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Influence of temperature, strain, alloy composition, doping, and film thickness on the dielectric function of semiconductors

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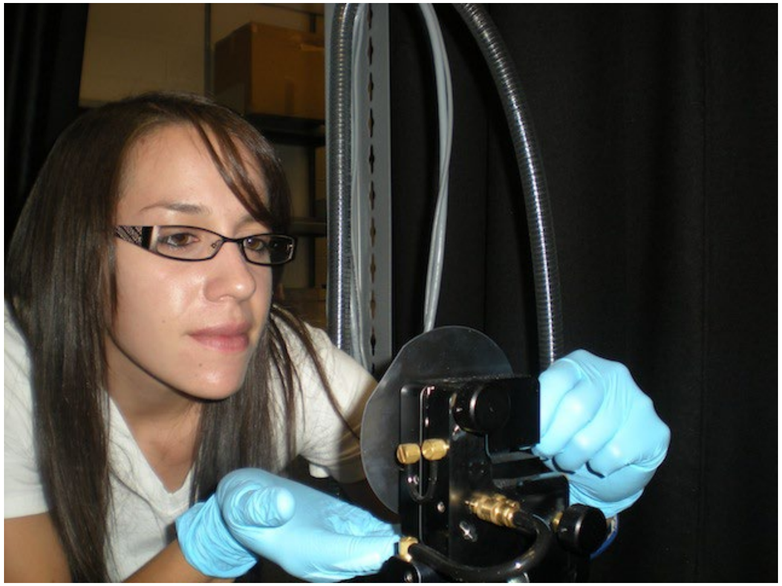
Department of Physics
New Mexico State University, Las Cruces, NM



DMR-1505172

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Call for Abstracts

Spectroscopic Ellipsometry Abstracts Due: May 2, 2018

Awards **Submit Abstract**

The Spectroscopic Ellipsometry Focus Topic integrates themes ranging from classical material science and thin film characterization to nanometer scale science and novel optical sensing concepts. We will host two oral sessions dedicated to traditional applications of spectroscopic ellipsometry in optical materials and thin film characterization as well as new and emerging topics. The first session will focus on classical research topics of ellipsometry as for instance optical coatings and inorganic thin films characterization.

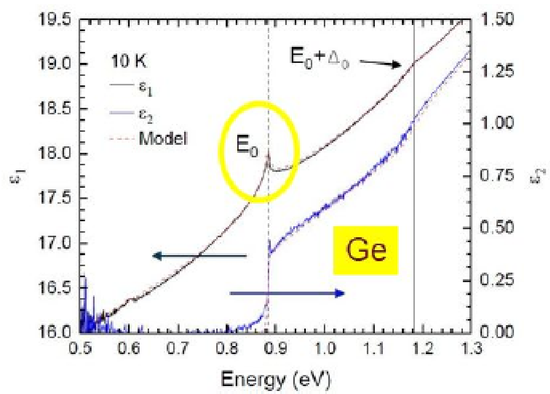


Figure courtesy Carola Emminger, Dept. of Physics, New Mexico State Univ., Las Cruces, NM

Furthermore, presentations on the ellipsometric investigation of novel optical and electronic materials and materials with subwavelength structures will be included. In the second oral session, we will host presentations on novel experimental and theoretical approaches including for instance imaging ellipsometry or optical critical dimension analysis techniques. As a highlight of our Spectroscopic Ellipsometry focus topic, the best student paper, which is selected based on the quality of the research, its presentation, and the discussion during the symposium, will be awarded with the Spectroscopic Ellipsometry Focus Topic student award. Spectroscopic Ellipsometry will also host a poster session. Click here for past recipients of the award and rules for entering the competition.

Eighth International Conference on SPECTROSCOPIC ELLIPSOMETRY

ICSE 8 BARCELONA 2019

May 26 - 31, 2019
World Trade Center
Barcelona
Spain

Please submit a proceedings manuscript.

Biography


Regensburg/Stuttgart
Germany


Motorola (Mesa, Tempe)
Arizona, 1997-2005

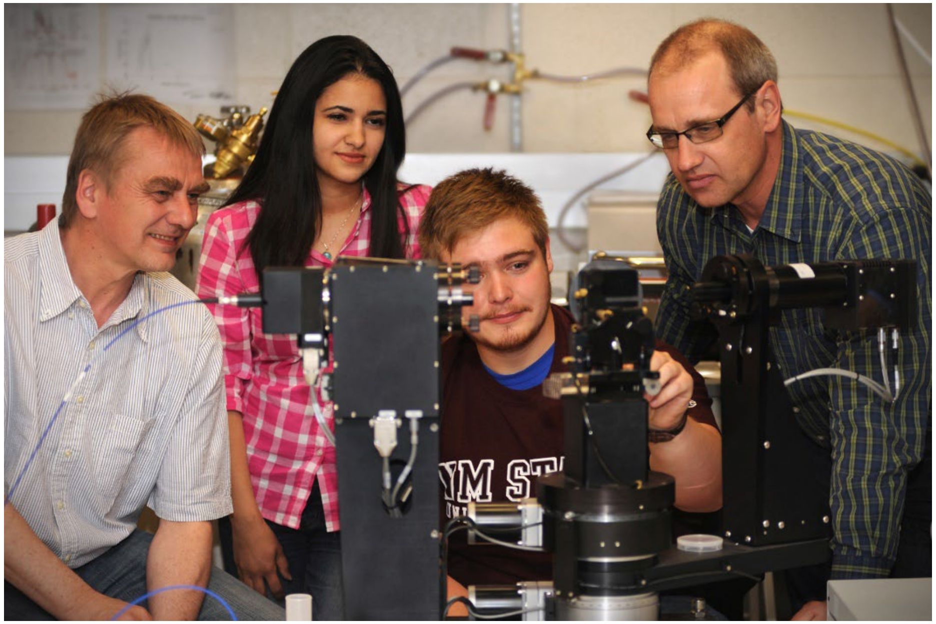

Freescale, IBM
New York, 91-92;07-10


Motorola, Freescale
Texas, 2005-2007

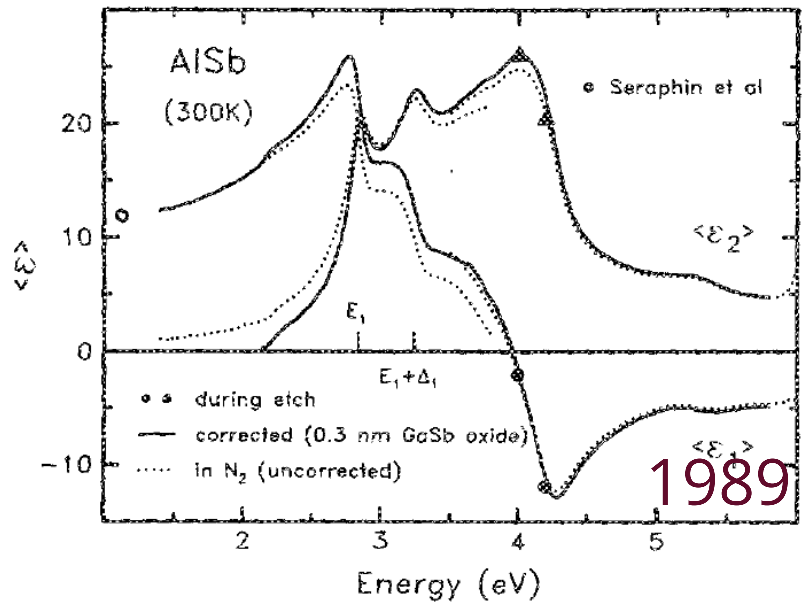

Las Cruces, NM
Since 2010

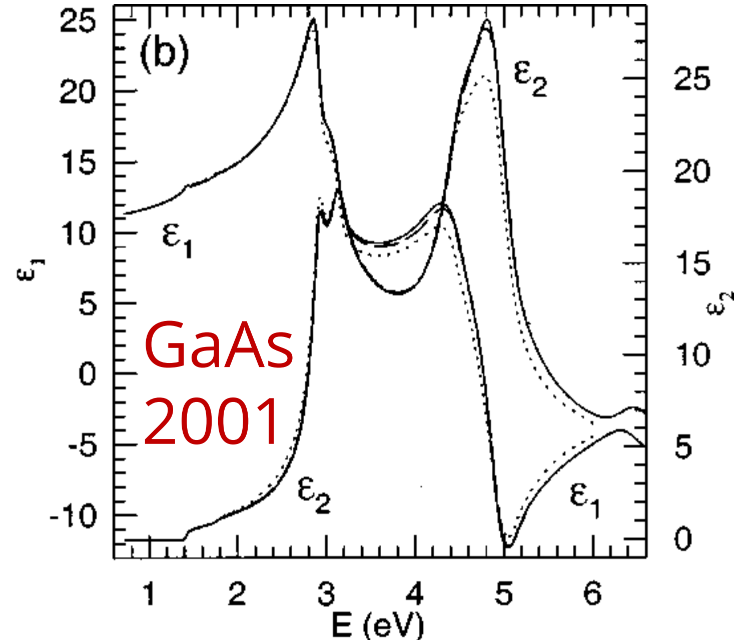
Outline

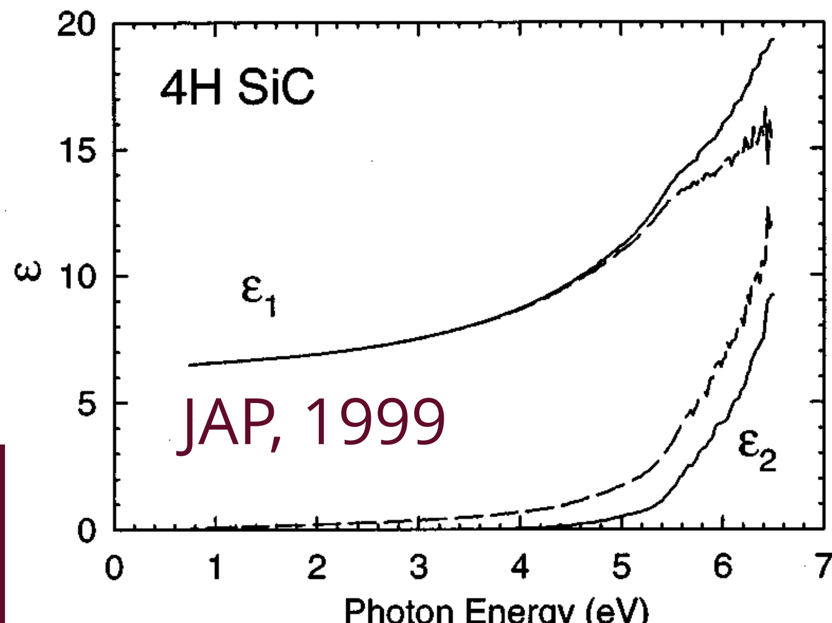
- Examples of **single-crystalline semiconductor** dielectric functions
- Temperature
- Strain
- Alloy composition
- Excitonic effects
- Film thickness
- Doping and carriers

