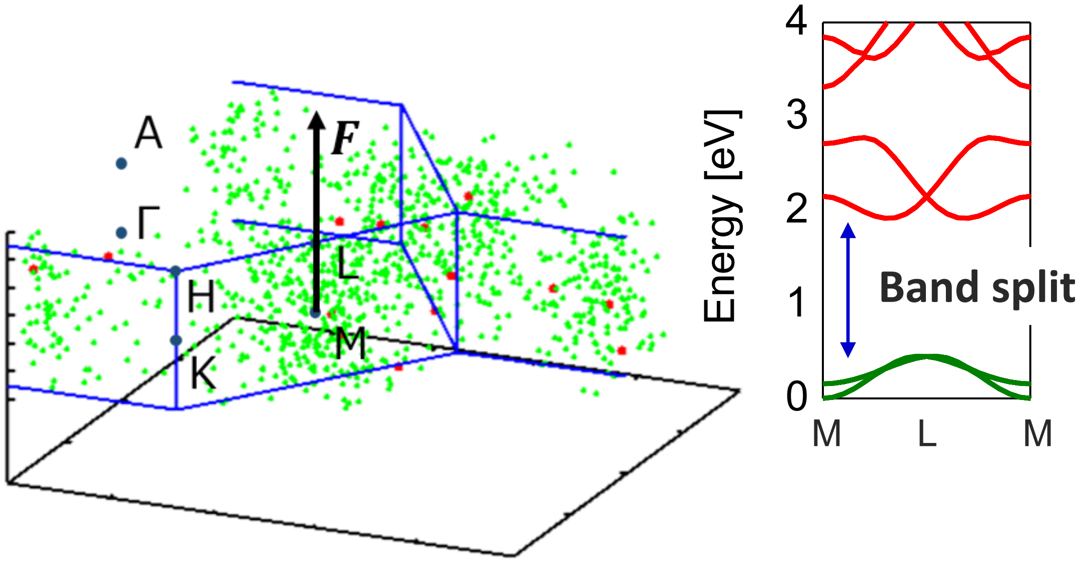


[1] R. Fujita *et al.*, SISPAD 2017
[2] T. Hatakeyama *et al.*, JAP **85**, 1380 (2004)
[3] H. Niwa *et al.*, IEEE TED **62**, 3326 (2015)
[4] A.O. Konstantinov *et al.*, APL **71**, 90 (1997)
[5] W.S. Loh *et al.*, IEEE TED **55**, 1984 (2008)
[6] R. Raghunathan *et al.*, Proc. IEEE ISPSD, 173 (1997)
[7] B.K. Ng, Ph.D. Thesis, Univ. Sheffield (2002)

Electron Distribution in *k*-space

$\boldsymbol{F} \parallel \langle 0001 \rangle$

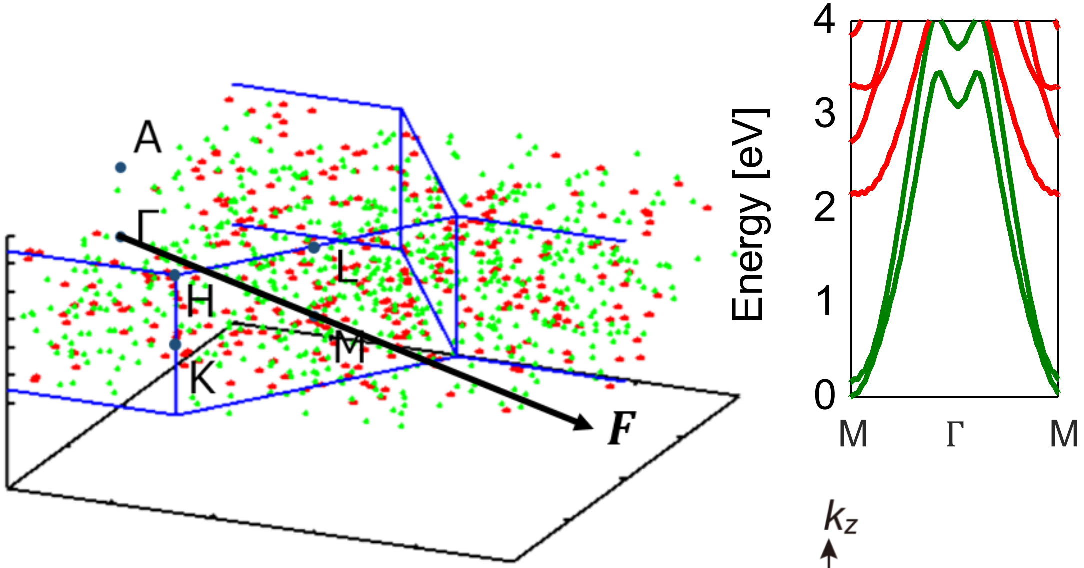
2 MV/cm along ML



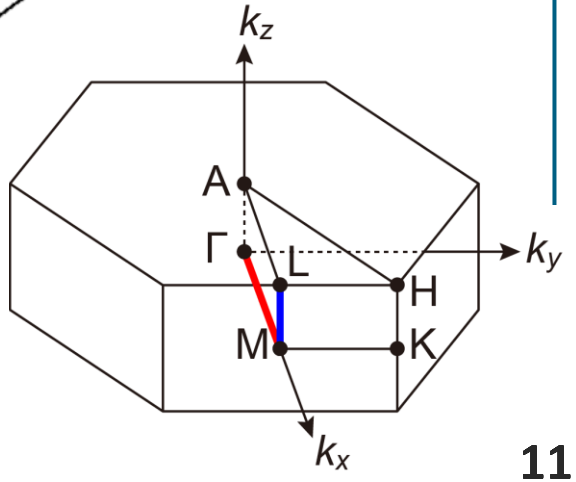
- 1st or 2nd bands
- higher bands

$\boldsymbol{F} \perp \langle 0001 \rangle$

2 MV/cm along MΓ



- 1st or 2nd bands
- higher bands



Synopsis

To systematically understand the impacts of band structures on the ionization coefficients, we have performed full-band Monte Carlo simulation using tunable band structure model.