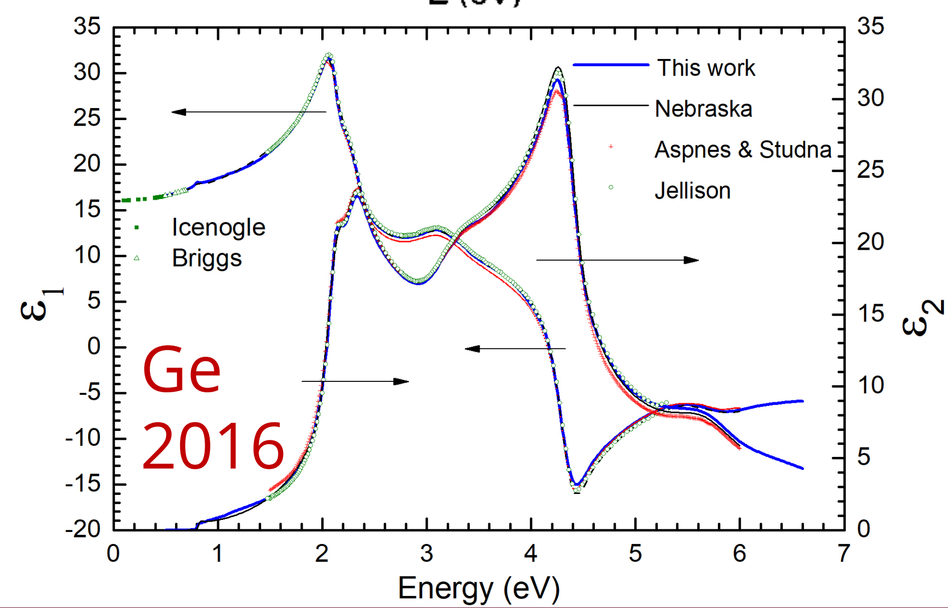


Semiconductor Dielectric Functions

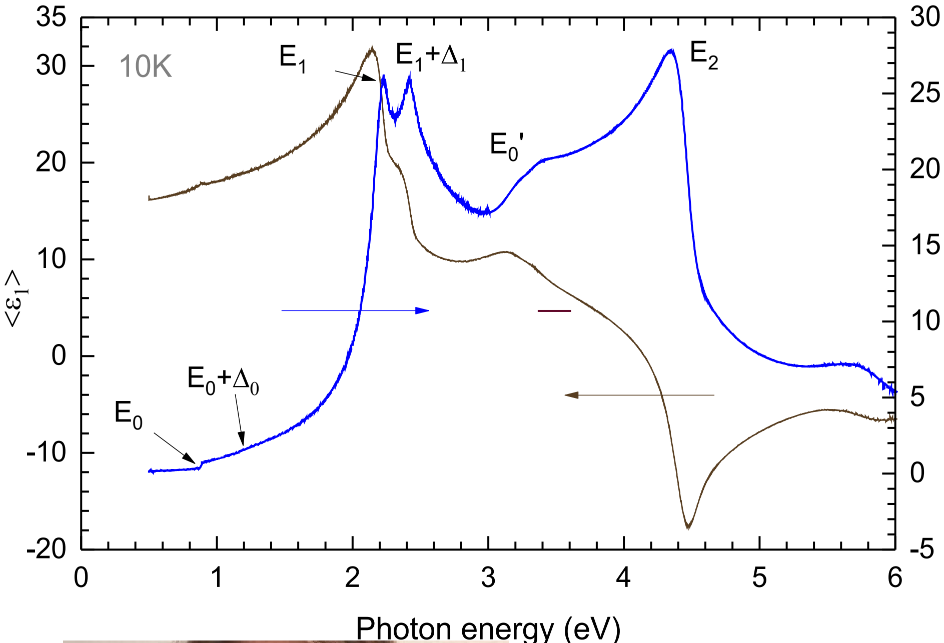


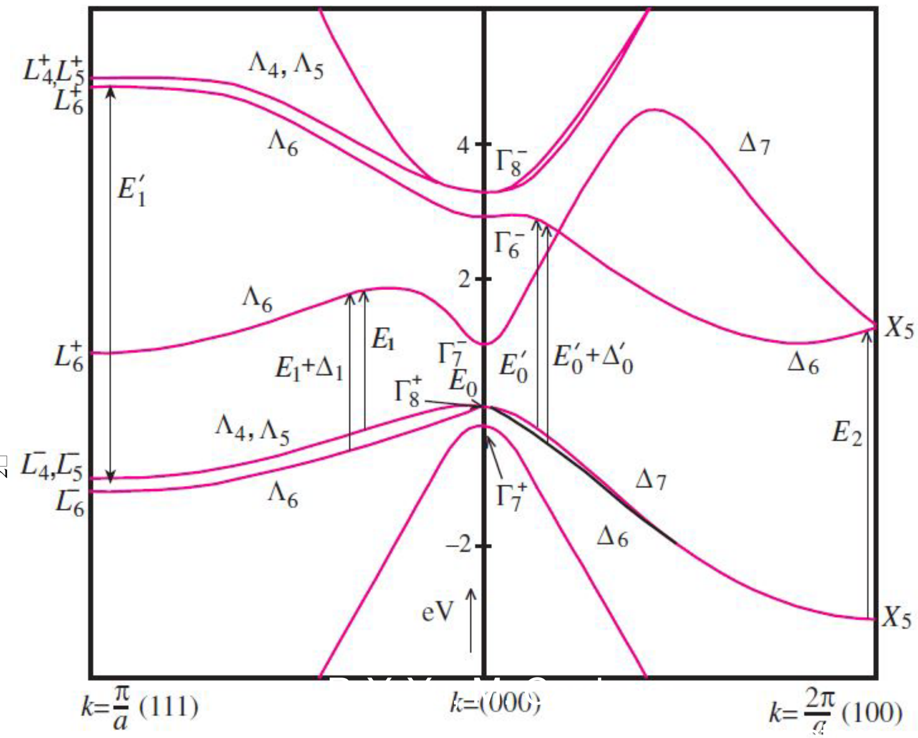




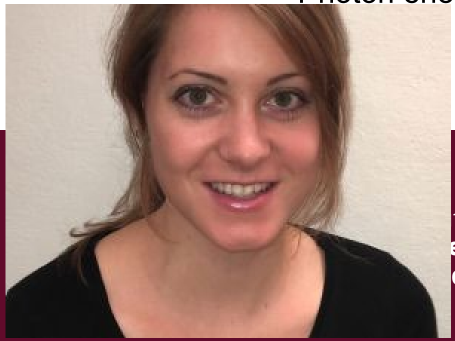


Critical points in the dielectric function are related to interband transitions





Band structure of Ge



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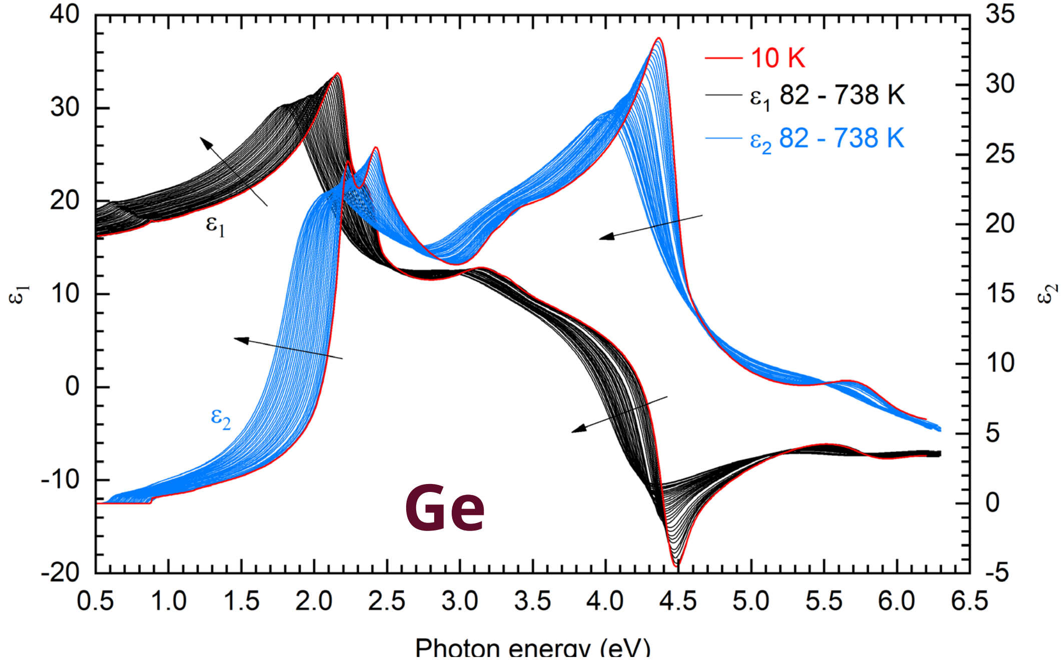
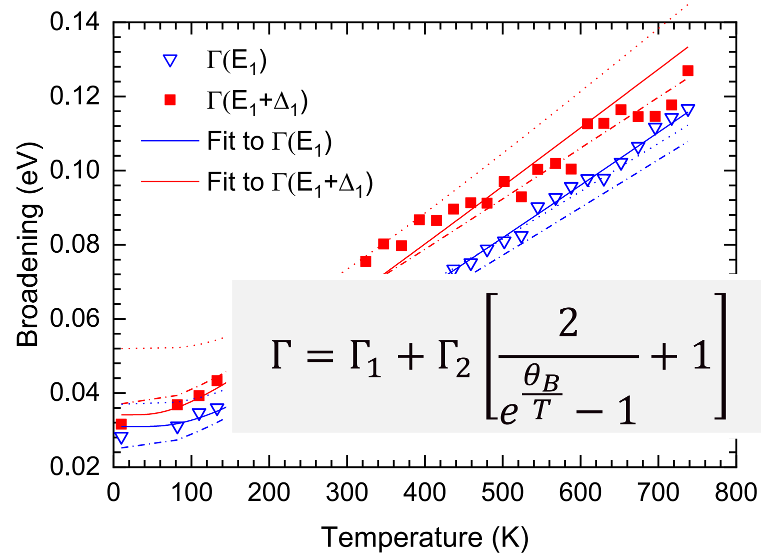
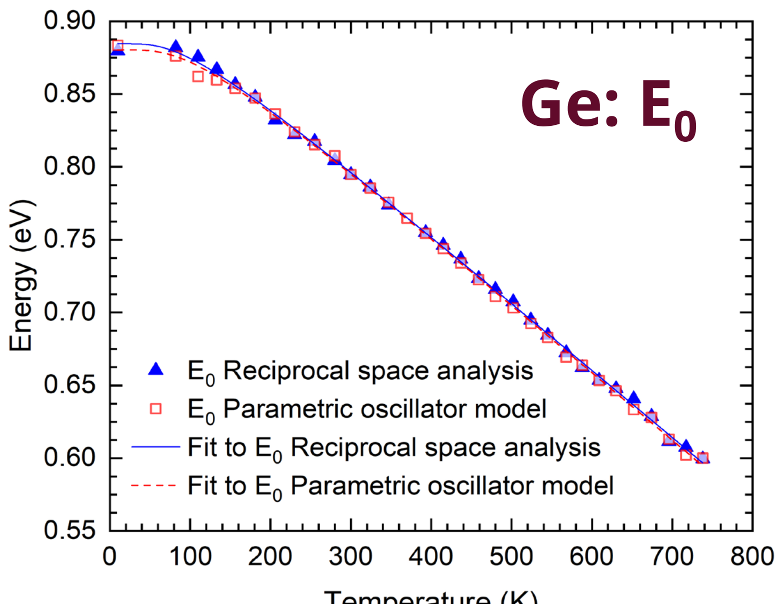
Carola Emminger, MS thesis (Linz)

Impact of Temperature





$$\Gamma = \Gamma_1 + \Gamma_2 \left[\frac{2}{e^{\frac{\theta_B}{T}} - 1} + 1 \right]$$



Thermal expansion (small)

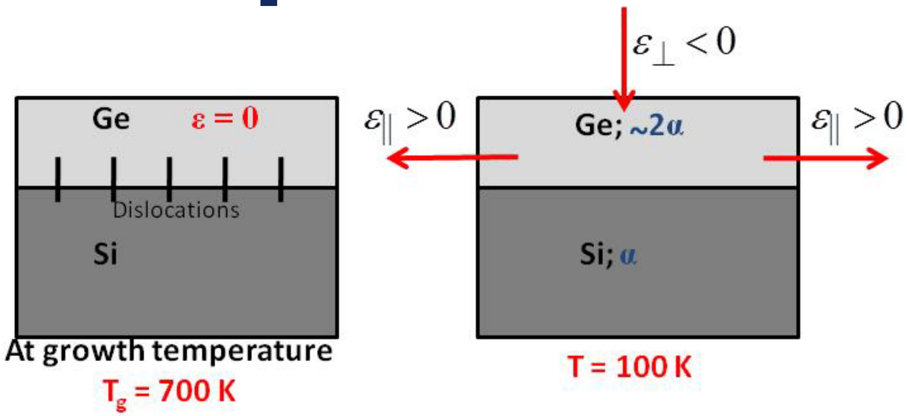
Electron-phonon interaction (dynamic disorder)

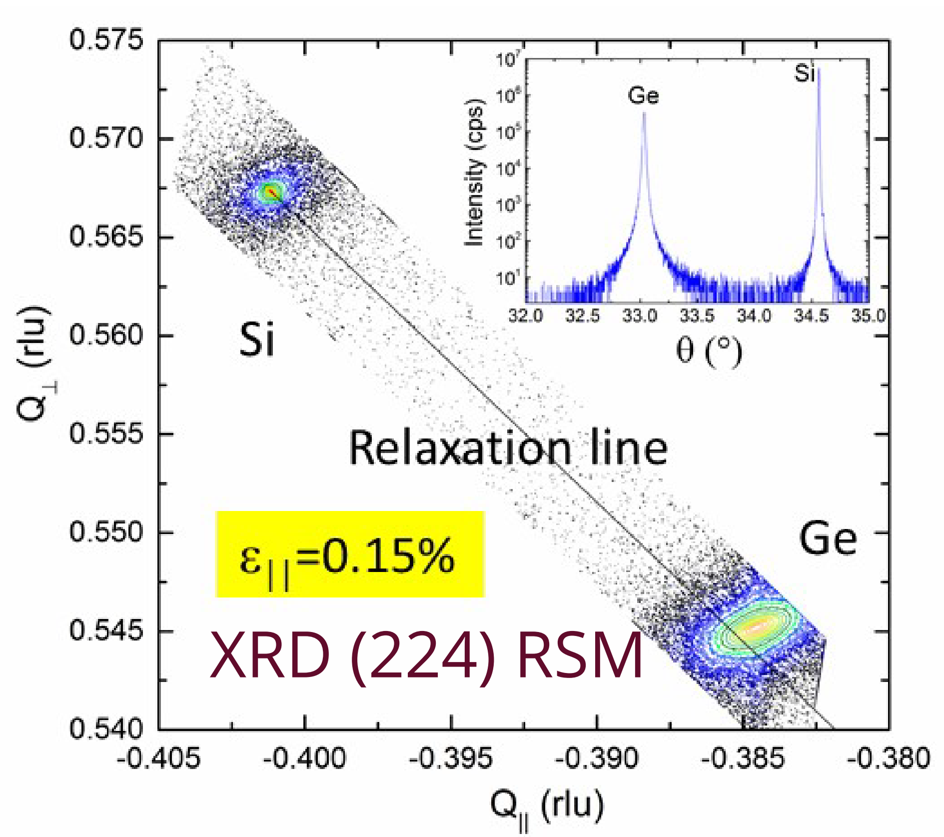
Red-shift and broadening of CPs

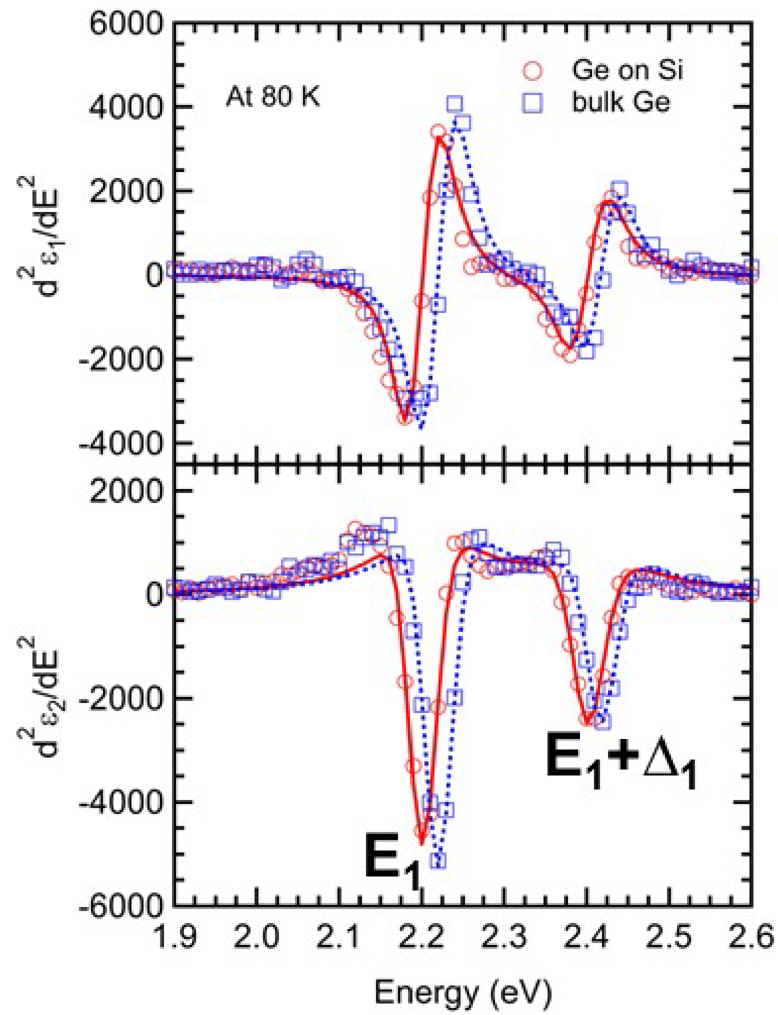
Theory exists (e-phonon coupling)

Carola Emminger, MS thesis (Linz)

Impact of Strain and Stress

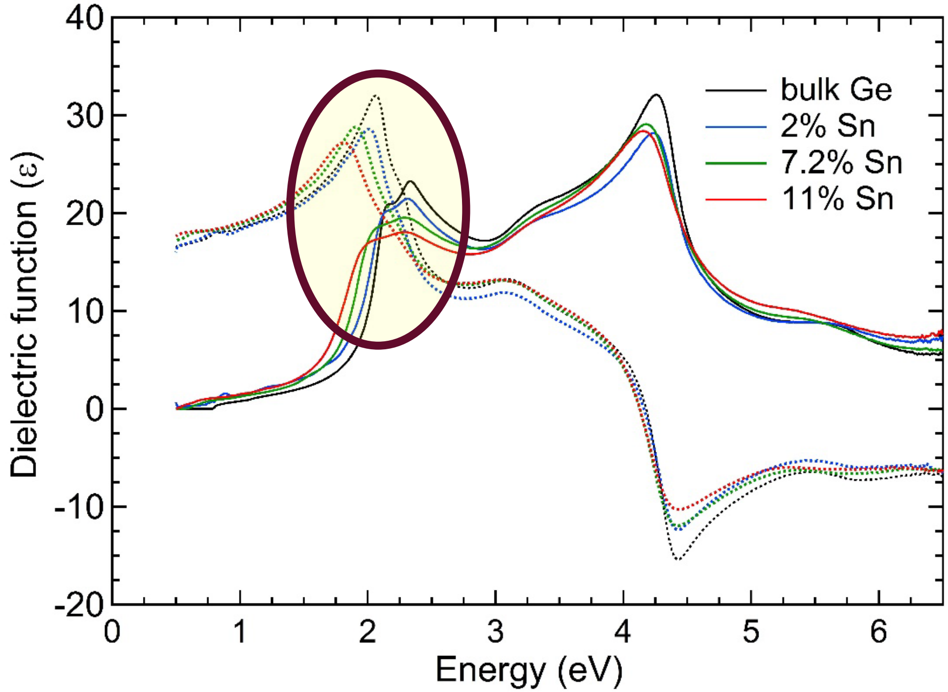


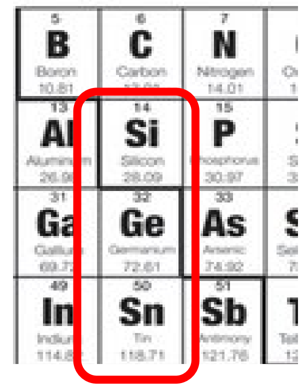




Continuum elasticity theory
Deformation potentials
Nalin Fernando, Appl. Surf. Sci. **421** (2017)

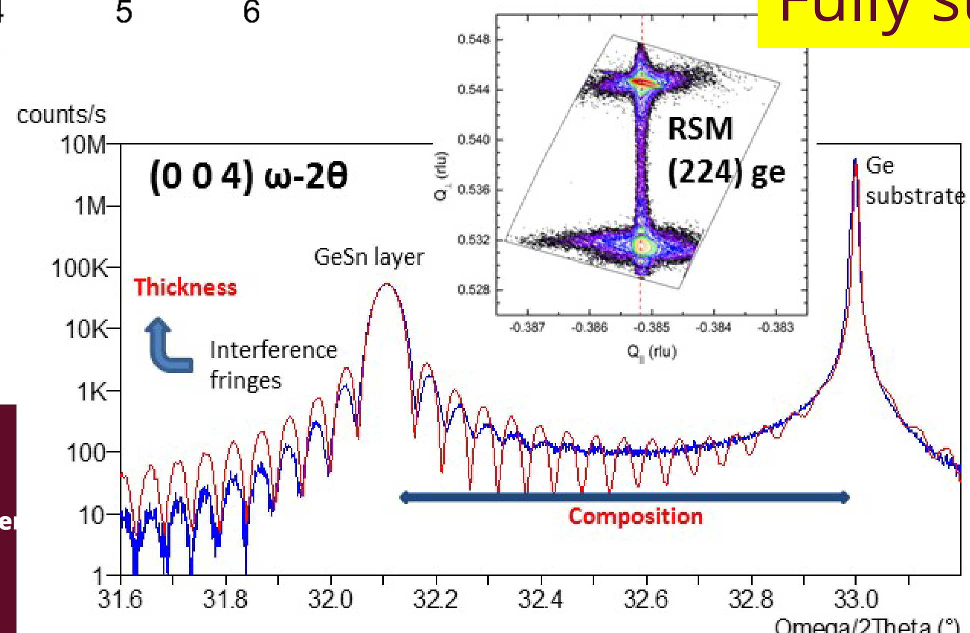
Impact of Composition: Ge-Sn Alloys





N. Fernando, JVST B **36** (2018)

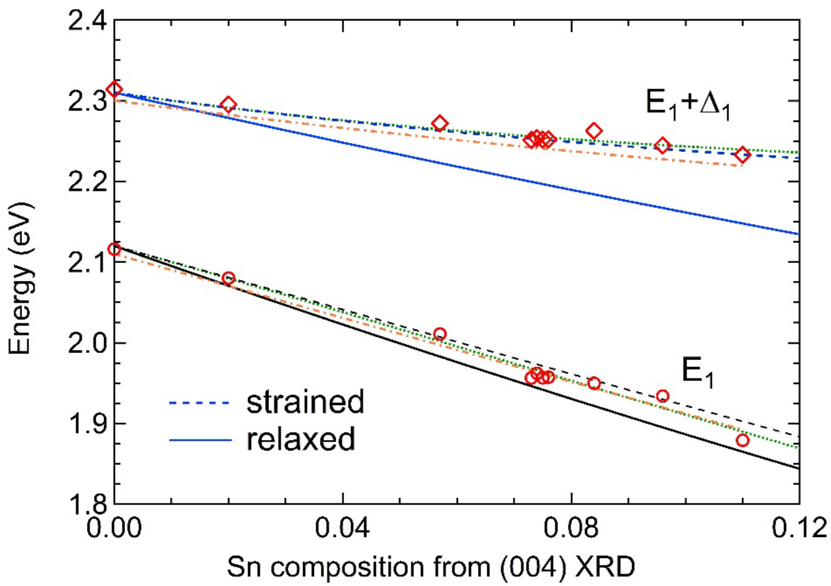
Fully strained

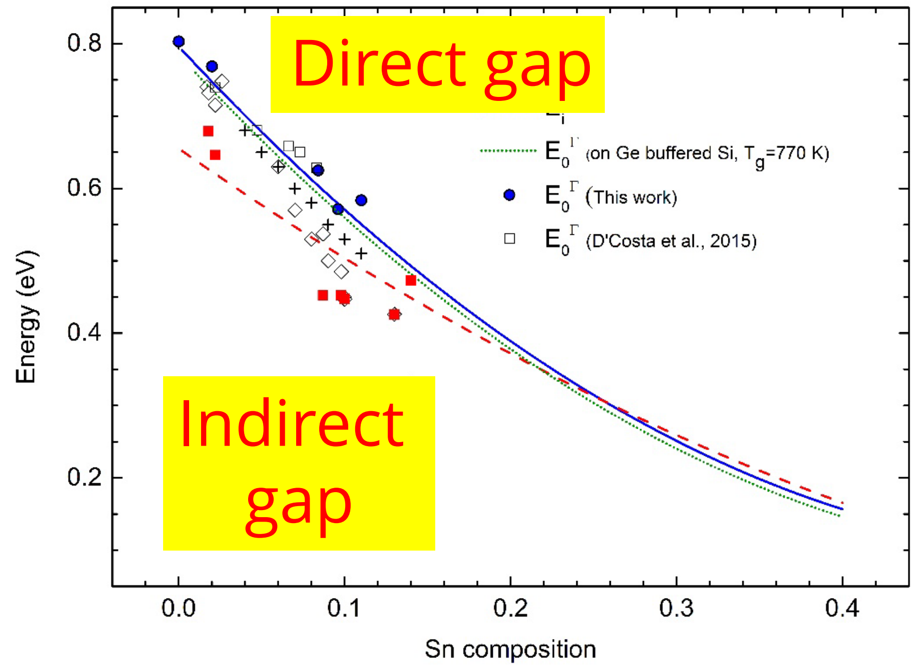


Impact of Sn:

- Redshift
- Broadening
- Increase of Δ_1
- Same theory as temperature effects

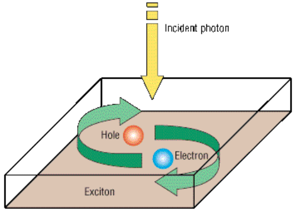
Impact of Composition: Ge-Sn Alloys





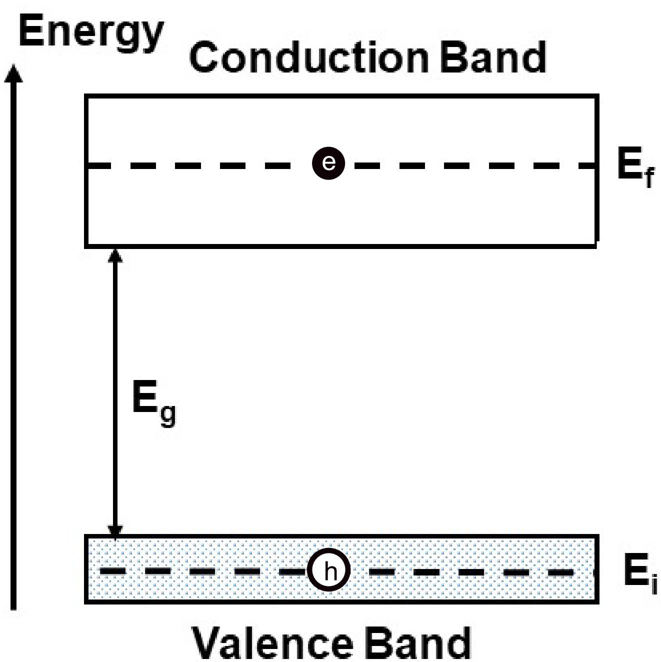
Significant difference between **pseudomorphic** Ge-Sn alloys (grown on Ge) and **relaxed alloys** (grown on Si). Only relaxed Ge-Sn alloys become direct semiconductors (10% Sn).

Nalin Fernando, SZ, Ph.D. thesis (2017).
Nalin Fernando, SZ, JVST B (submitted).



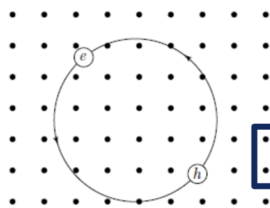
The Concept of an Exciton

Exciton: bound electron – hole pair



Wannier exciton

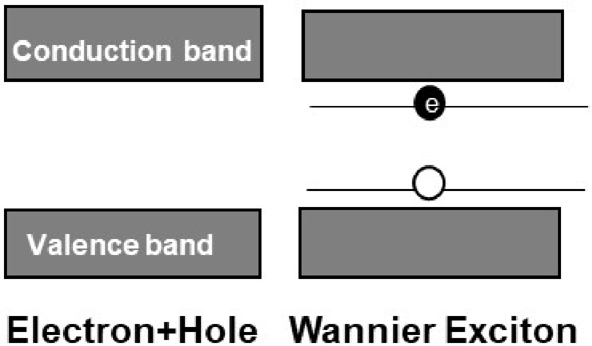
(typical of inorganic semiconductors)



	Excitonic Radius(Å)	Lattice Constant(Å)	Excitonic Binding Energy (meV)
GaAs	130	5.6532	4.2
$SrTiO_3$	62.5	3.9050	20
GaP	50	5.4505	21
ZnO	20	a=3.2500, c=5.2040	60

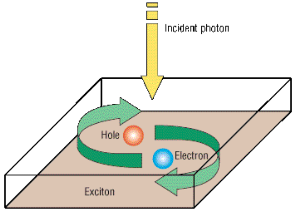
- Large radius (larger than atomic spacing)
- Weakly bound

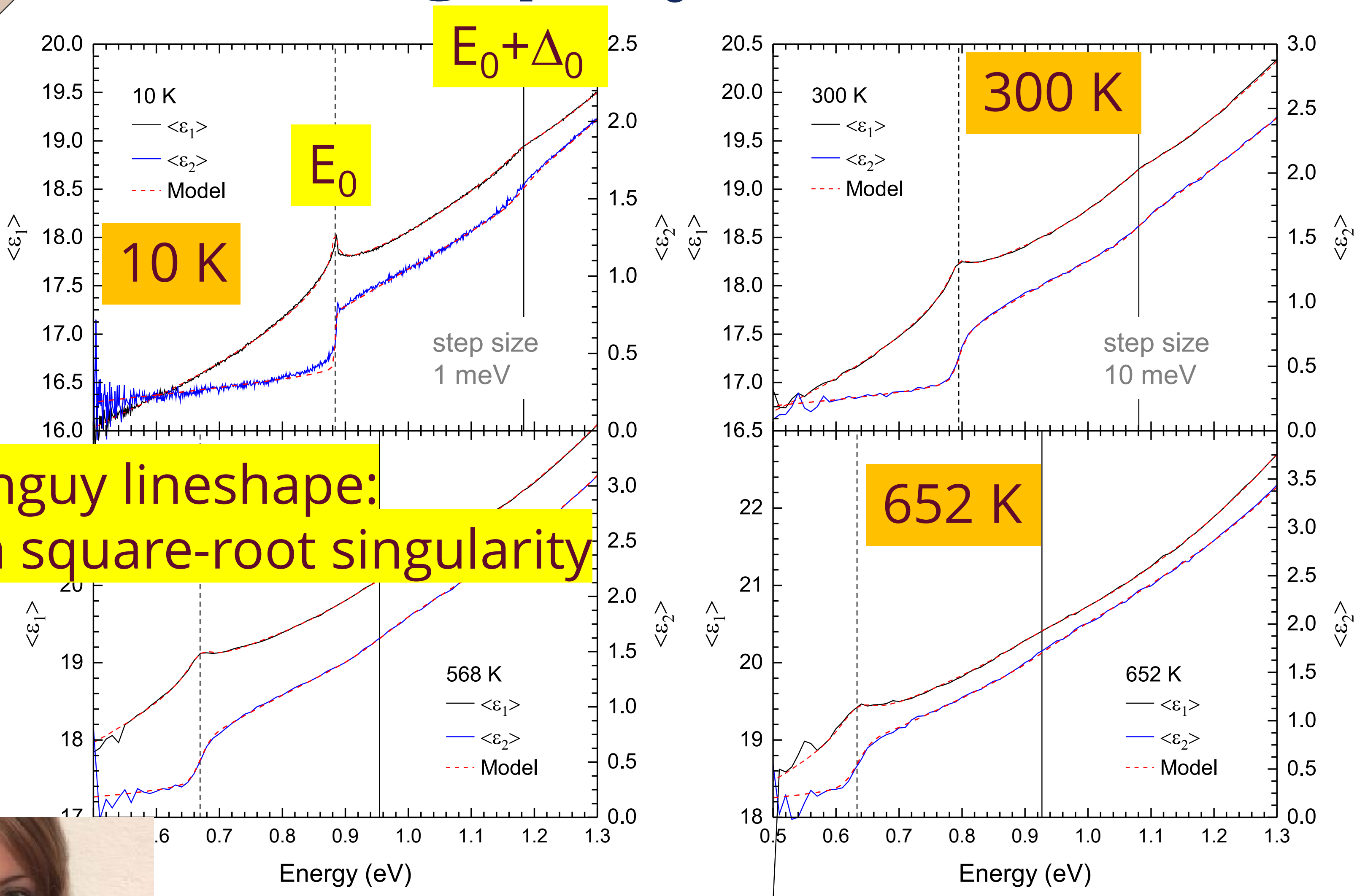
Semiconductor Picture



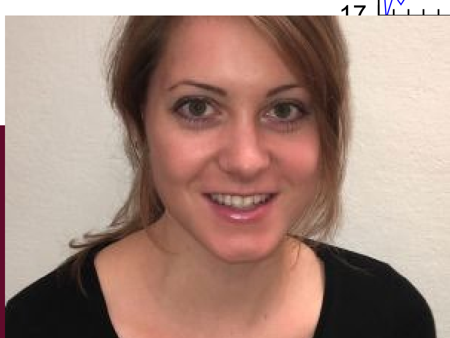
Mark Fox, *Optical Properties of Solids* (Oxford University Press, Oxford, 2010).
S.L. Pyshkin, L. Zv. Zifudin, J. Luminescence **9,** 302 (1974).

Direct gap (E_0) exciton in Ge



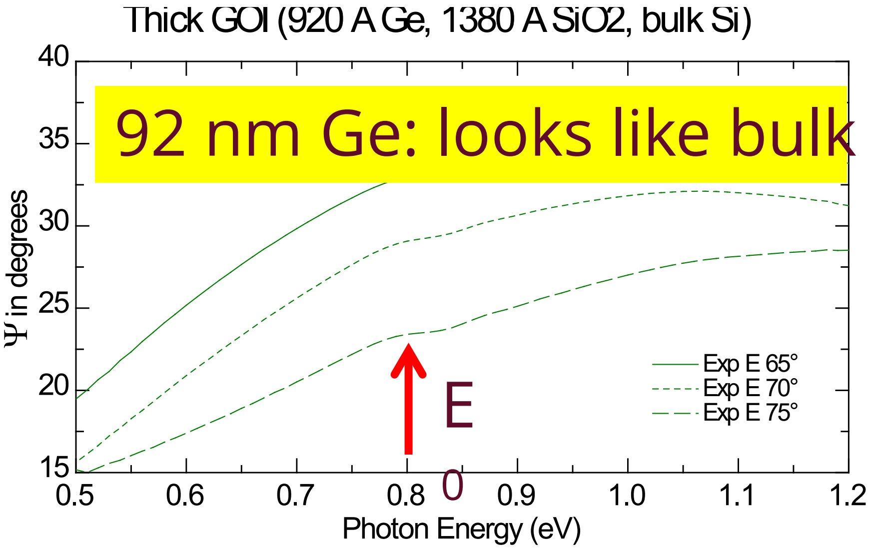


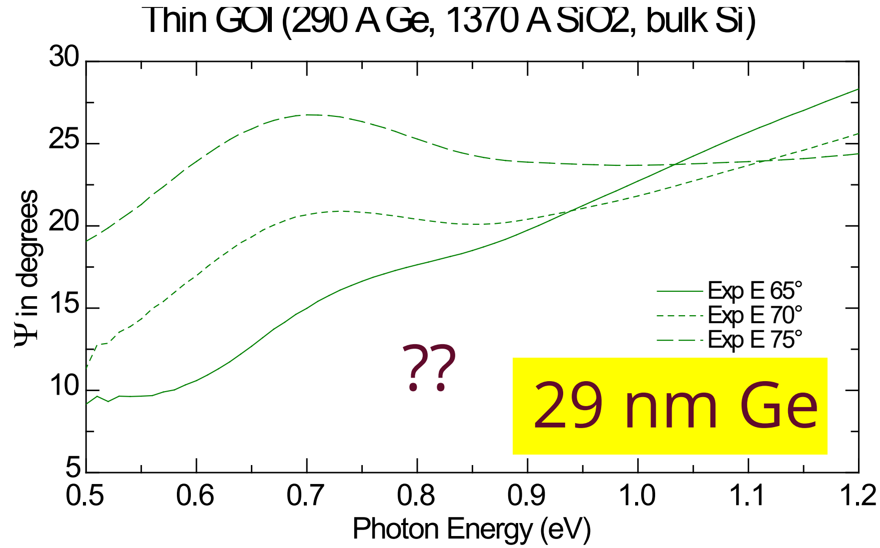
Elliot-Tanguy lineshape:
Far from square-root singularity

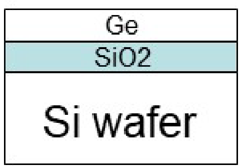


Carola Emminger, MS thesis (Linz)

Impact of Film Thickness: Ge on SiO_2







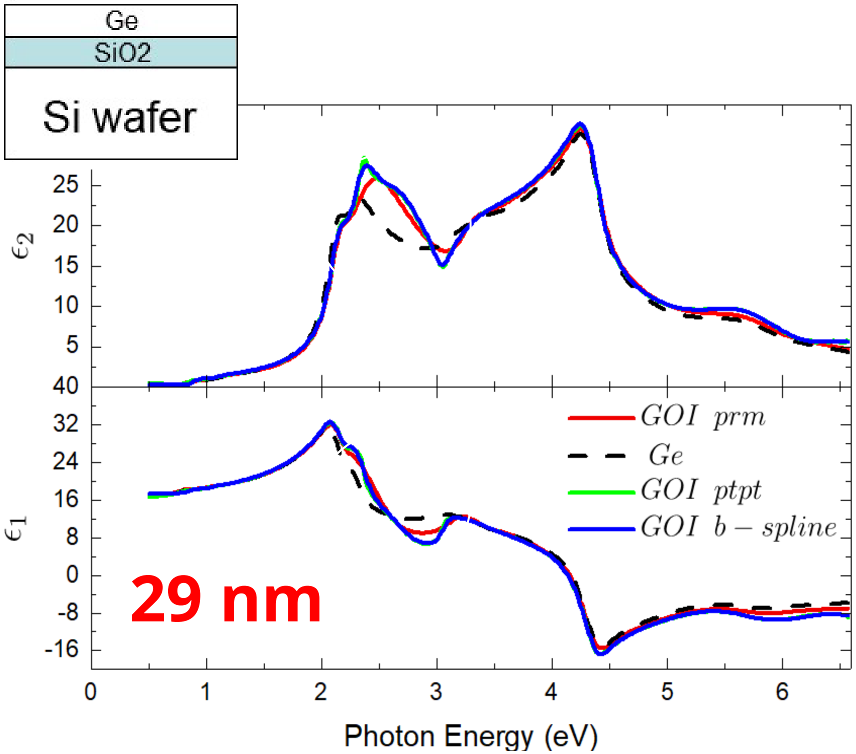
GOI: Ge on insulator, produced by SmartCut process

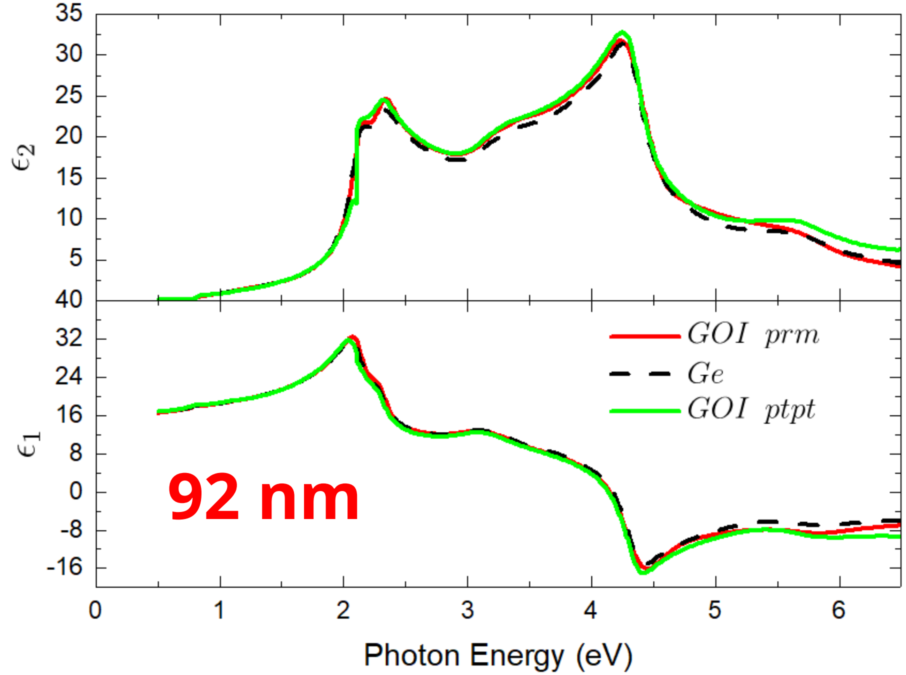
Possible confinement shift of E_0 by 10-30 meV

(very hard to see at 300 K, need low temperature data)

Rigo Carrasco, SZ (unpublished).

Impact of Film Thickness: Ge on SiO_2





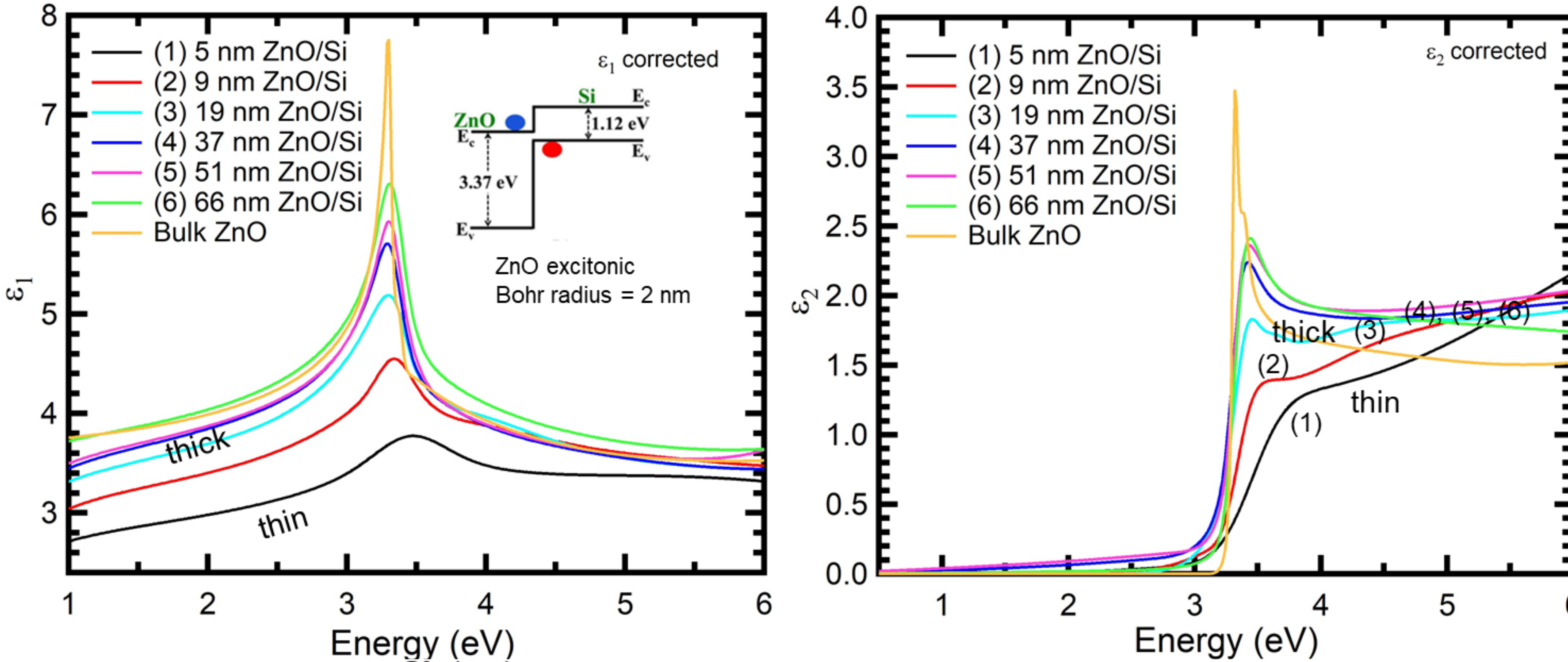
Thin GOI: Blueshift of E_1 and $E_1+\Delta_1$ (about 100 meV)