1. Tunable band structure model and simulated models
2. Scattering mechanisms
3. Impacts of Brillouin zone width
4. Impacts of phonon scattering rates

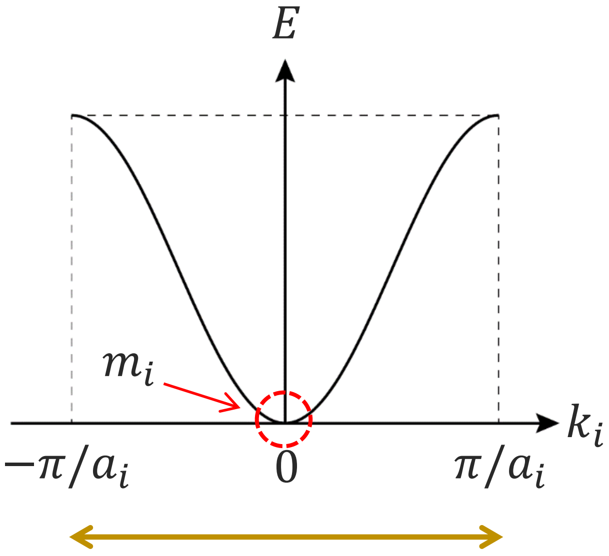
Tunable Band Structure Model

E-k dispersion of the j^{th} conduction band is given by

$$E_j(k_x, k_y, k_z) = \sum_{i=x,y,z} \frac{\hbar^2}{m_i a_i^2}(1 - \cos k_i a_i) + (n-1)\Delta E, \qquad (j = 1,2,\dots,N)$$

Parameters:

a_i	lattice constant along the i-direction $(i = x, y, z)$
m_i	band-edge effective mass along the i-direction
ΔE	energy interval between adjacent bands
N	total number of bands



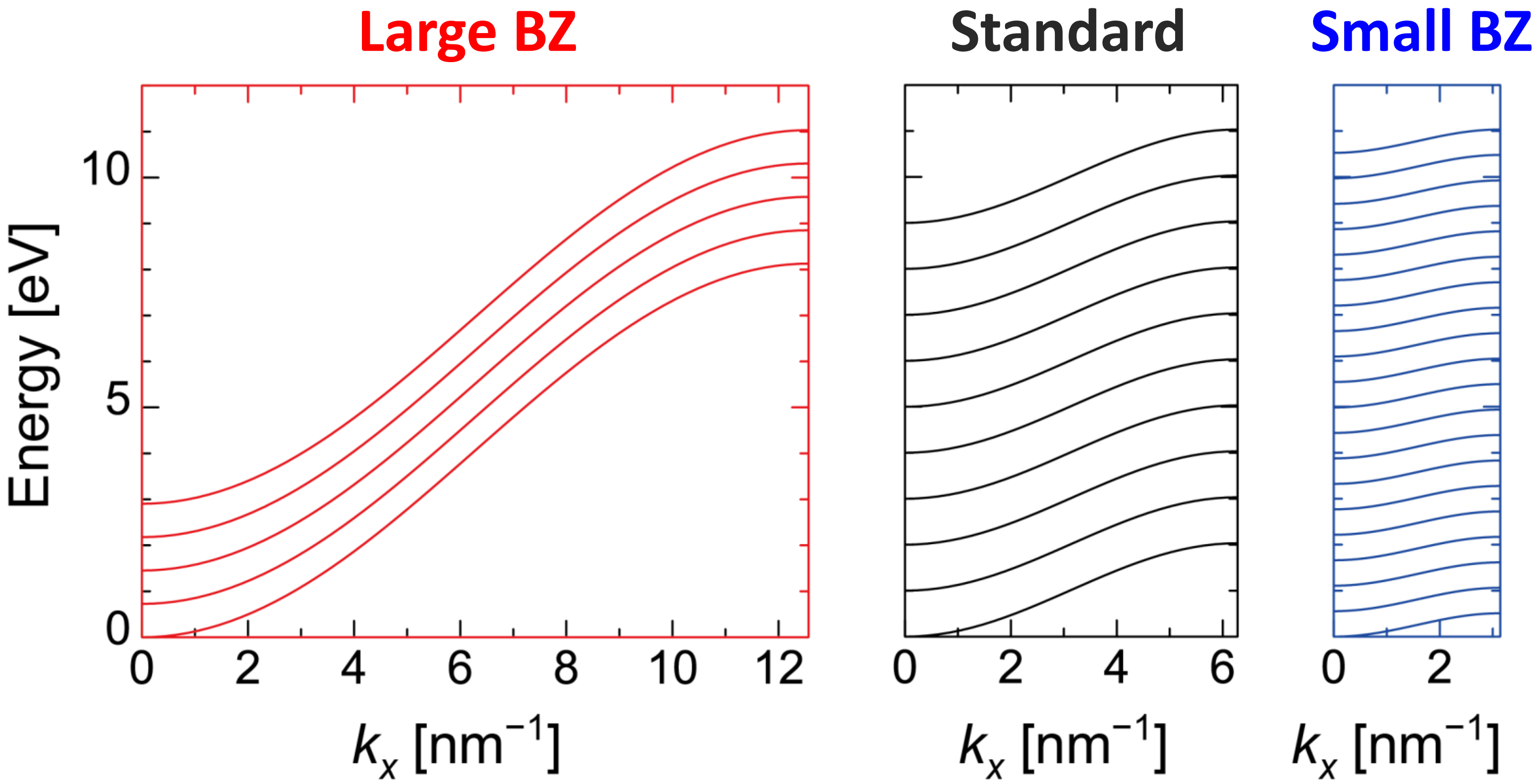
Brillouin zone (BZ) width $G_i = 2\pi/a_i$

Simulated Models

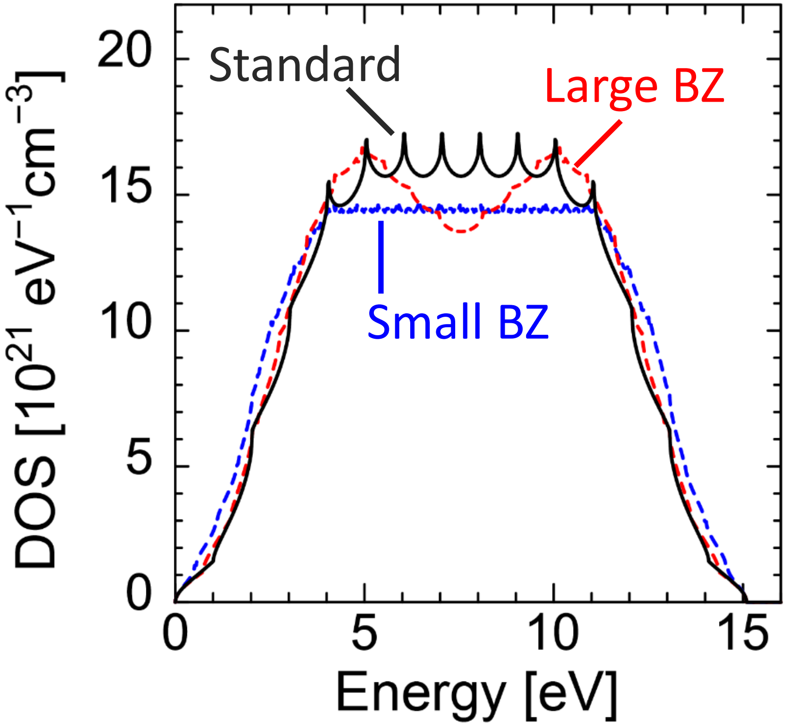
	a_x (nm)	$a_y = a_z$ (nm)	m^* (m_0)	N	ΔE (eV)
Standard	0.5	0.5	0.3	10	1
Small BZ	1	0.5	0.3	20	0.73
Large BZ	0.25	0.5	0.3	5	0.55