Thick GOI: Similar to bulk Ge

Observed blueshift (100 meV) in thin GOI hard to explain with strain of confinement

Rigo Carrasco, SZ (APS March 2018).
J. Price and A.C. Diebold, JVST B 24, 2156 (2006)

Impact of Film Thickness: ZnO on Si

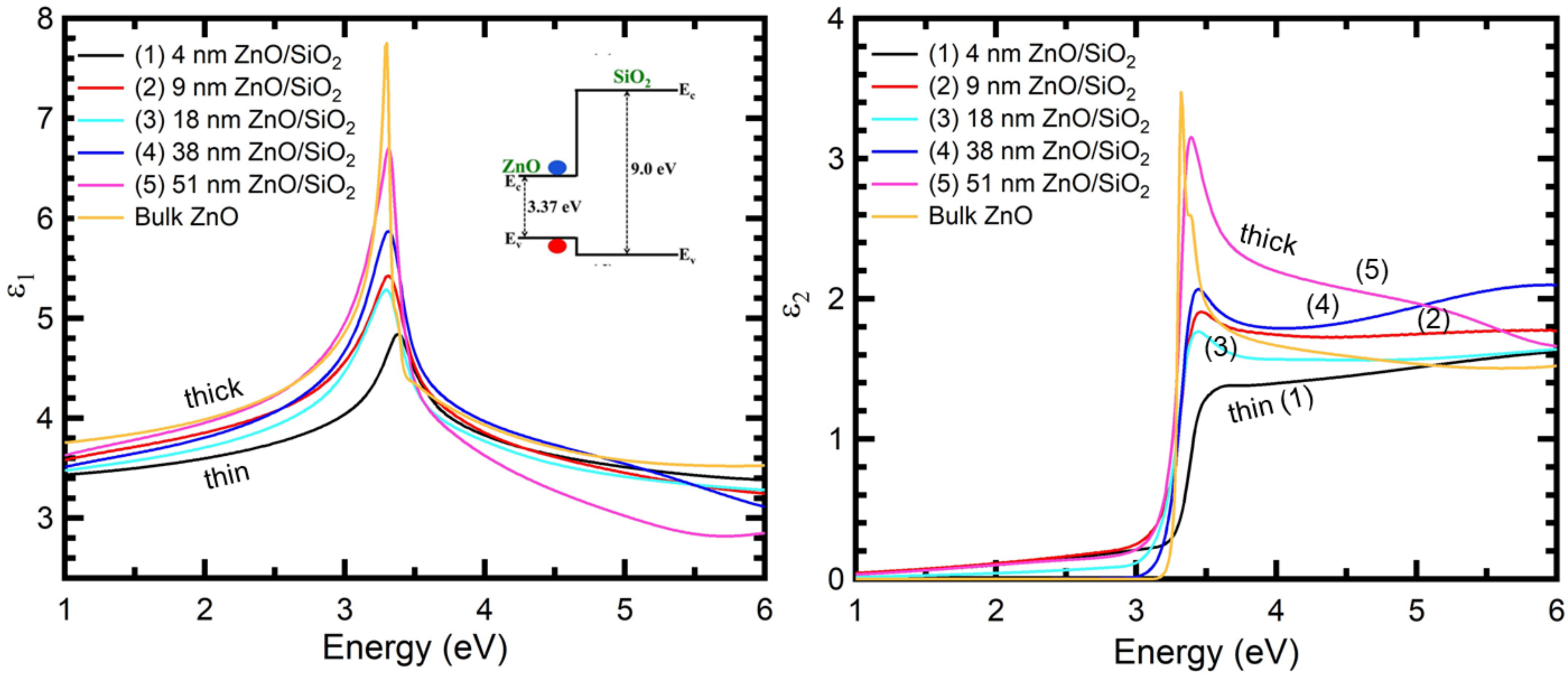


Kramers–Kronig consistent modeling with Tauc-Lorentz oscillators.

- Real and imaginary parts of dielectric function of ZnO layers on Si decrease monotonically with decreasing thickness.

N. Samarasingha, SZ (DPG 2018).

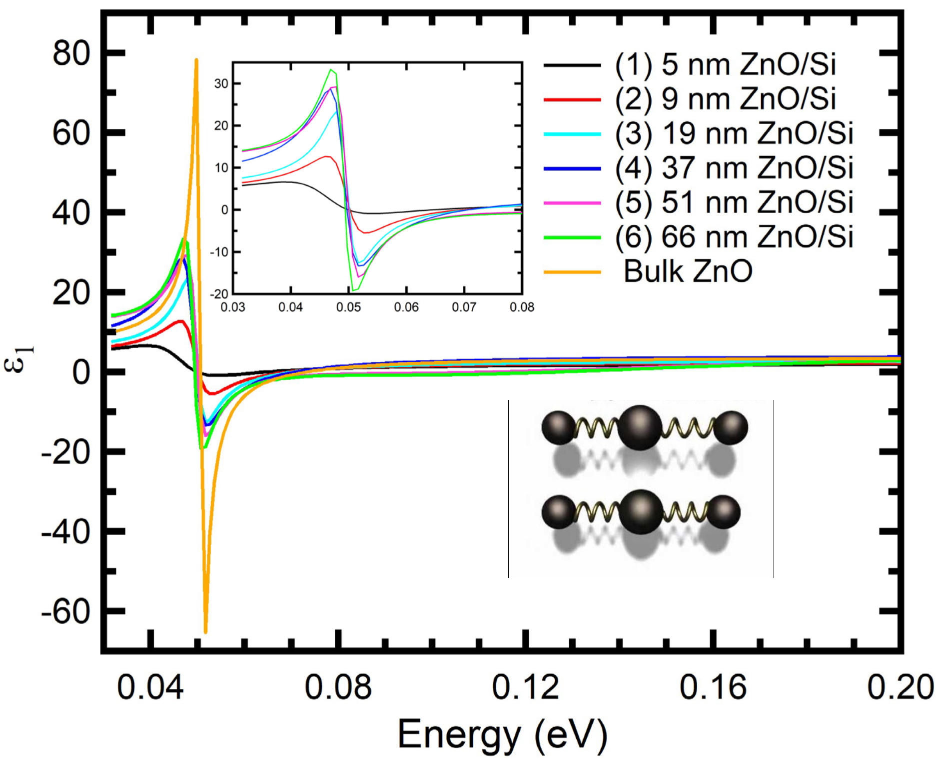
Impact of Thickness: ZnO on SiO_2

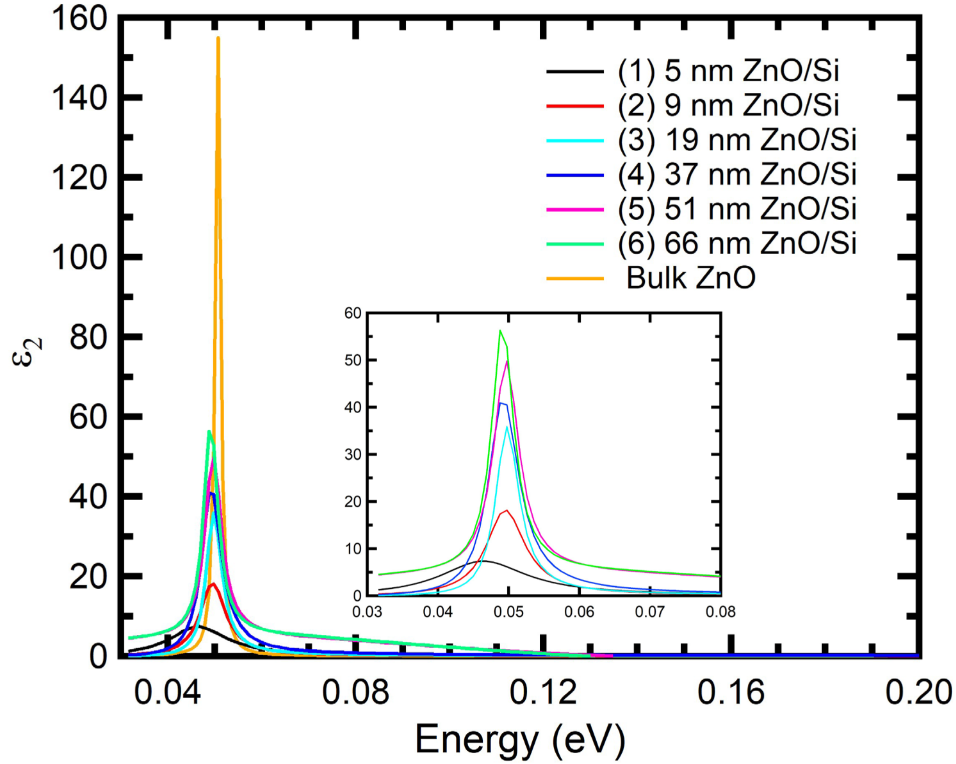


- Real and imaginary parts of dielectric function of ZnO layers on SiO_2 also decrease monotonically with decreasing thickness.
- Explanation: Exciton dephasing at type-II quantum well interface.

N. Samarasingha, SZ (DPG 2018).

Lattice vibrations in thin ZnO on Si





- TO absorption in thin films is broader and redshifts.
- Explanation: Damping of oscillations, if thickness below mean free path

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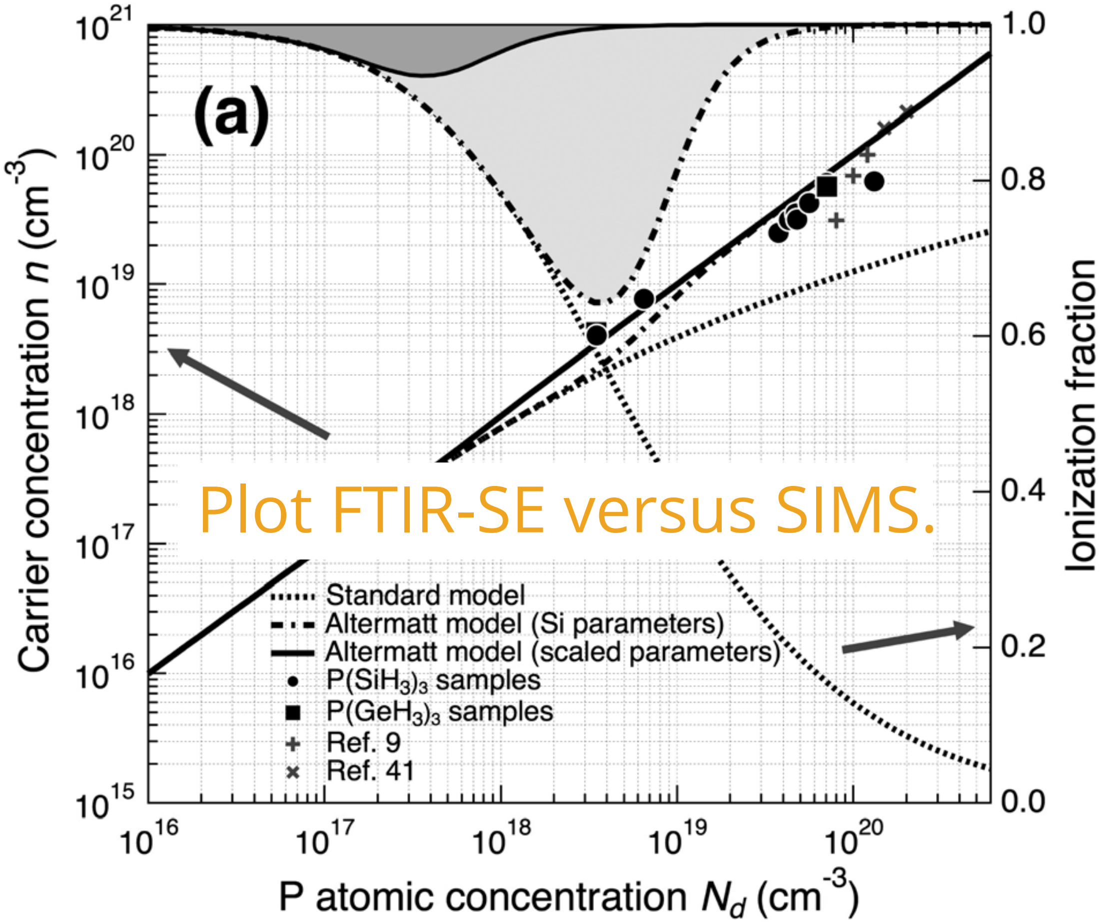
N. Samarasingha, SZ (DPG 2018).

Impact of Doping

- **Doping:** Impurities plus free carriers
- **Dopant activation:** How many impurities are ionized, produce free carriers?
- **Impurities:**
  - Impurity (alloy) scattering due to lattice potential disorder
  - *Compensation doping (electrons plus holes)*
  - Strain effects if atomic radii of impurity and host differ
- **Free carrier effects:**
  - Drude response
  - Band gap renormalization (BGR)
  - Band gap filling or Pauli blocking
  - Burstein-Moss shift
  - **Reduction of excitonic effects**
- **Photoexcitation:** Equal number of electrons and holes add to existing carriers (from doping)

Dopant Activation (Ge:P)



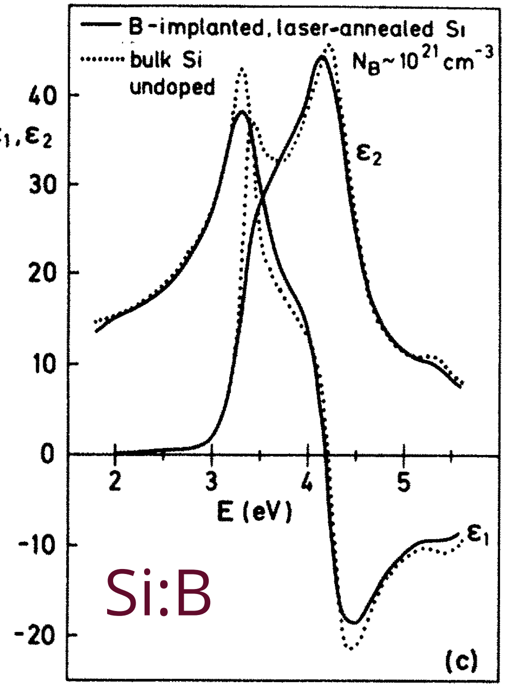
Nearly complete donor ionization is possible in Ge:P, as long as all donors are in substitutional lattice sites (avoid donor clusters and interstitial donor atoms).

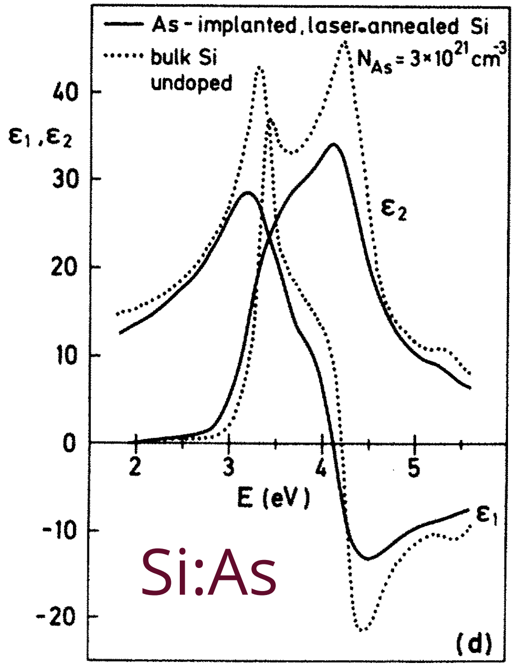
Ionization fraction only depends on quality of samples.

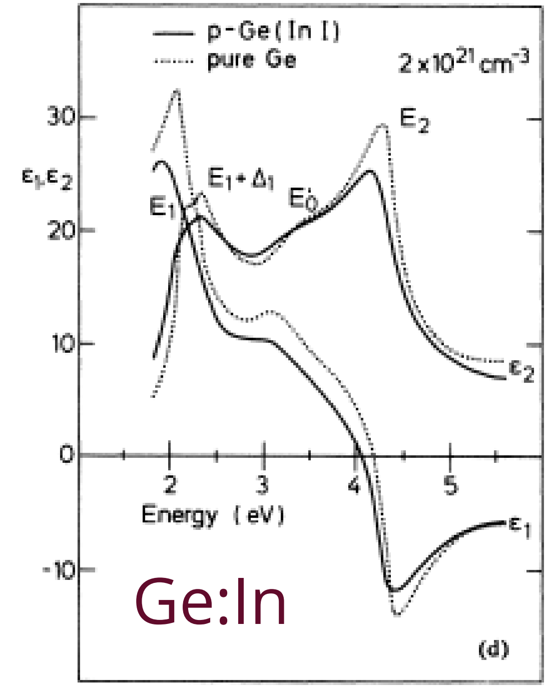
In situ doping methods preferred.

C. Xu, C.L. Senaratne, J. Kouvetakis, and J. Menendez, APL 105, 232103 (2014)

Highly doped Si and Ge







E_1 Exciton weakened

E_1 Exciton weakened
Broadening

Broadening
No amplitude reduction

E_1 excitonic enhancement strong in Si, weak in Ge.