- ✓ The x-direction is defined along the electric field direction
- ✓ Isotropic band-edge effective mass
- ✓ N and ΔE are determined so that the total number of states and the total band width are equal in all the models

Band Structures and DOS



Band structures at $k_y = k_z = 0$



Density of states

Scattering Mechanisms

- Elastic acoustic phonon scattering

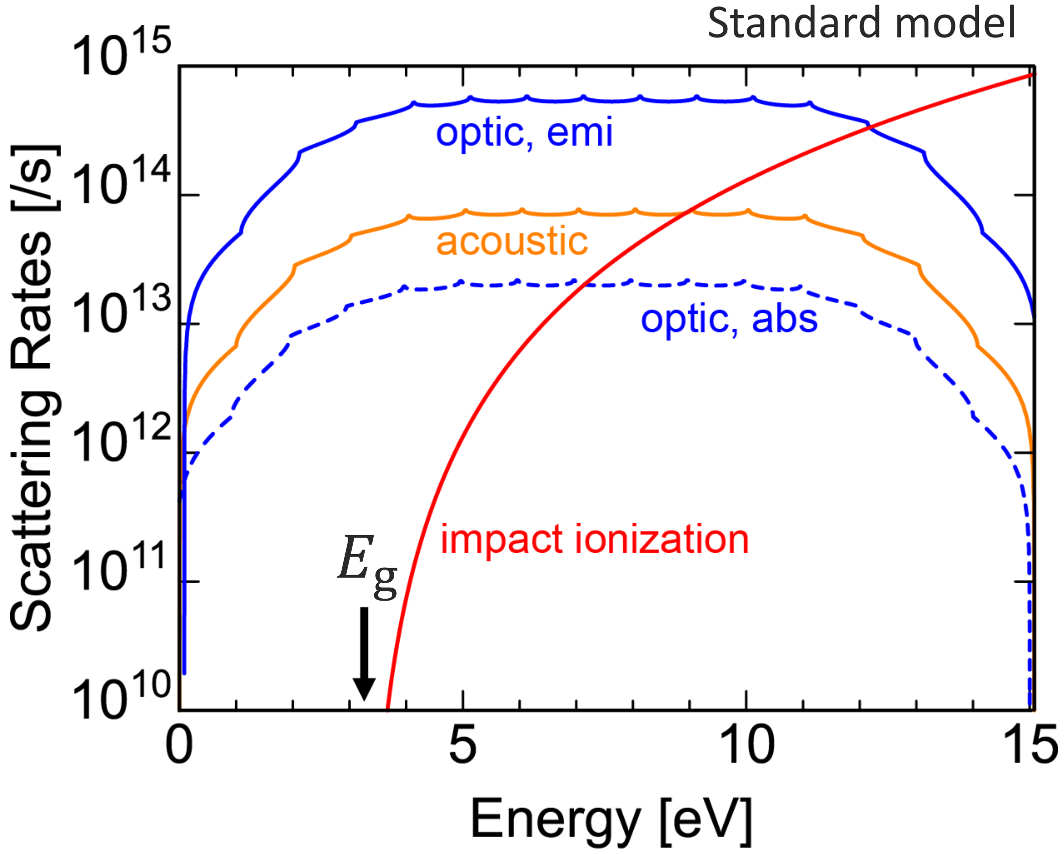
$$W_{\mathrm{ac}}(E) = \frac{\pi D_{\mathrm{ac}}^2 kT}{\hbar \rho v_{\mathrm{s}}^2}\mathrm{g}(E)$$

- Inelastic optic phonon scattering

$$W_{\mathrm{op}}^{\pm}(E) = \frac{\pi D_{\mathrm{op}}^2}{2\rho\omega_{\mathrm{op}}}\left(N_{\mathrm{op}} + \tfrac{1}{2}(1 \mp 1)\right)\mathrm{g}(E \pm \hbar\omega_{\mathrm{op}})$$

- Impact ionization

$$W_{\mathrm{ii}}(E) = a\left(\frac{E - E_{\mathrm{g}}}{E_{\mathrm{g}}}\right)^{b}$$