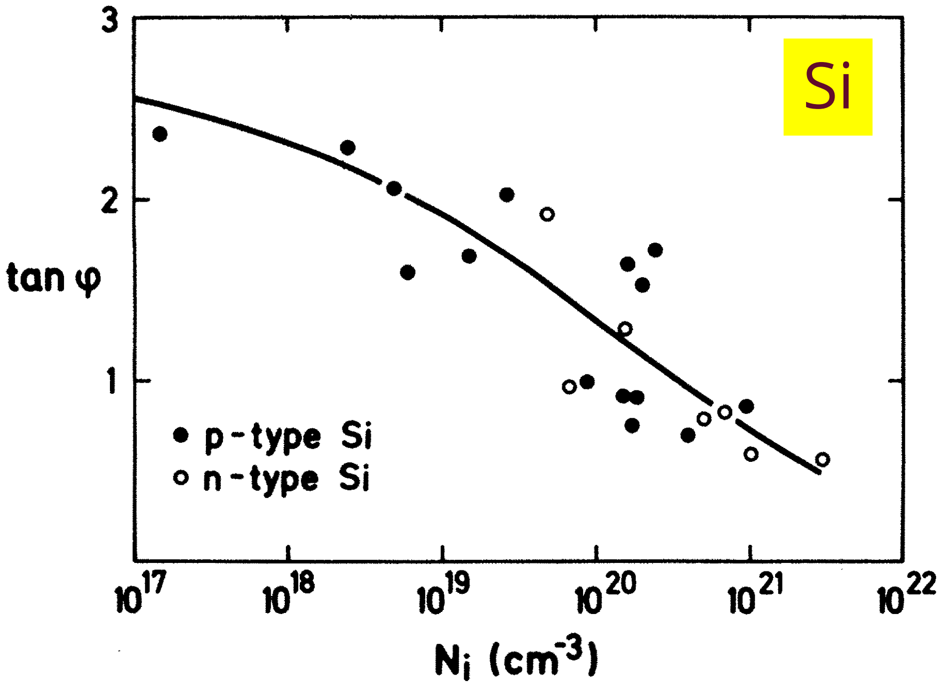
Viña and Cardona, PRB, 1984 and 1986

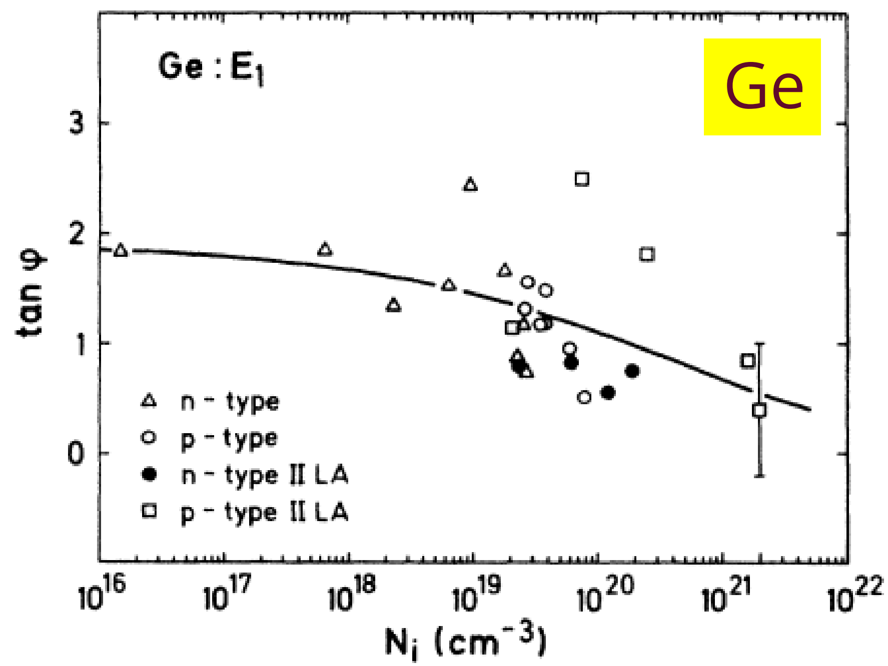
Excitonic Effects (doping)

- In some semiconductors, strong excitonic contributions to the E_1 and $E_1+\Delta_1$ critical points.
- **Si and GaAs: Strong E_1 excitons; Ge: Weak E_1 excitons.**
- Si: Strong dephasing at 6E20 P doping, when the Thomas-Fermi screening length (0.5 nm) is smaller than the excitonic radius (3 nm).
- Si: **Strong reduction of E_1 amplitude, but no shift.**
- Ge: Not much amplitude reduction (band filling), but redshift and broadening due to impurities.
- Excitonic screening changes the E_1 **phase angle** (Si, Ge, alloys) due to impurities and alloy disorder.
- Compare Raman scattering in doped Ge at E_1 resonance.

Excitonic Effects: E_1 phase angle

- Excitonic screening changes the E_1 phase angle (Si, Ge, alloys) due to impurities and alloy disorder.

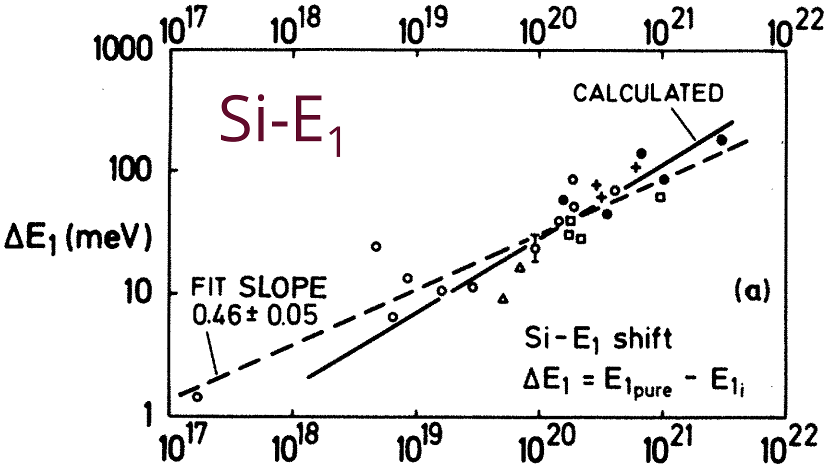


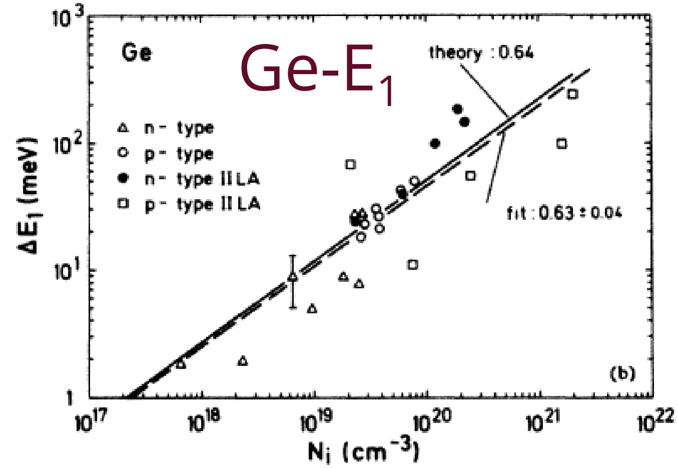


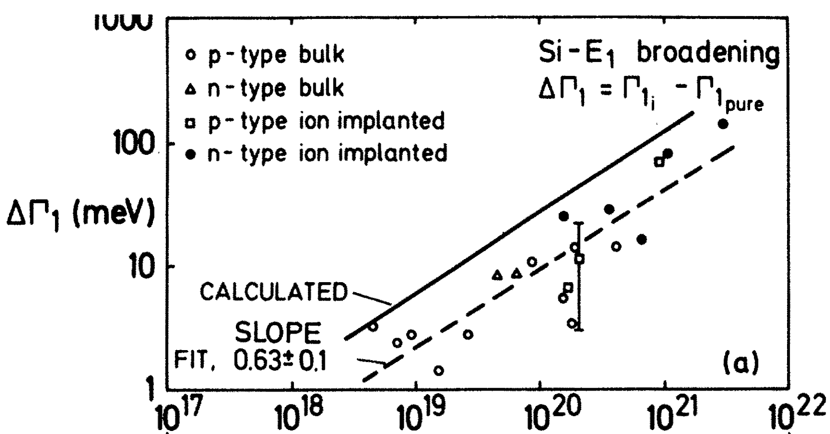
Similar reduction in E_1 phase angle for Si and Ge.

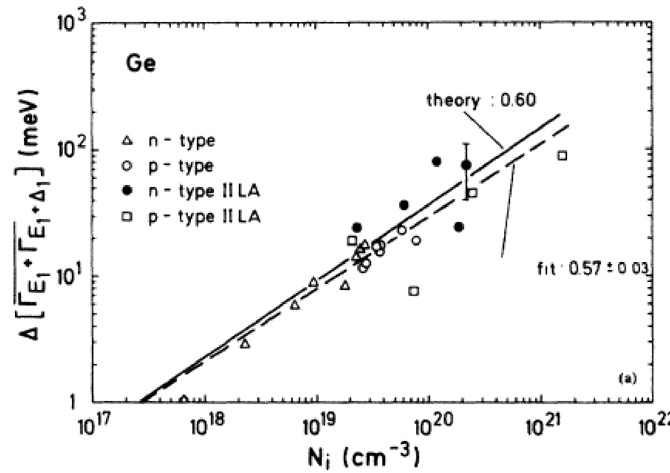
Vina and Cardona, PRB, 1984 and 1986

Impurity Scattering: Si and Ge







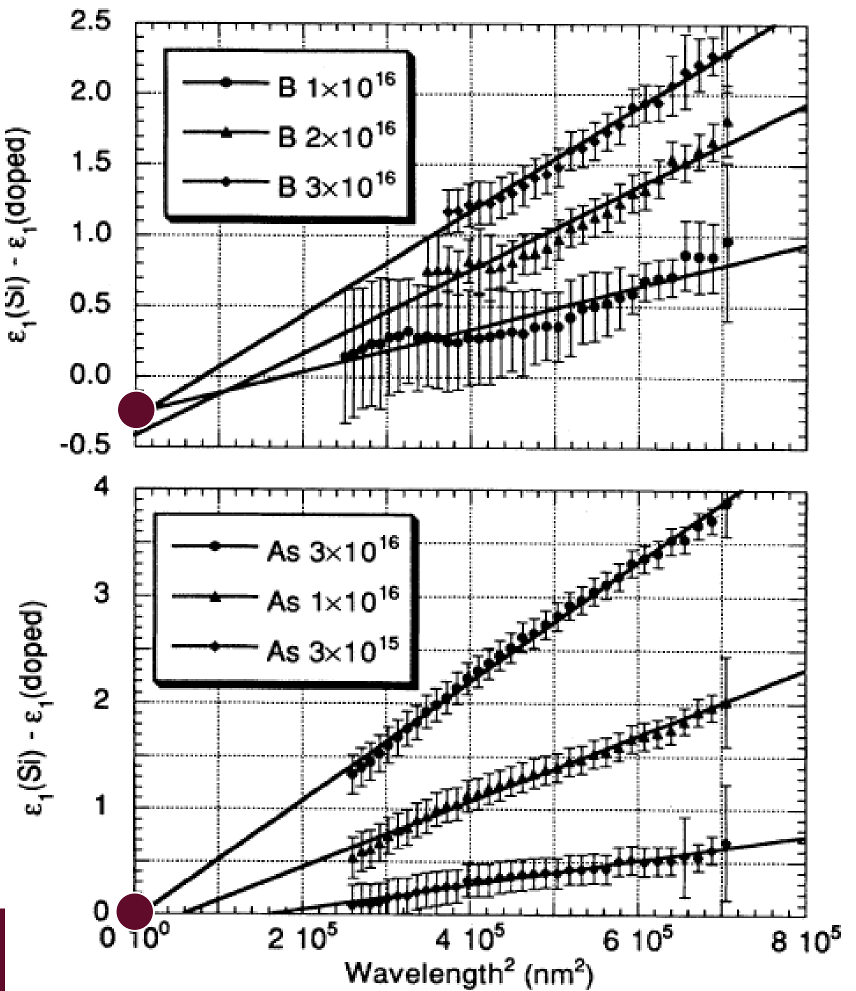


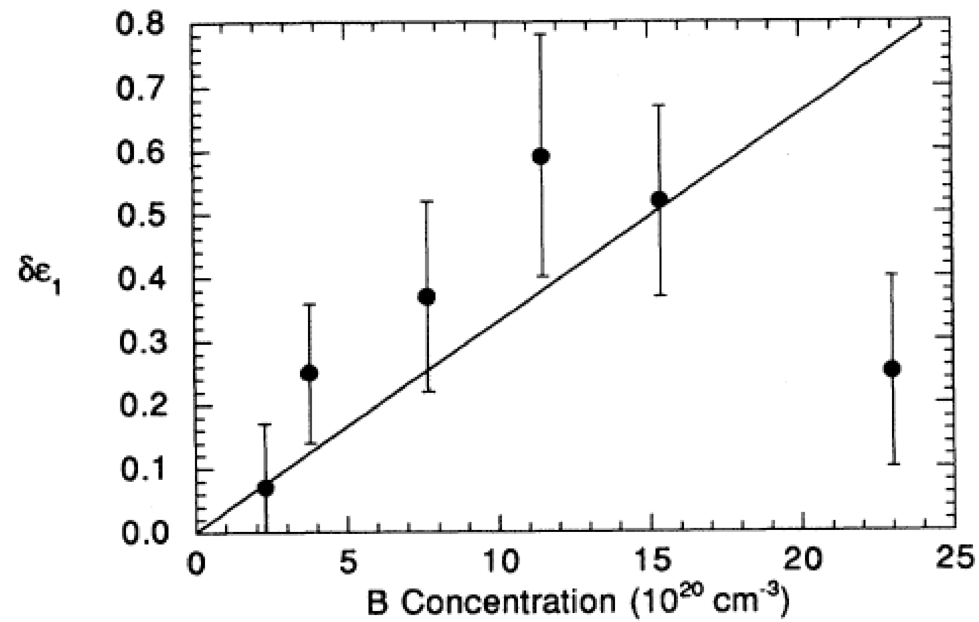
Static Disorder (alloy scattering):
Similar redshift and broadening as with temperature.

Vina and Cardona, PRB, 1984 and 1986

Strain Effects in doped Si

- Measurable if atomic radii of impurity and host differ





Boron doping 2.3E21 cm^{-3}

Out-of-plain strain $\varepsilon_{\perp}$=1.1%

ε_1 changes (piezo-optic coefficients)

G.E. Jellison, Jr., et al., PRB **52**, 14607 (1995).
P. Etchegoin, J. Kircher, M. Cardona, PRB **47**, 10292 (1993).

Strain Effects in doped Ge

Covalent atomic radii (Phillips)

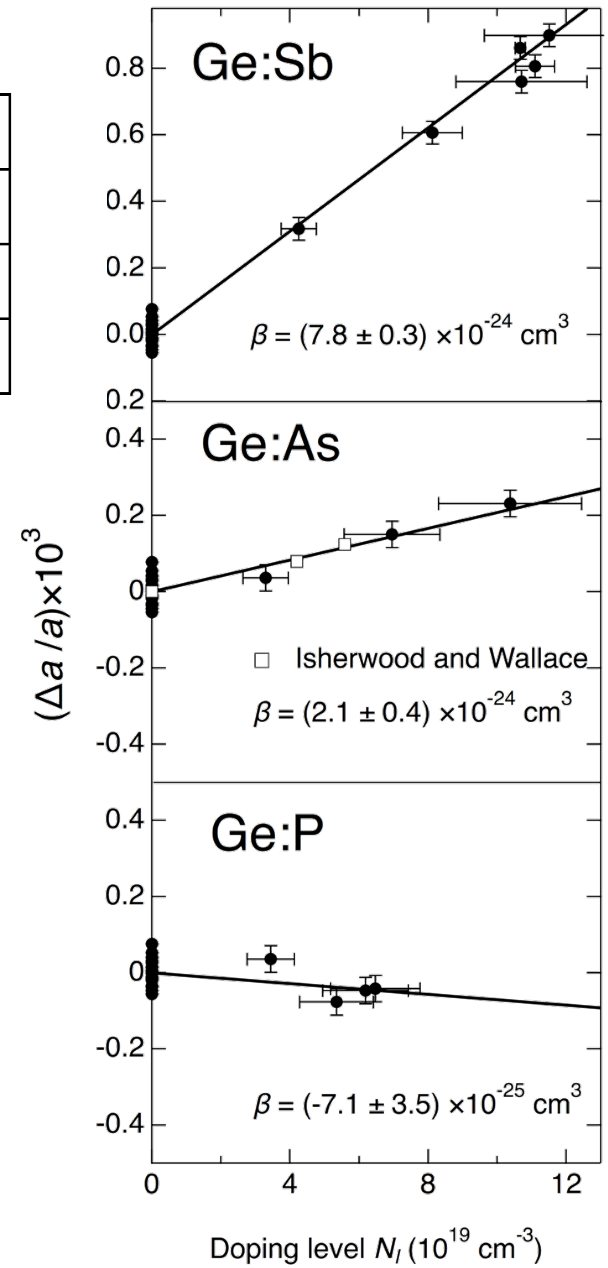
B 0.853	C 0.744	N 0.719
Al 1.230	Si 1.173	P 1.128
Ga 1.225	Ge 1.225	As 1.225
In 1.405	Sn 1.405	Sb 1.405

$$\beta_{\mathrm{P}}^{\mathrm{Ge}} = \left(\frac{2}{4.418\times10^{22}\ \mathrm{cm}^{-3}}\right)\left(\frac{1.128-1.225}{1.225}\right) =$$

$$= 4.527\times10^{-23}\ \mathrm{cm}^3 \times \left(-0.0791\right) = -3.58\times10^{-24}\ \mathrm{cm}^3$$

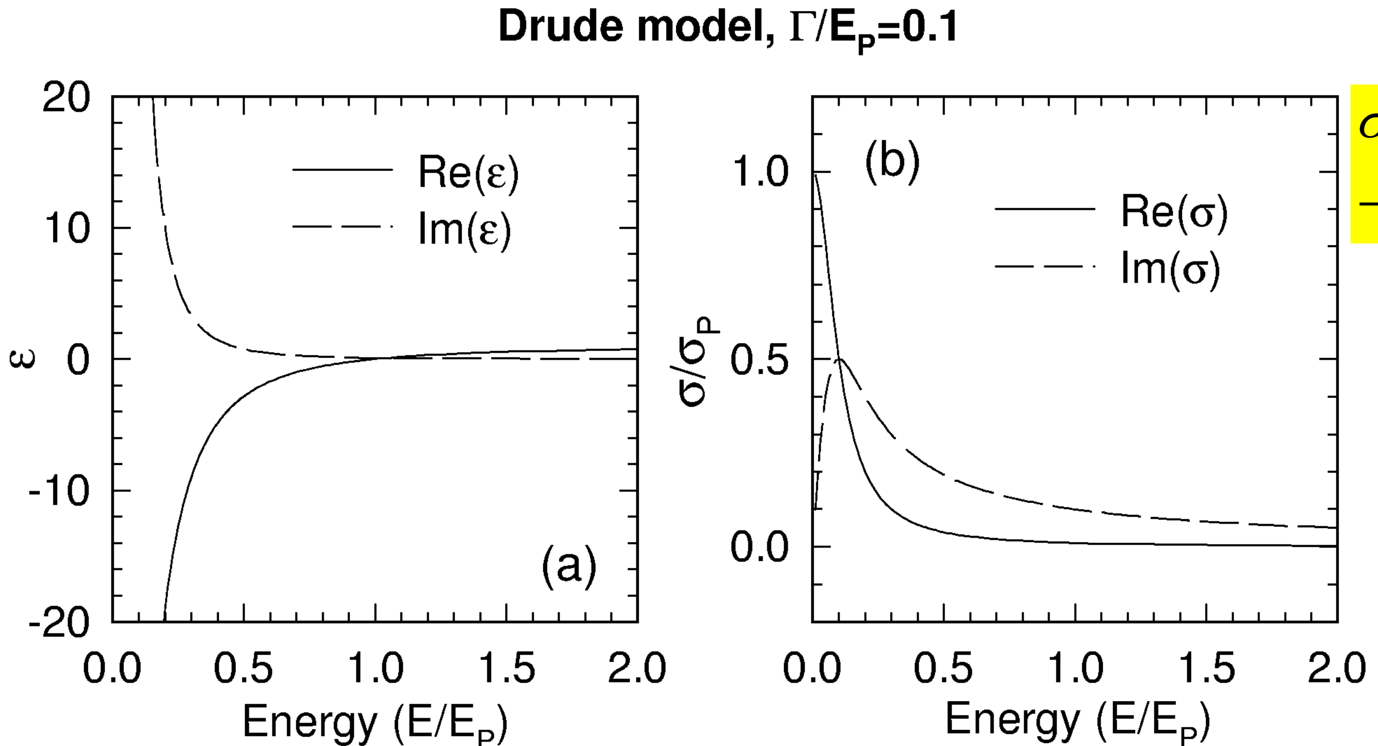
$$\beta_{\mathrm{As}}^{\mathrm{Ge}} = 4.527\times10^{-23}\ \mathrm{cm}^3 \times \left(\frac{1.225-1.225}{1.225}\right) = 0\ \mathrm{cm}^3$$

$$\beta_{\mathrm{Sb}}^{\mathrm{Ge}} = 4.527\times10^{-23}\ \mathrm{cm}^3 \times \left(\frac{1.405-1.225}{1.225}\right) = 6.65\times10^{-24}\ \mathrm{cm}^3$$