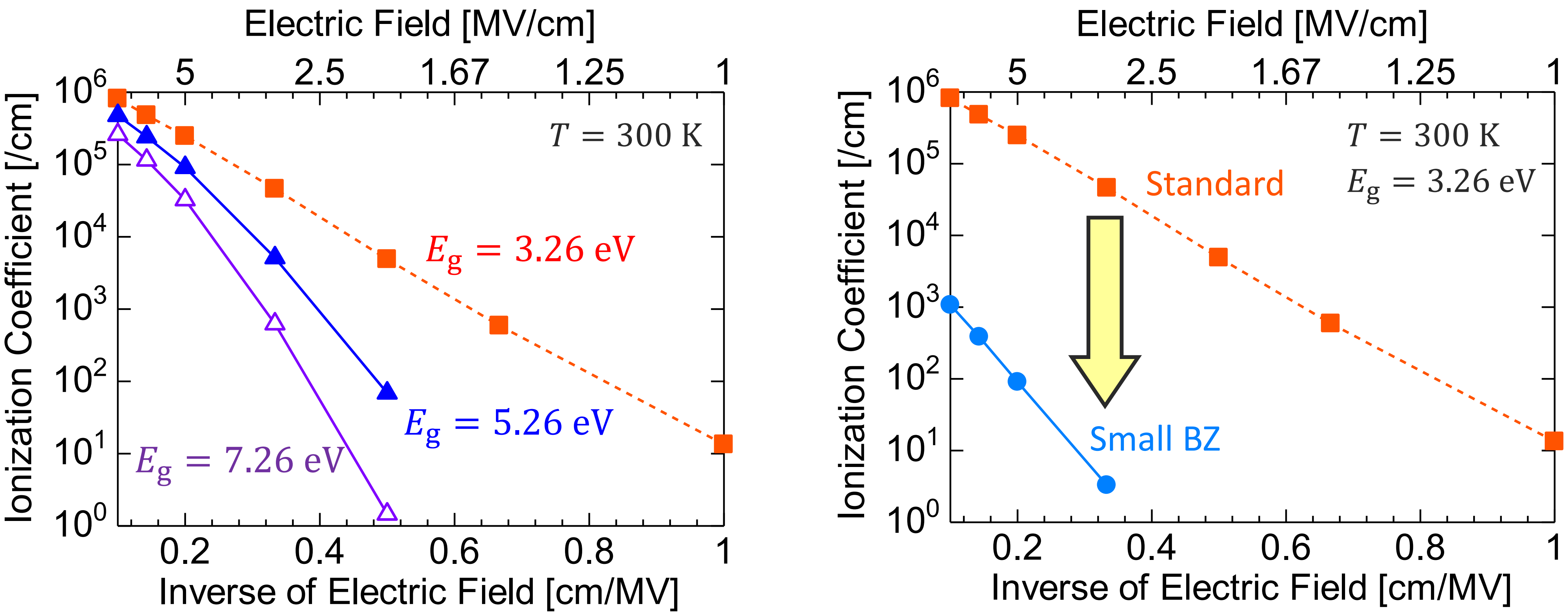


✓ Material parameters are adopted from 4H-SiC values

✓ a, b were determined by fitting to the QSGW results

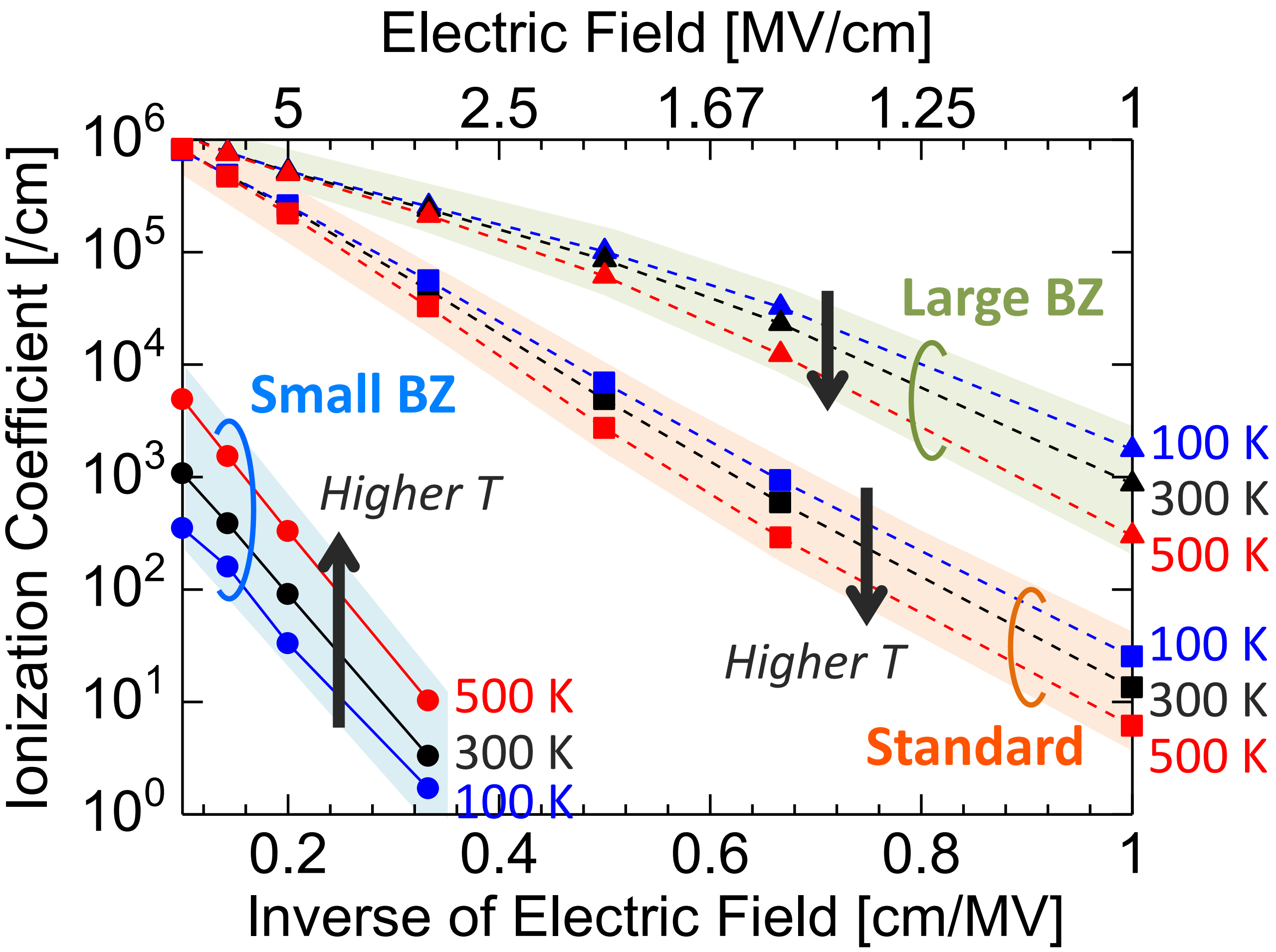
(Quasiparticle Self-consistent GW Method)