J. Menendez (ASU)

Drude Model for Metals



$$\sigma_1 = E\varepsilon_0\varepsilon_2$$

$$-\sigma_2 = (1-\varepsilon_1)E\varepsilon_0$$

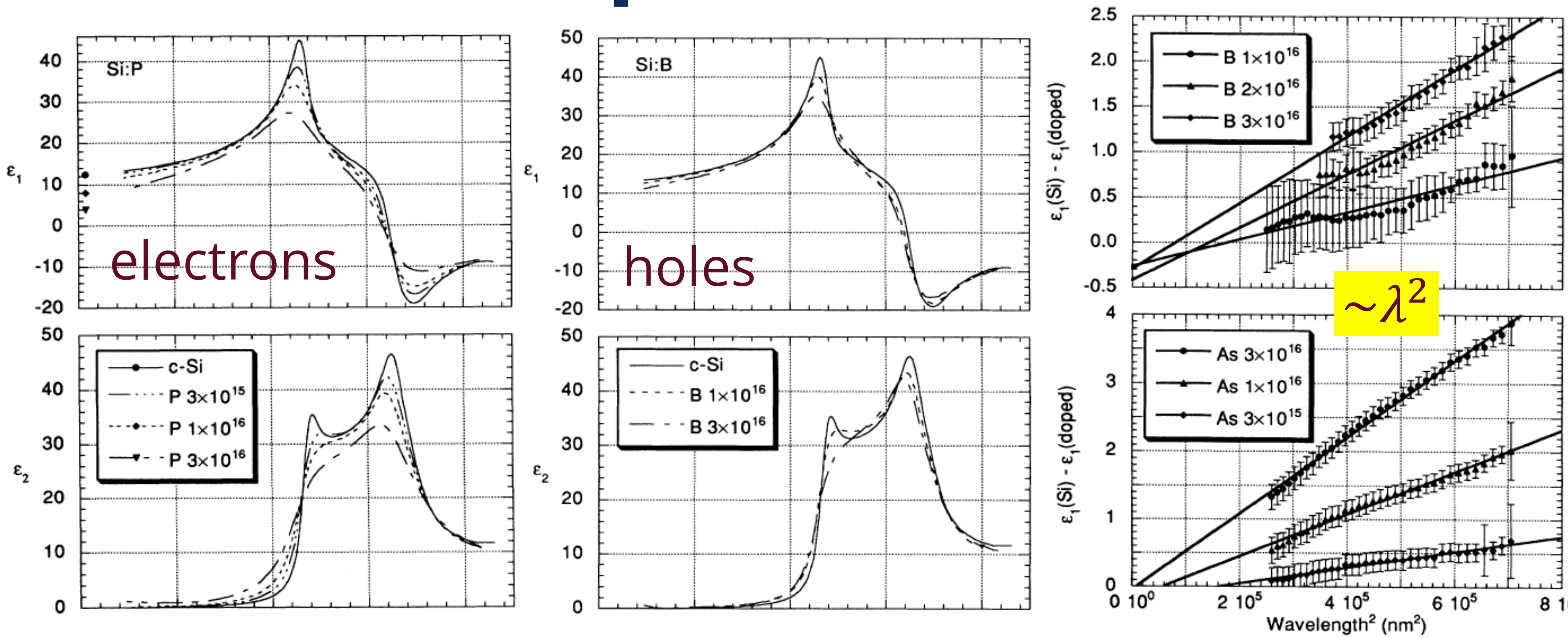
$$\Delta\varepsilon(E) = -\frac{E_P^2}{E^2+\Gamma^2} + i\,\frac{E_P^2}{E^2+\Gamma^2} \times \frac{\Gamma}{E}$$

$$E_P^2 = \frac{\hbar^2 ne^2}{m\varepsilon_0}$$

$\Delta\varepsilon$ proportional to λ^2 for small Γ (slope n/m).
Only $\Delta\varepsilon_1$ measurable for small Γ.

H. Fujiwara and M. Kondo, PRB **71**, 075109 (2005)

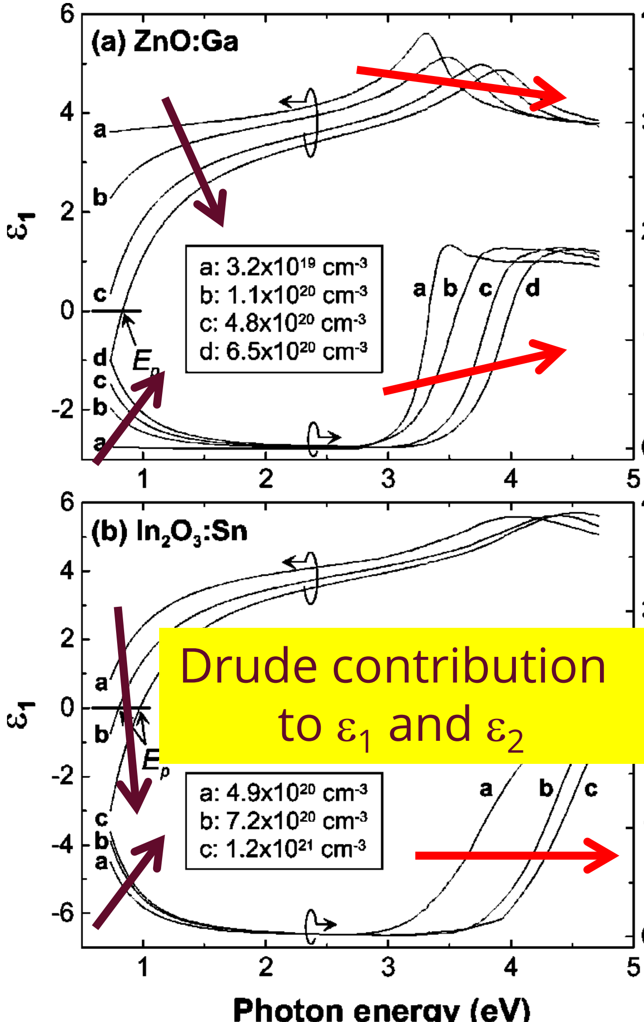
Drude Response for doped Si



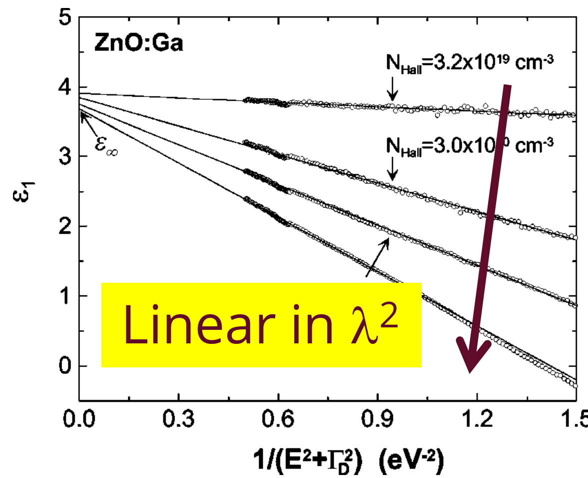
Clear reduction of ε_1 below the direct gap due to free carriers.
Change in ε_2 is due to impurity scattering, not free carriers.
Electrons contribute more than holes (smaller mass).
Doping with P and As has similar results (not shown).

G.E. Jellison, Jr., et al., PRB **52**, 14607 (1995).

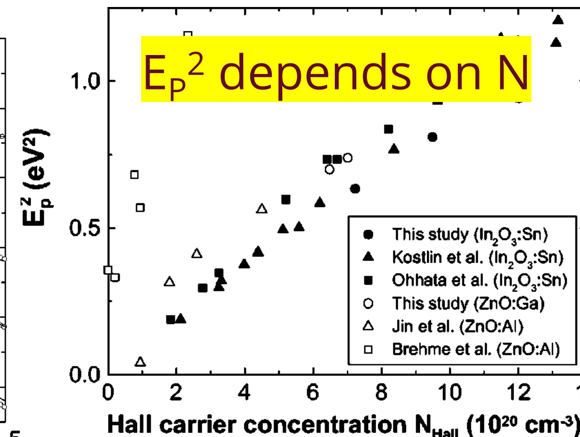
Drude Response for doped ZnO and ITO



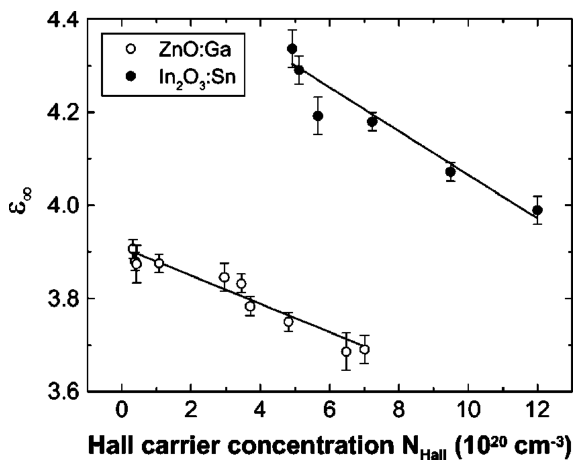
Drude contribution to ε_1 and ε_2



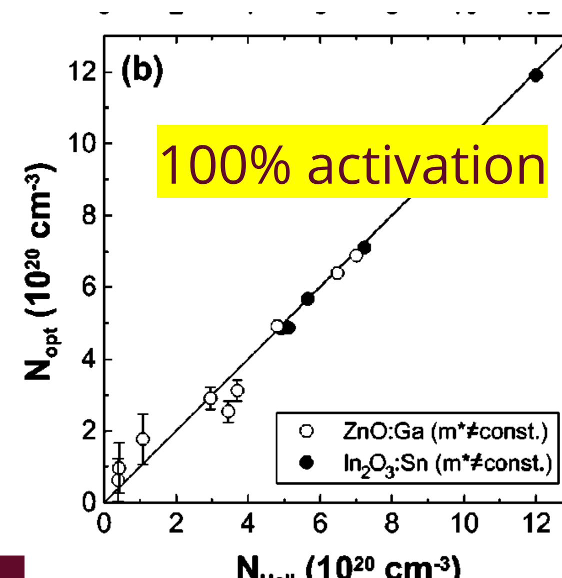
Linear in λ^2



E_P^2 depends on N



Linear in n

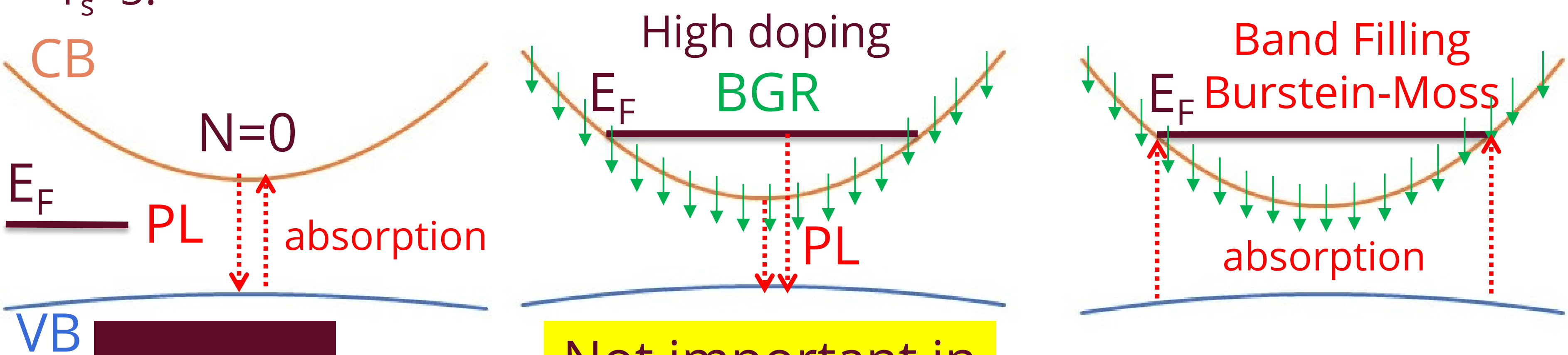


100% activation

H. Fujiwara and M. Kondo, PRB **71**, 075109 (2005)

Many-Body Effects

- **Band gap renormalization** (BGR)
  - Band gap is lowered at high carrier density
  - Measurable with photoluminescence
- **Band filling** or **Pauli blocking**
  - Band filling affects absorption measurements
- **Burstein-Moss shift**
  - Absorption threshold affected by both BGR and band filling
- **Mott transition:** Individual excitons versus electron-hole liquid (EHL) at r_s~5.

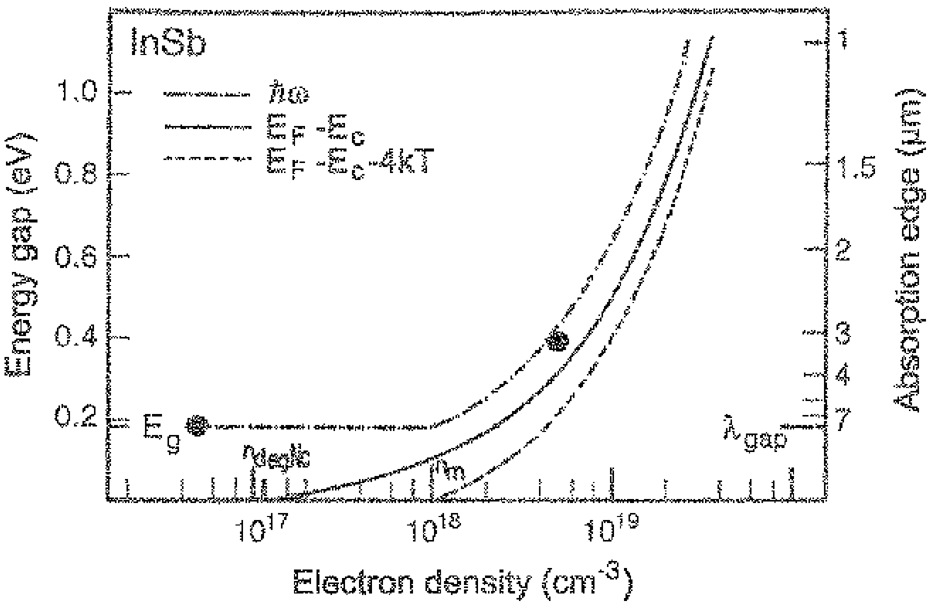


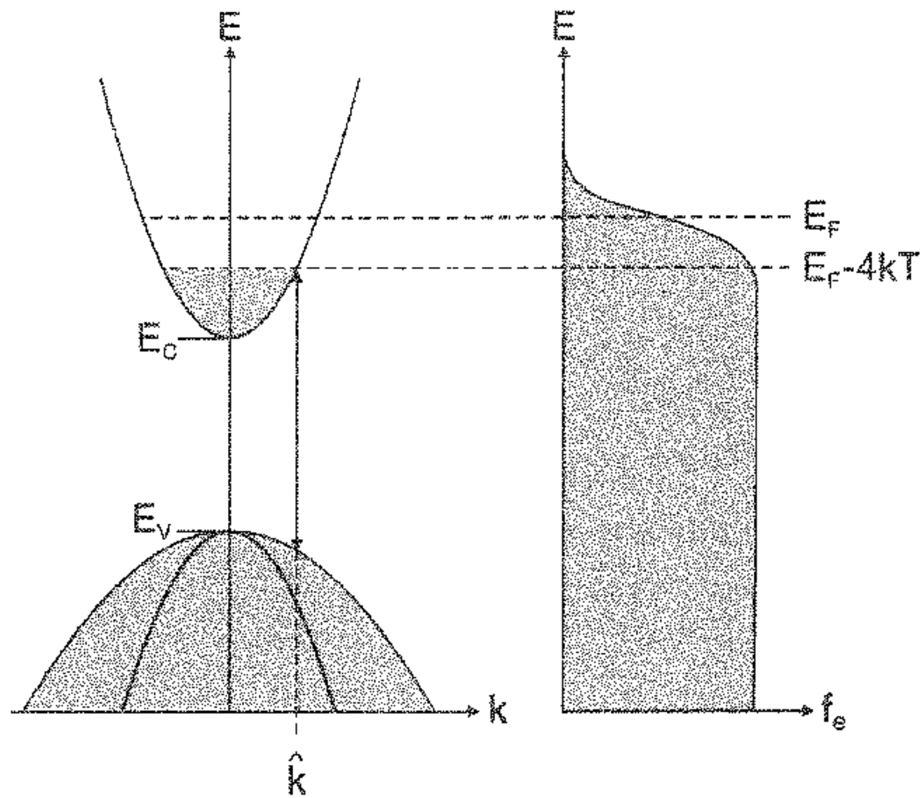
Not important in ellipsometry

Band gap filling

- Filled electron and hole states reduce absorption probability by a factor **$1\text{-}f_e\text{-}f_h$**, where f is the population of the state.
- Also known as **Pauli blocking**.
- Bleaches the absorption, spectral hole burning.
- Purely quantum mechanical effect (Fermi statistics).

Burstein-Moss Shift: n-type InSb



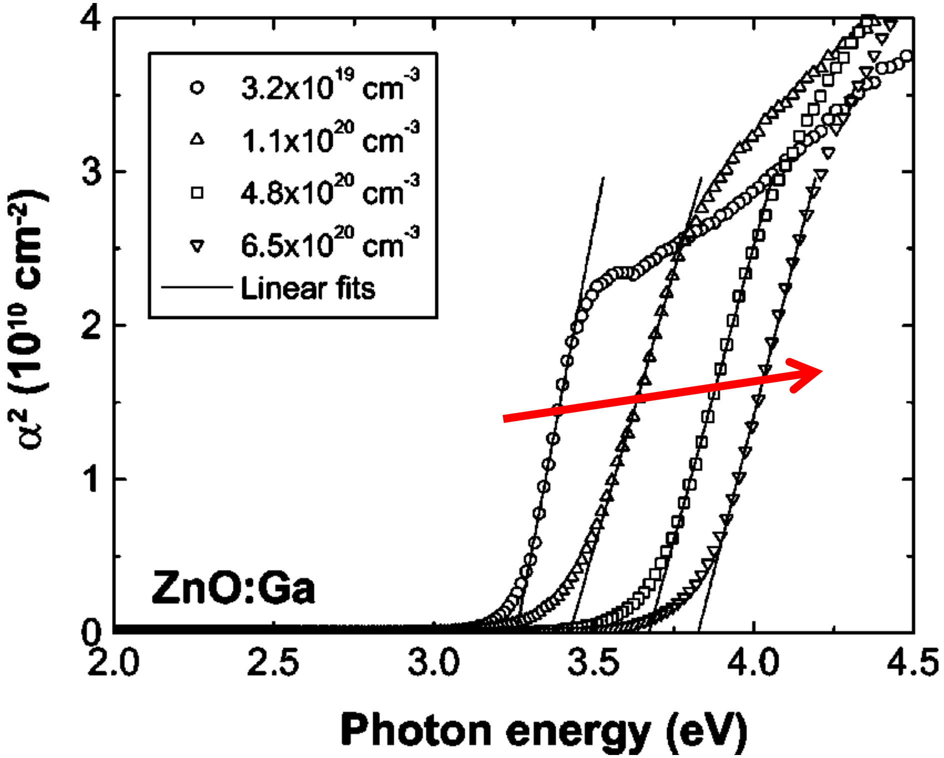


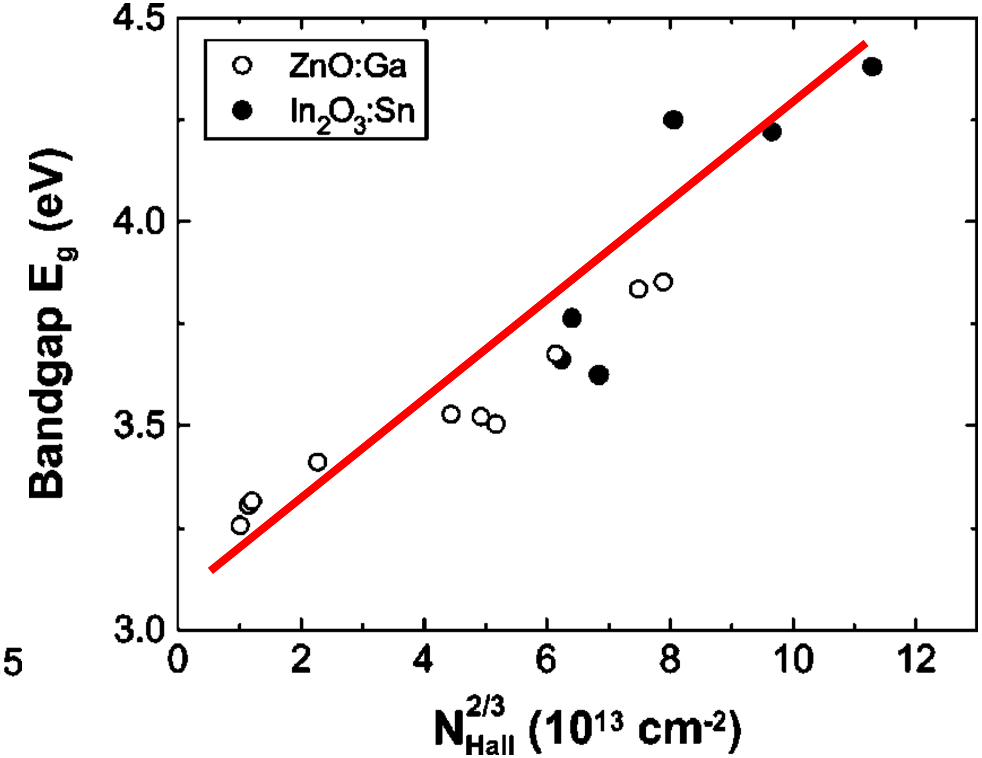
Absorption threshold increases, because CB bottom is filled with electrons (Pauli blocking).

$$\Delta E = (E_F - 4kT - E_{CB})\left(1 + \frac{m_e}{m_h}\right) \approx \frac{h^2}{8m_r} n^{2/3}$$

E. Burstein, Phys. Rev. **93**, 632 (1954).
T.S. Moss, Proc. Phys. Soc. (London) B **67**, 775 (1954).
M. Grundmann, *The Physics of Semiconductors*

Burstein-Moss Shift in ZnO and ITO

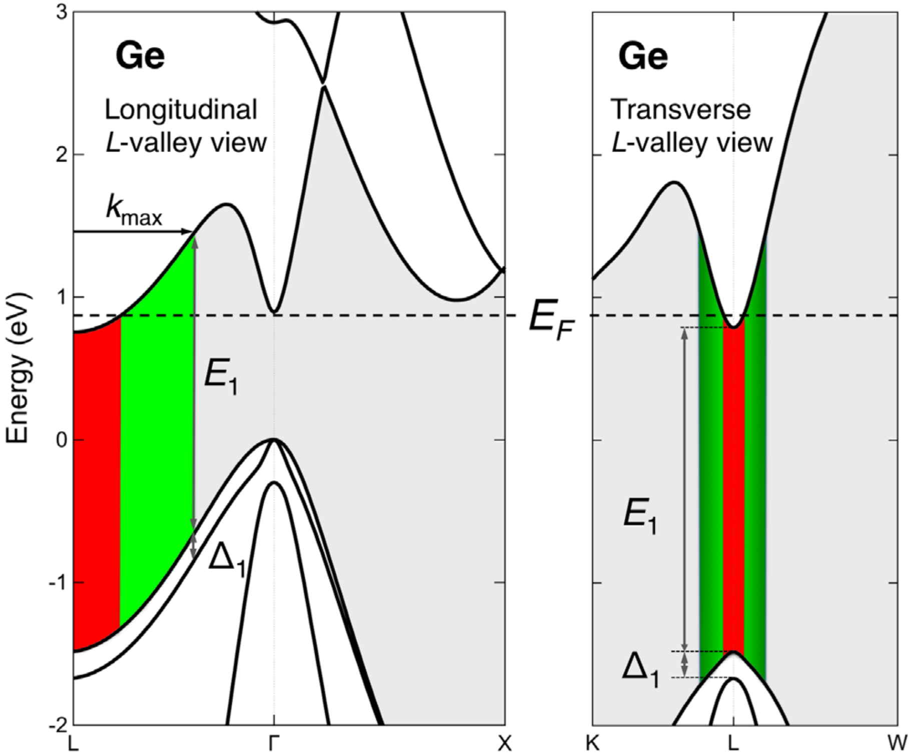




Band gap **increases** with increasing dopant concentration.
Band gap renormalization (decrease) PLUS band filling (increase
Shift is proportional to $n^{2/3}$ (many-body effect).

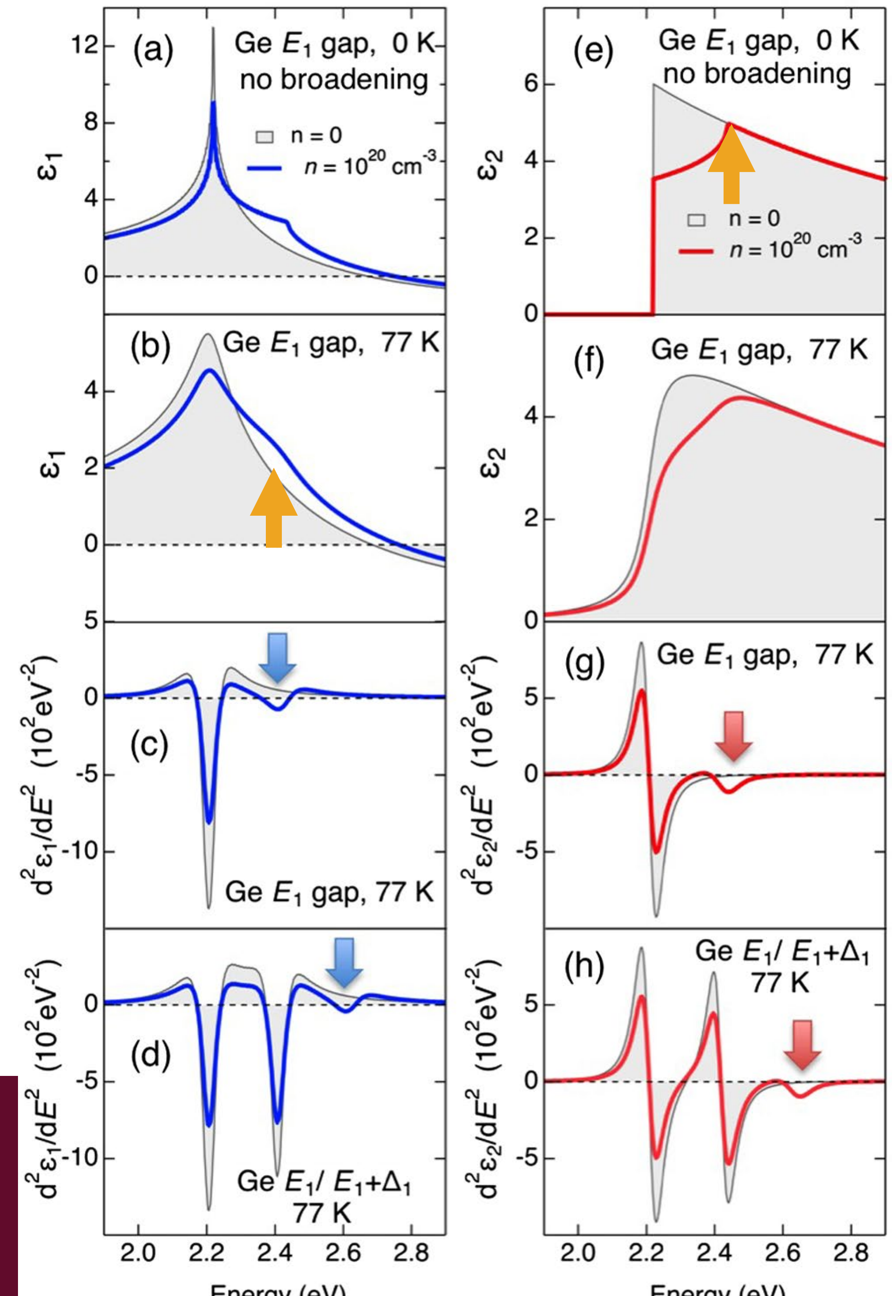
H. Fujiwara and M. Kondo, PRB **71**, 075109 (2005)

E_1 gap in highly doped Ge:P



$$\varepsilon_2(E) = \frac{8e^2\bar{P}^2\mu_\perp}{3m^2E^2} H(E-E_1) \times$$

$$\times \int_{-k_{max}}^{k_{max}} dk_z \{1 - f[E_c(E,k_z^2)]\}$$



Phase-filling singularity

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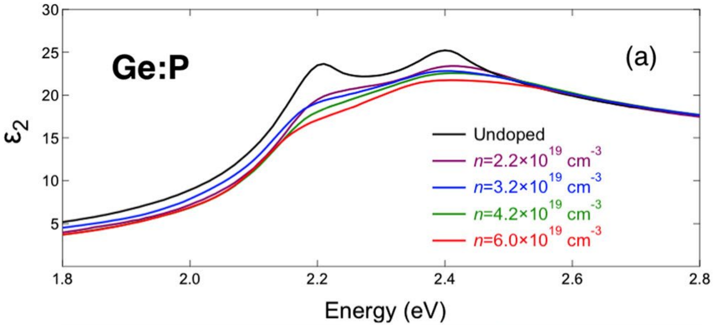
C. Xu, NF, SZ, JK, J. Menendez, PRL **118**, 267402 (2017)

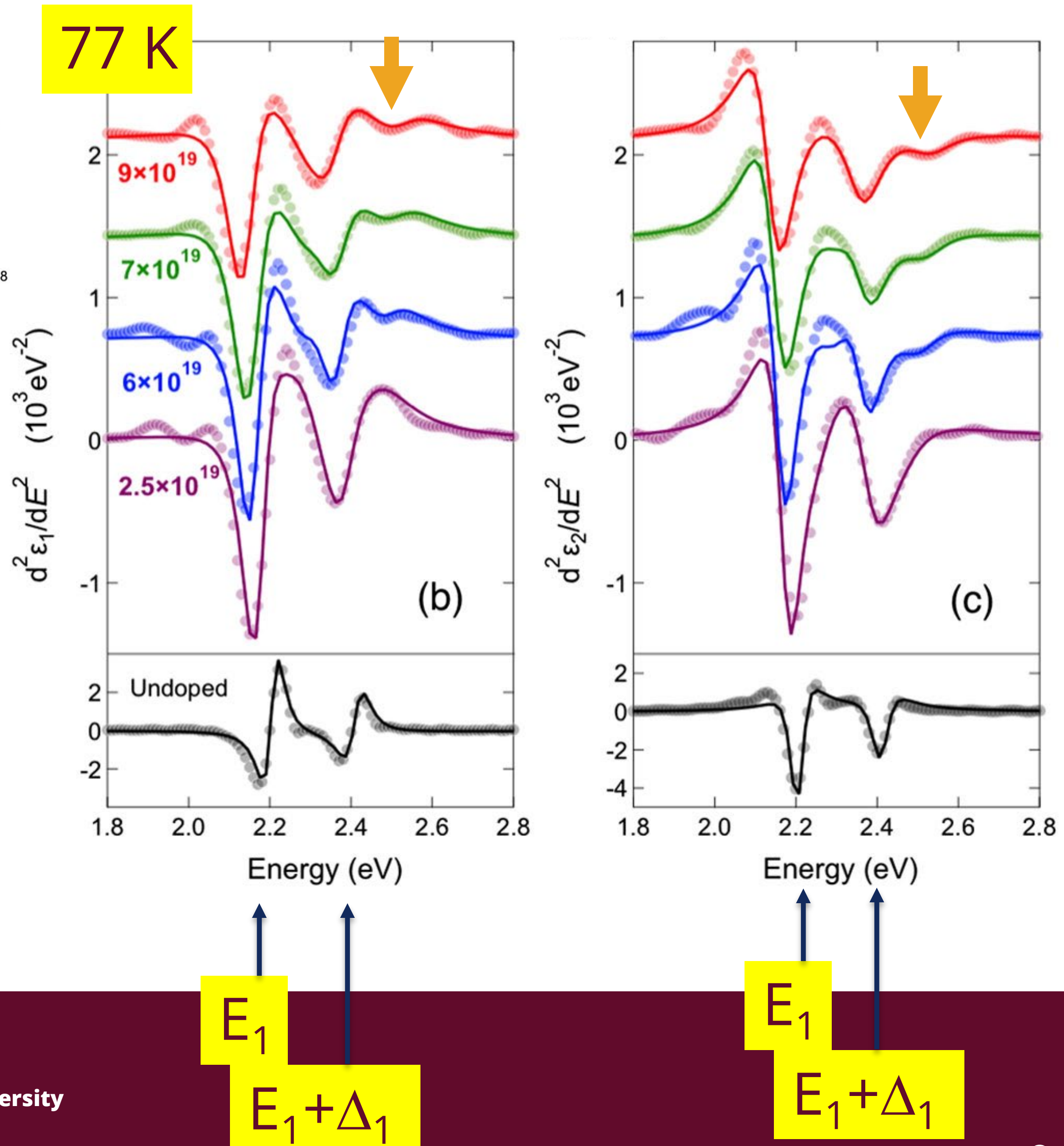
Phase-filling singularity in highly doped Ge:P



$$\varepsilon_2(E) = \frac{8e^2\bar{P}^2\mu_\perp}{3m^2E^2} H(E - E_1) \times$$

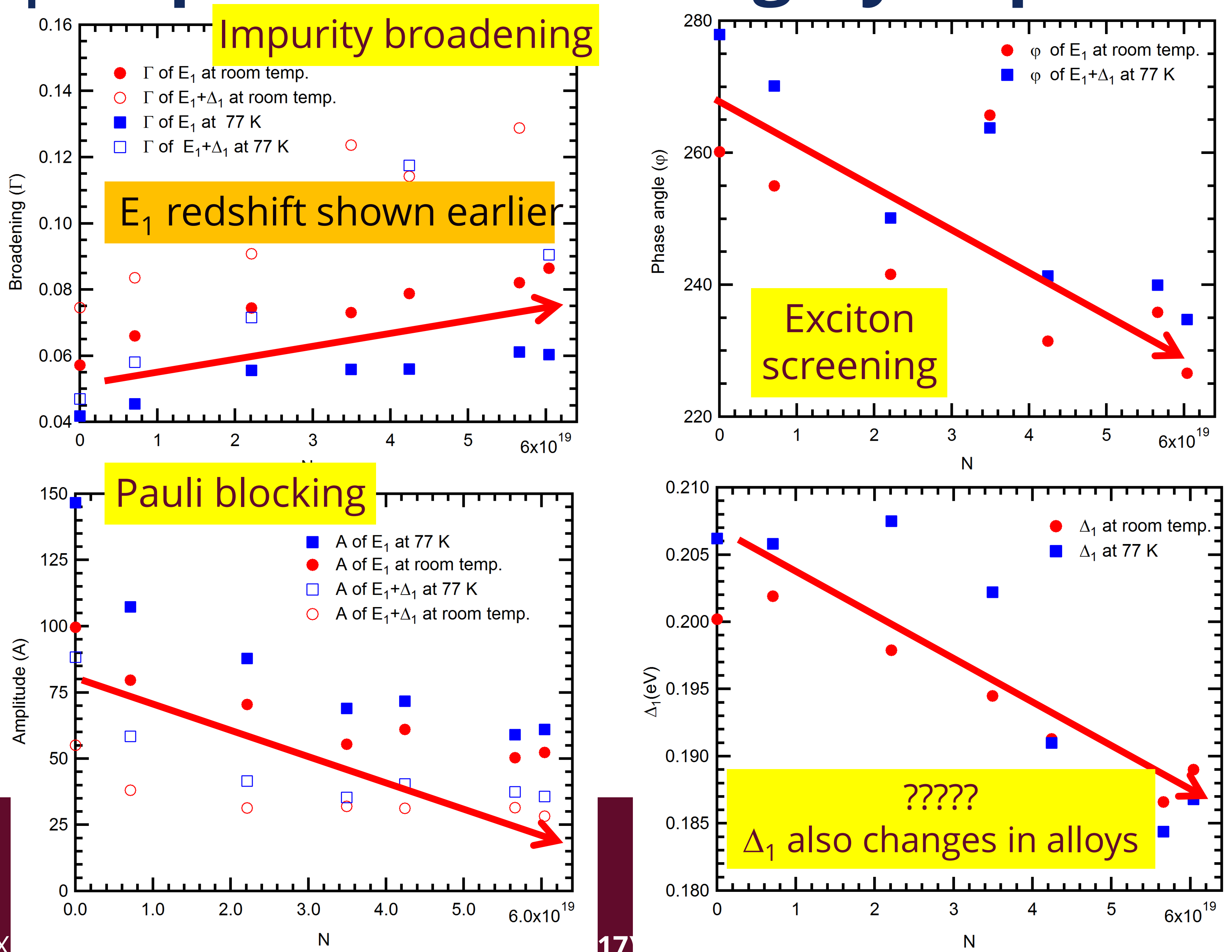
$$\times \int_{-k_{max}}^{k_{max}} dk_z \{1 - f[E_c(E, k_z^2)]\}$$