Bandgap *vs* Brillouin Zone Width



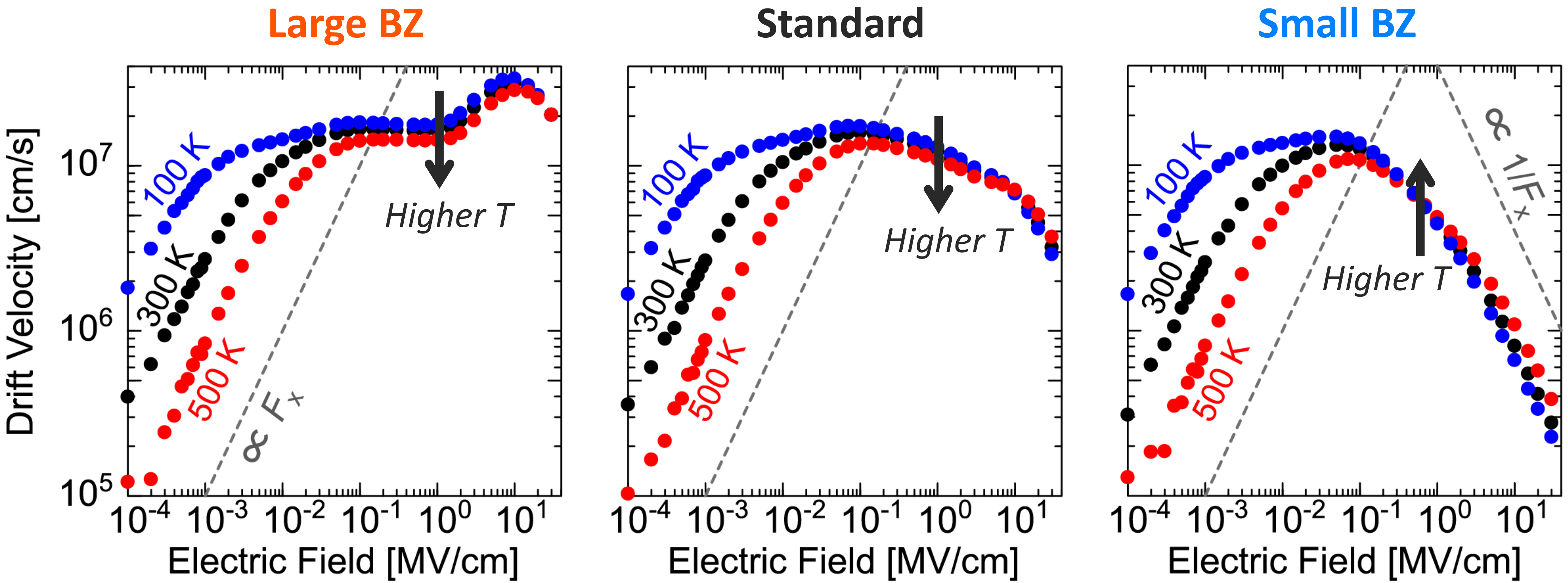
- ✓ BZ width strongly affects ionization coefficients
- ✓ It is not enough just focusing on the bandgap

Temperature Dependence



Positive temperature dependence of α for small BZ

Velocity-Field Relations



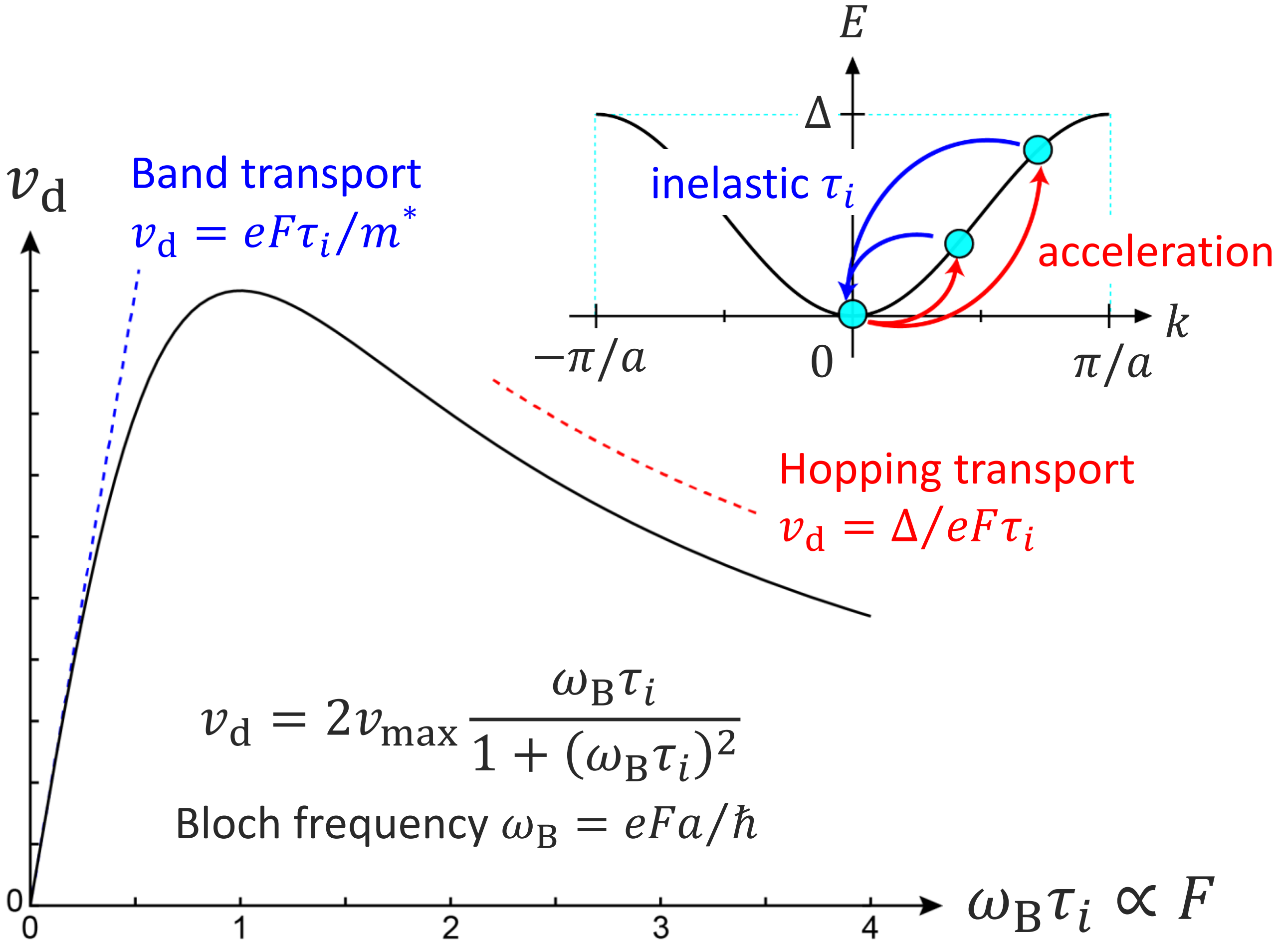
Large BZ

Standard

Small BZ

For small BZ width, v_d steeply decreases ($\propto F_x^{-1}$) and shows positive T dependence at high field → Bloch oscillation

Esaki-Tsu Model and Bloch Oscillation



$$v_\mathrm{d} = 2v_\mathrm{max}\frac{\omega_\mathrm{B}\tau_i}{1+(\omega_\mathrm{B}\tau_i)^2}$$

Bloch frequency $\omega_\mathrm{B} = eFa/\hbar$

Velocity-field curve

L. Esaki and R. Tsu, IBM J. Res. Dev. **14**, 61 (1970)

Bloch oscillation

✓ Electrons are confined in a small spatial region

↓

cannot gain energy from the field

↓

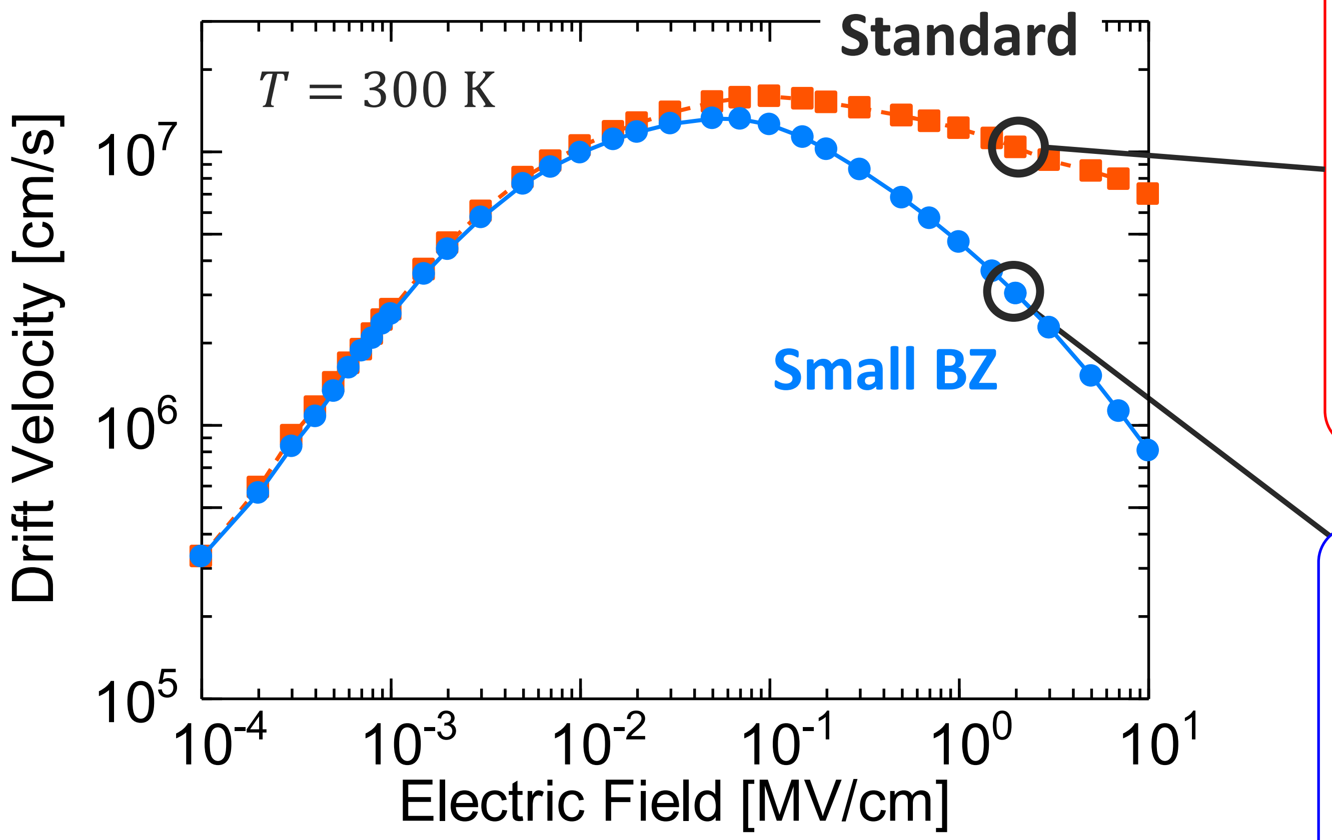
small ionization coefficients

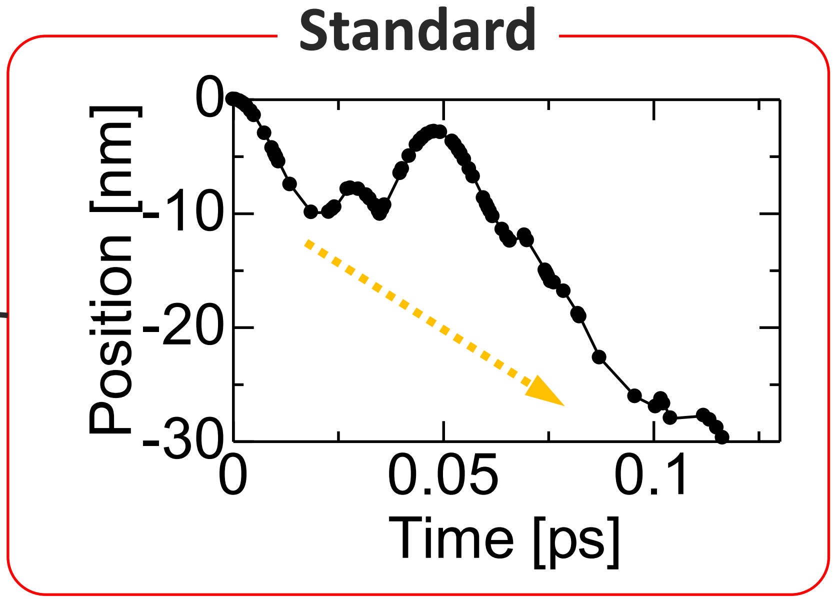
✓ Scatterings enhance the transport

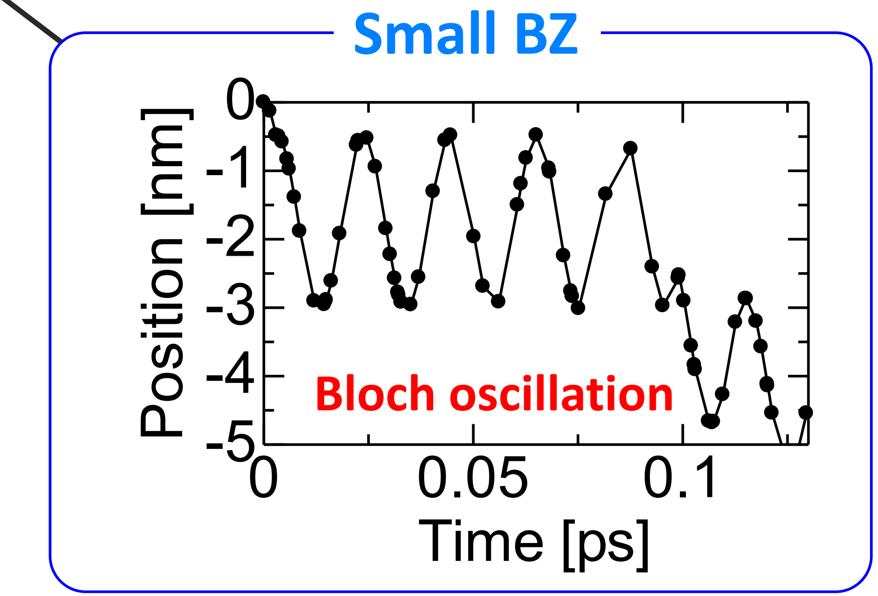
↓

positive T dependence

Electron Trajectories





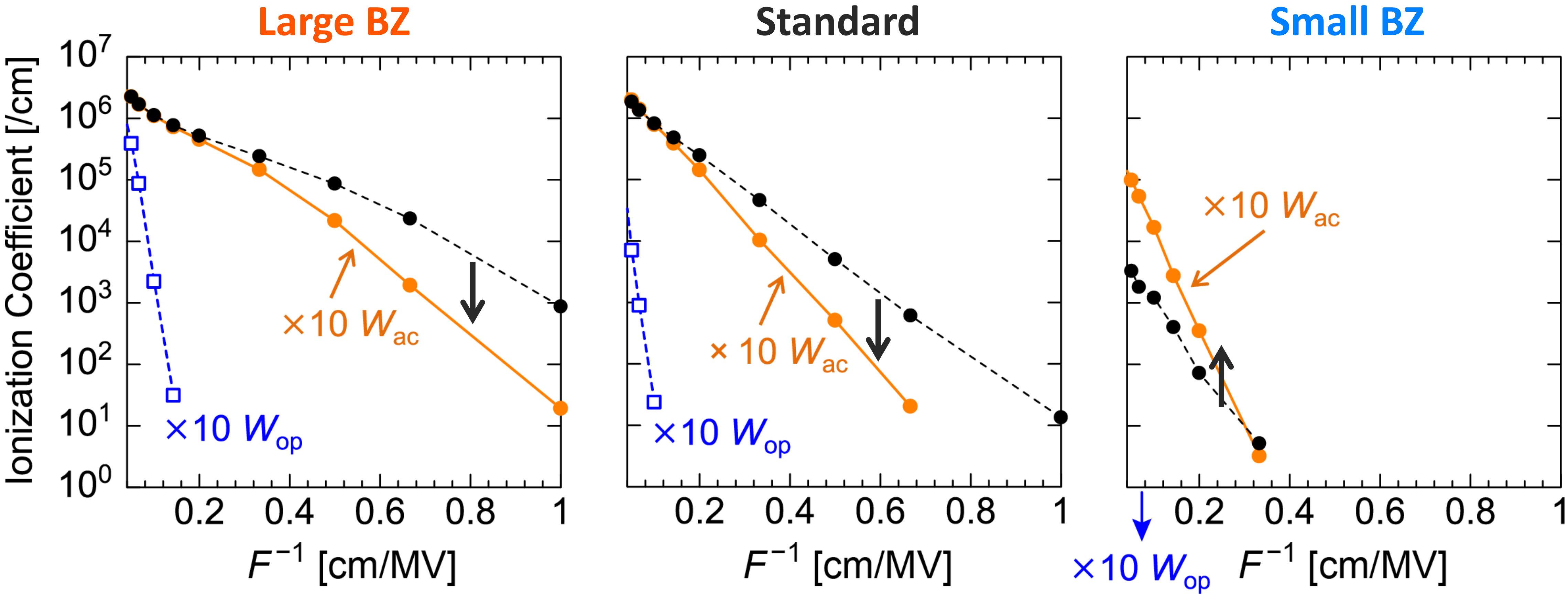


◆ **For small BZ**, Bloch oscillation occurs

→ Smaller ionization coefficient α

→ Positive T dependence of α

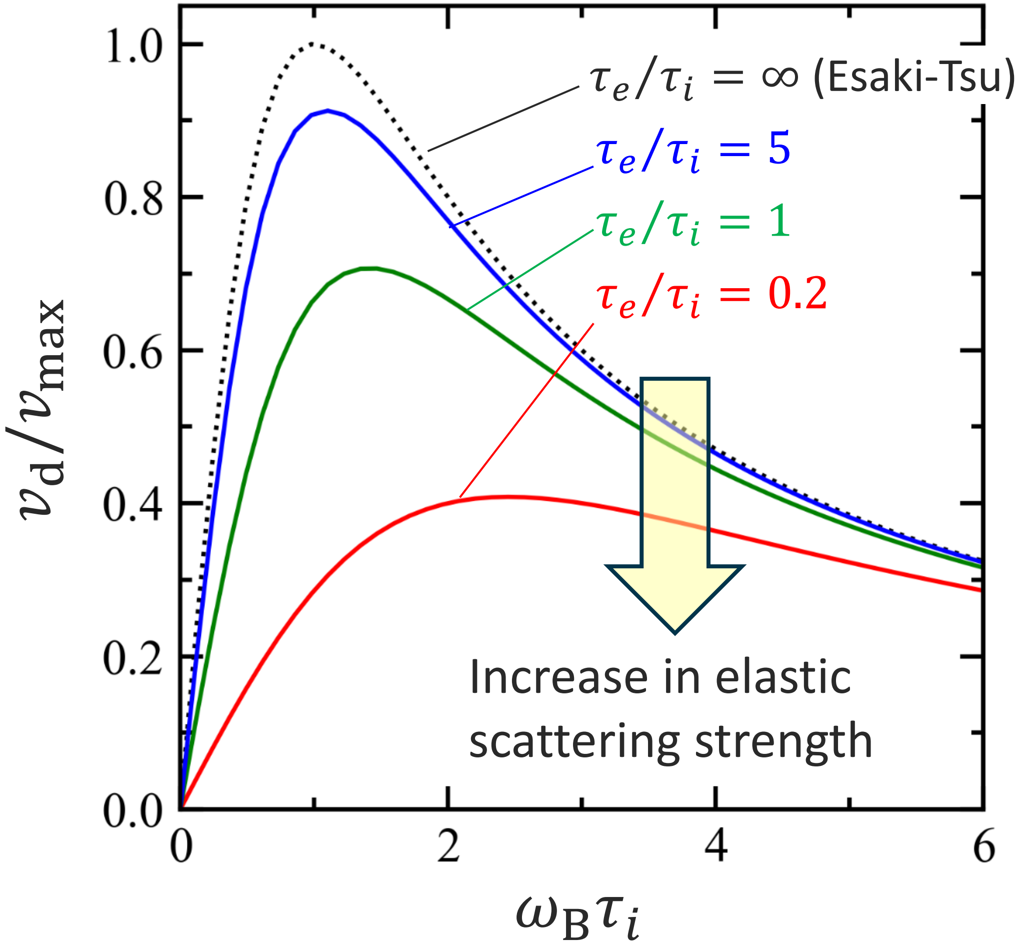
Impacts of Phonon Scattering Rates on α

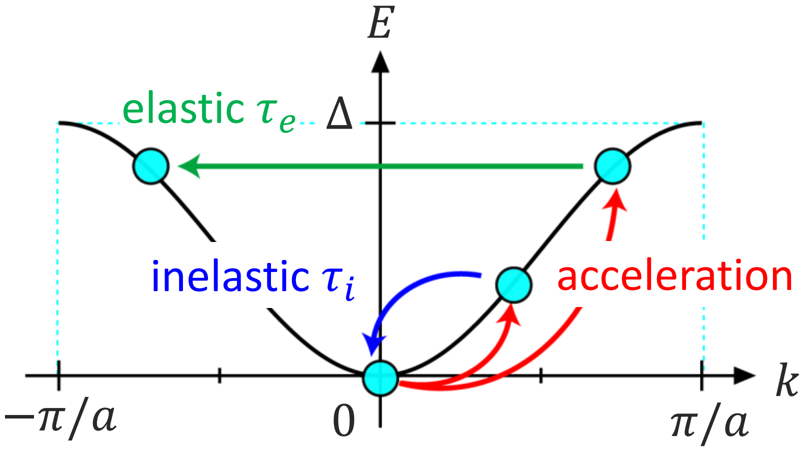


✓ $\times 10\ W_{\mathrm{op}}$ → faster energy relaxation → smaller α

✓ $\times 10\ W_{\mathrm{ac}}$ → different trend for small BZ

Ignatov Model





$$v_\mathrm{d} = 2\delta v_\mathrm{max}\frac{\omega_\mathrm{B}\tau}{1+(\omega_\mathrm{B}\tau)^2}$$

$$\left(\tau = \delta\tau_i,\quad \delta = \frac{1}{\sqrt{1+\tau_i/\tau_e}}\right)$$

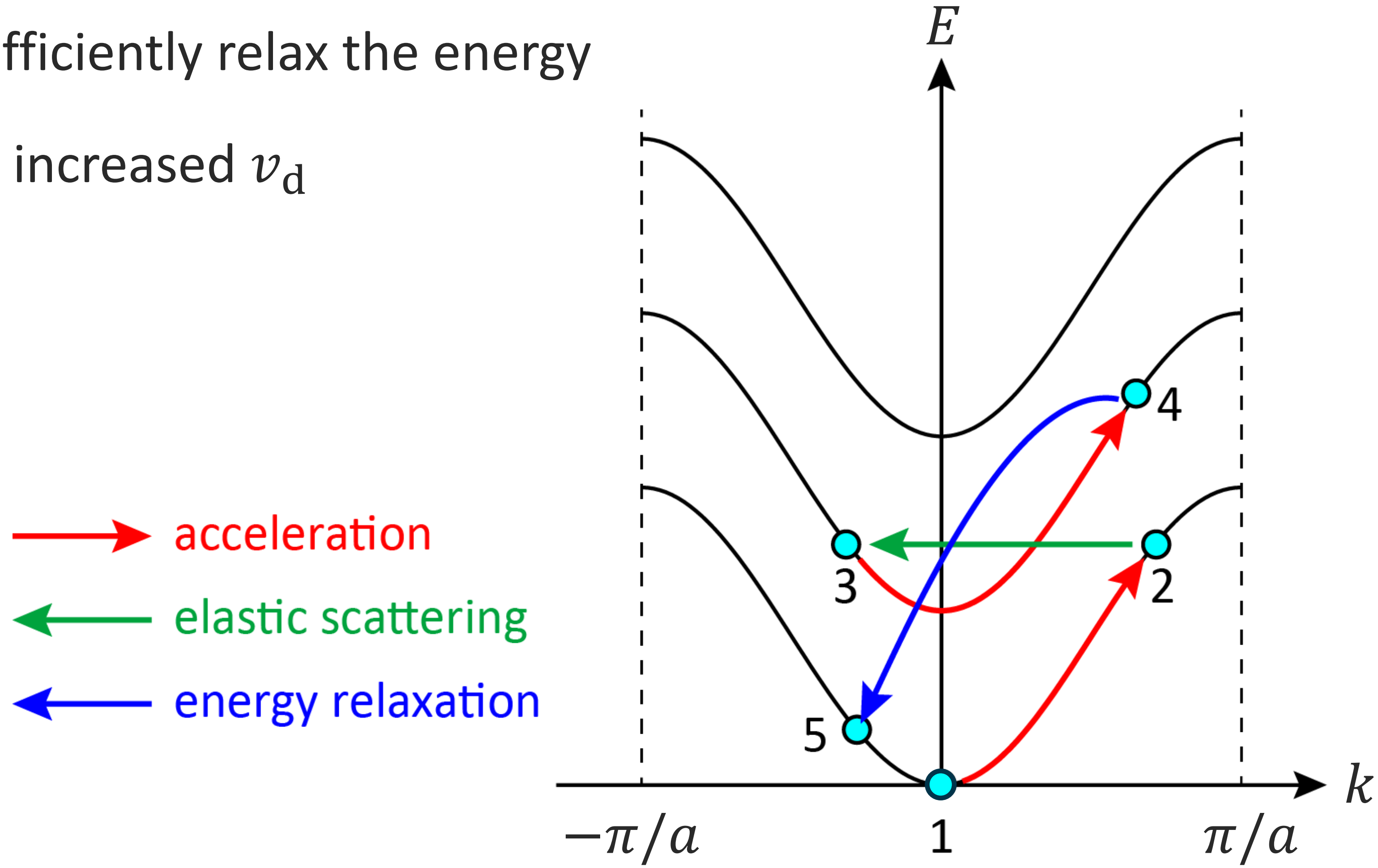
A.A. Ignatov *et al.*, Mod. Phys. Lett. **5**, 1087 (1991)

Elastic Scattering Assisted Energy Relaxation

Elastic scattering transfers an electron to the upper bands

→ The hot electron can efficiently relax the energy

→ This process may have increased v_d



Conclusion

- We analyzed the ionization coefficients assuming the tunable band structures.
- Smaller Brillouin zone width could give rise to the Bloch oscillation which results in a significant reduction and the positive temperature dependence of the ionization coefficient.
- The impacts of the Brillouin zone width on ionization coefficients can be stronger than those of the bandgap.
- Elastic scattering can contribute to both energy gain and loss processes by transferring electrons to upper bands.
- Our results show the importance of considering the E-k dispersion rather than just focusing on the bandgap when discussing the materials for high-power devices.

Ref: H. Tanaka, T. Kimoto, N. Mori, APEX **13**, 041006 (2020); JAP **131,** 225701 (2022)