Phase-filling singularity



C. Xu, NF, SZ, JK, J. Menendez, PRL **118**, 267402 (2017)

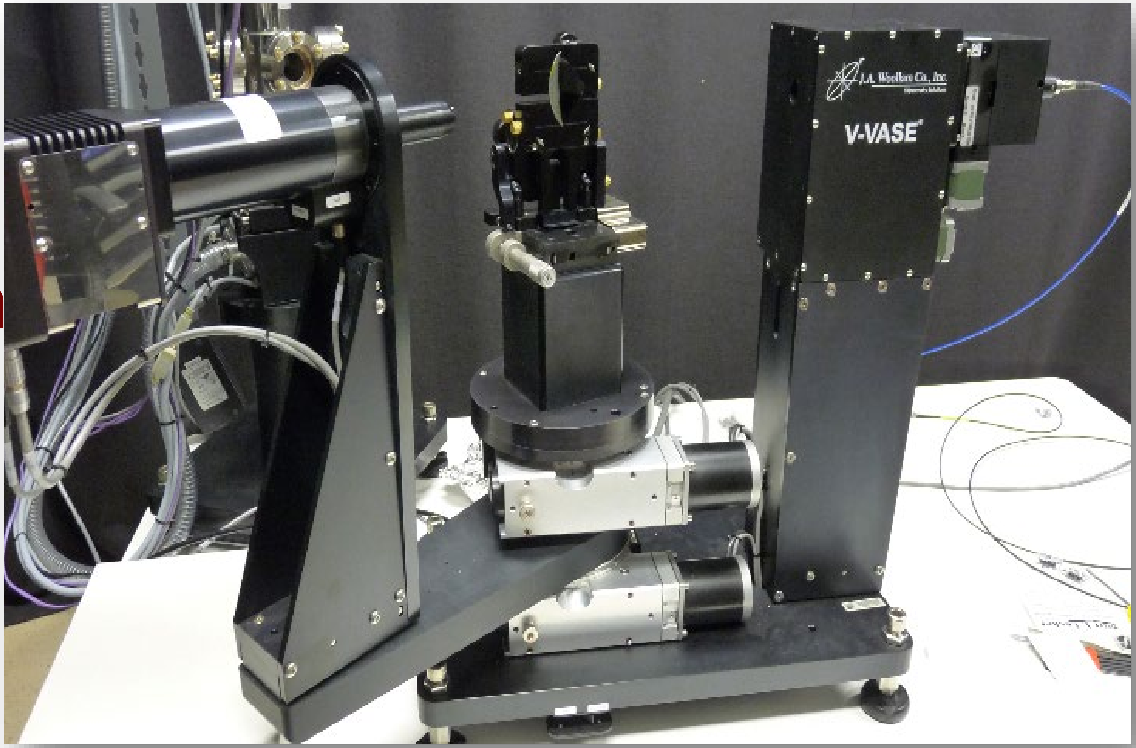
E_1 CP parameters in highly doped Ge:P



Summary

Dielectric functions of semiconductors depend on many parameters:

- Temperature
- Strain
- Alloy composition
- Doping
- Free carriers
- Excitonic effects
- Film thickness



Graduate Students (Spring 2017):

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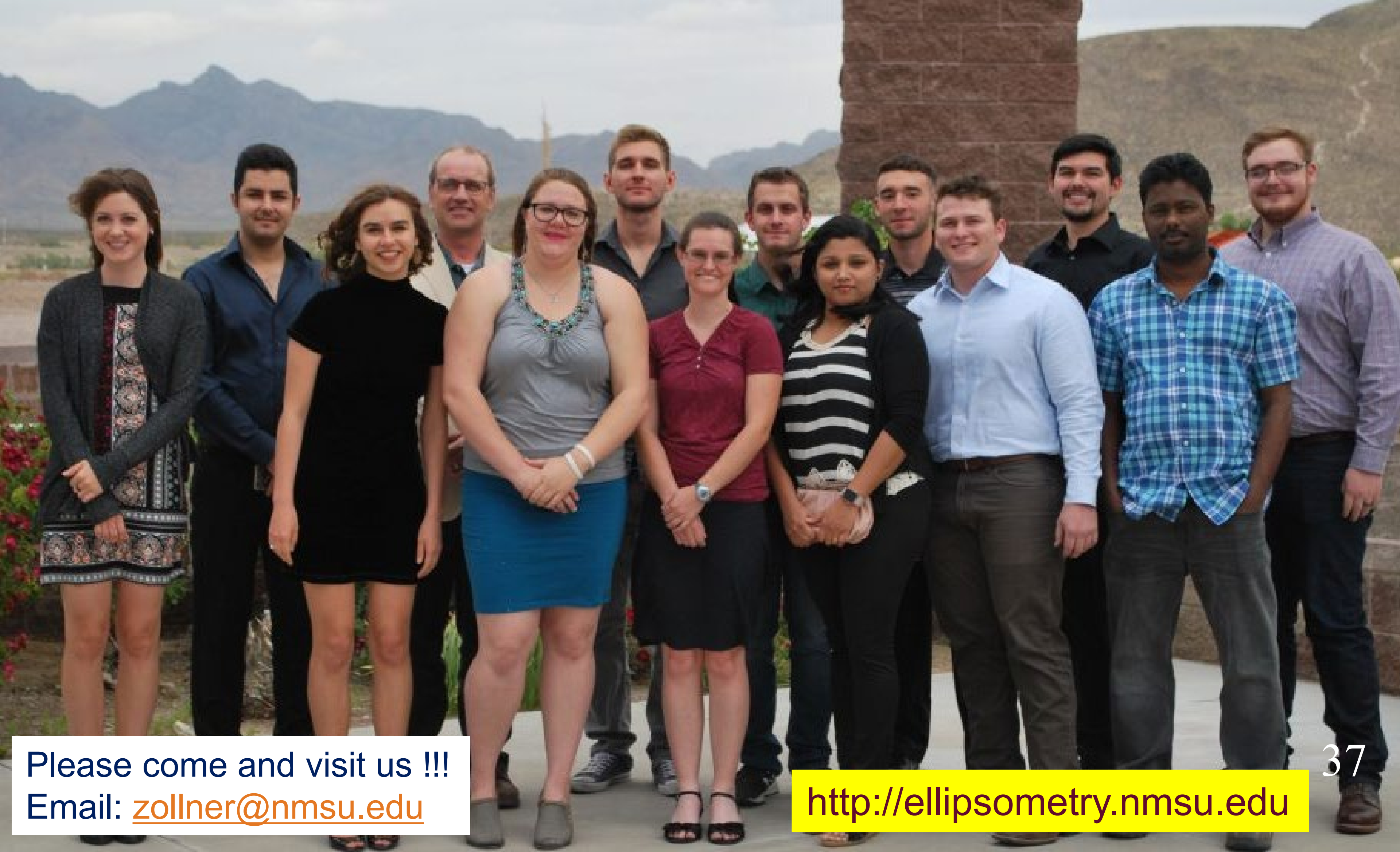
Undergraduate Students:

Nica Richard-Vasquez, Alexandra Hartman, Dominik Martens, Jacqueline Cooke, Troy Powell, Pablo Paradis, *Jaime Moya, Luis Barrera*, Cesy Zamarripa, Zachary Yoder



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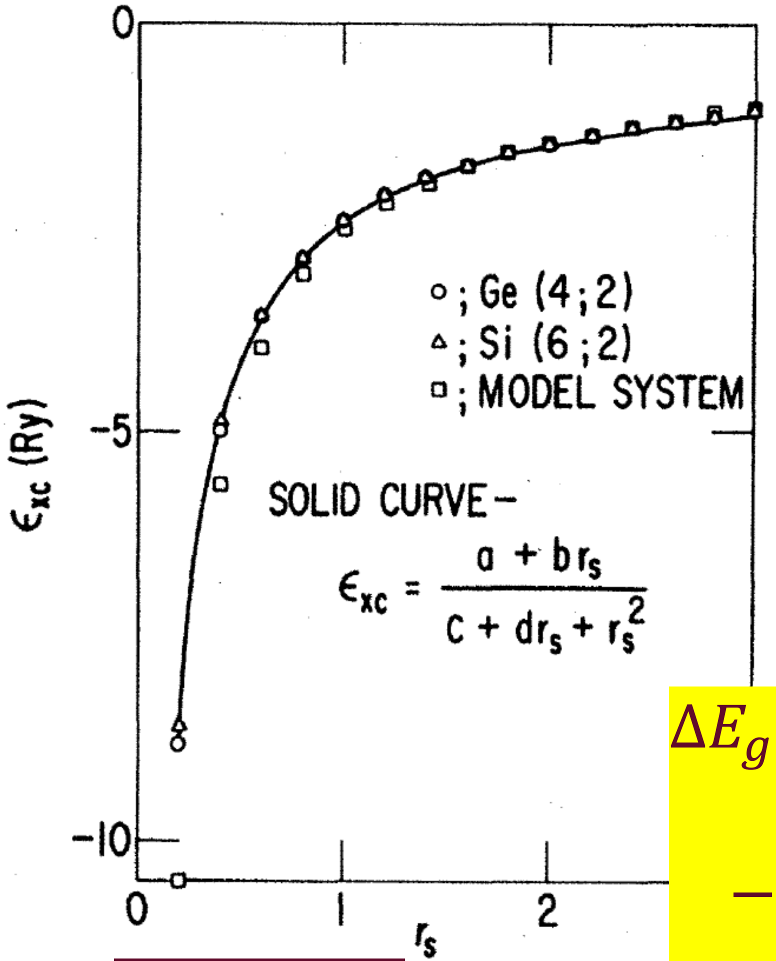
Backup

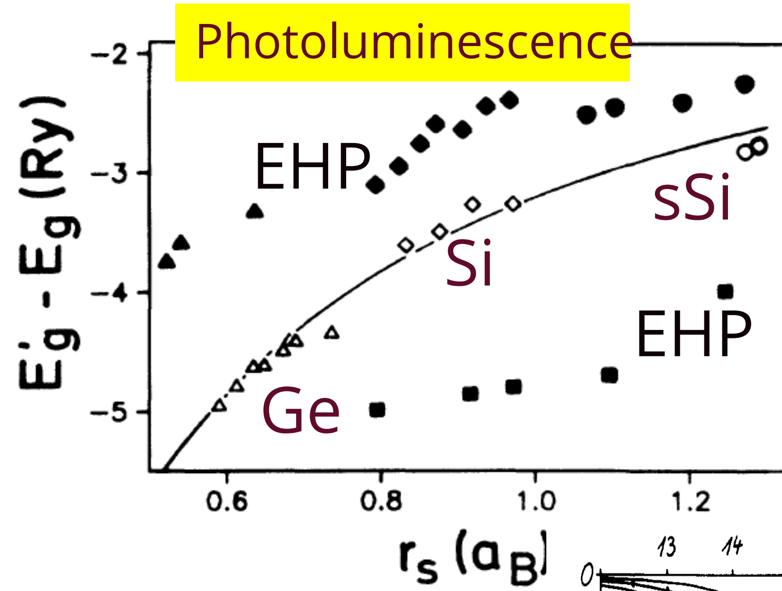
Band-gap renormalization (BGR)

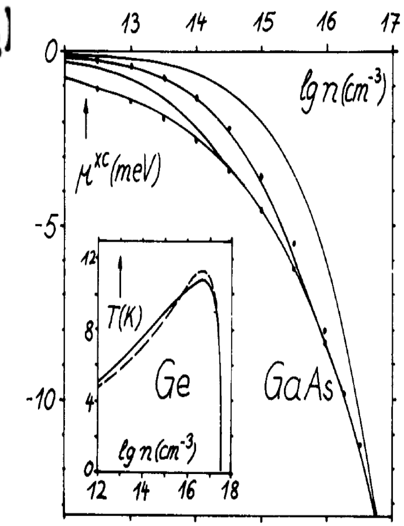
- **Modified Rydberg units make BGR independent of material:**
  - Excitonic Rydberg R (exciton binding energy: mass m* + screening ε)
  - Excitonic Bohr radius a_B
  - **Carrier separation** r_s: $n^{-1}=(4\pi/3)(r_s a_B)^3$
  - Reduced density: $\mathcal{N}=na_B^3$; reduced temperature: $\mathcal{T}=kT/R$.
- **Exchange energy:**
  - ΔE_g(exchange)$=-1.22/r_s$ (single isotropic valley), proportional to $n^{1/3}$.
  - Modify expression for multiple or anisotropic valleys
  - Ge at n=4.3E19cm^{-3}: ΔE_g(exchange)=–0.02 eV (observed: –0.07 eV)
  - Electrons in L-valley of Ge do not impact direct band gap BGR, because wave functions at L and Γ do not overlap. Exchange energy between electrons in different valleys vanishes. Compare Kalt&Rinker, PRB **45**, 1139 (1992).
- **Summary:**
  - Band gap renormalization in doped semiconductors is not important, because it is smaller than the impurity shifts observed by Vina.
  - BGR is the dominant influence in photoexcited semiconductors (PL experiments).

C. Haas, Phys. Rev. **125**, 1965 (1962).
P. Vashista and R.K. Kalia, Phys. Rev. B **25**, 6492 (1982).
R. Zimmermann, phys. stat. solidi (b) **146**, 371 (1988).

Band-gap renormalization (BGR)



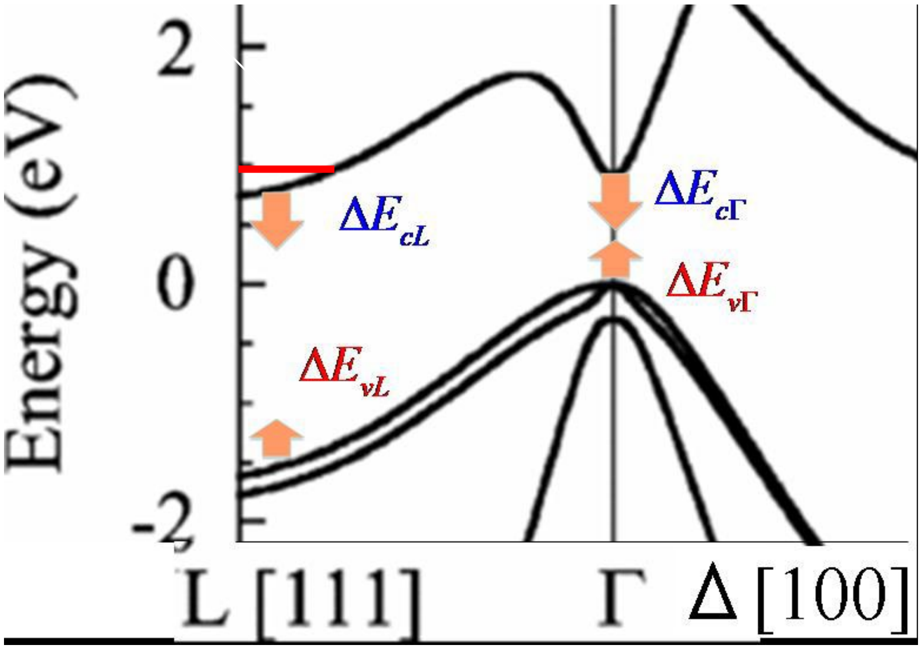


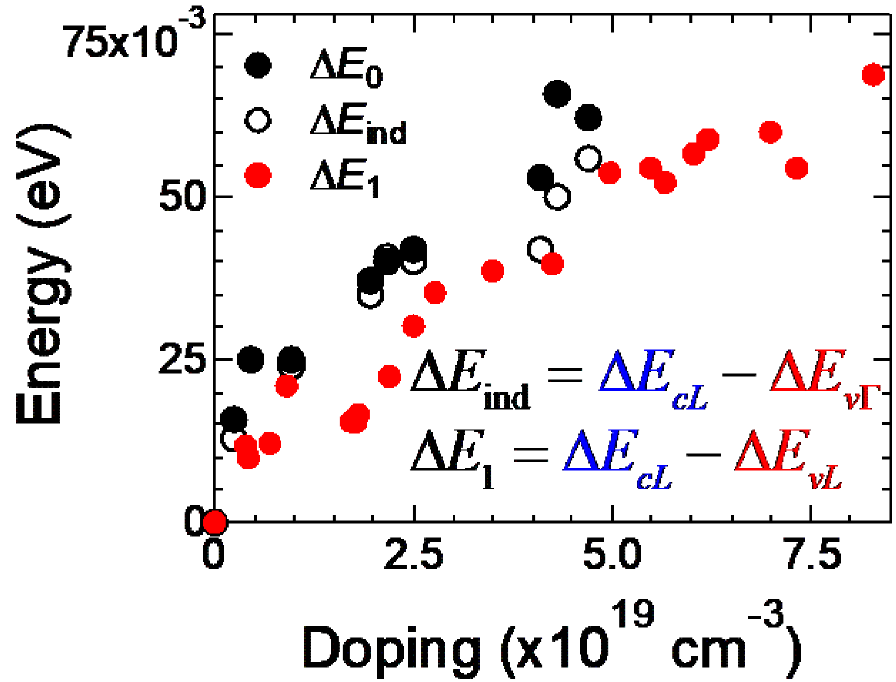


$$\Delta E_g(n,T) = -\frac{3.24 r_s^{-3/4}}{[1 + 0.0478 r_s^3 \mathcal{T}^2]^{1/4}}$$

P. Vashista and R.K. Kalia, Phys. Rev. B **25**, 6492 (1982).
A. Forchel, H. Schweizer, and G. Mahler, PRL **51**, 501 (1983).
R. Zimmermann, phys. stat. solidi (b) **146**, 371 (1988).
S.C. Jain and D.J. Roulston, Solid-State Electron. **34**, 453 (1991).

Band gap lowering in Ge:P





Band gap collapses in Ge:P and Ge:As. (Band filling subtracted.) E_{ind}, E_0 and E_0 collapse at about the same rate, nearly linear in doping density, independent of temperature. Depends on impurity density, independent of n.

Is this collapse due to free carriers or due to impurity scattering (Viña)?

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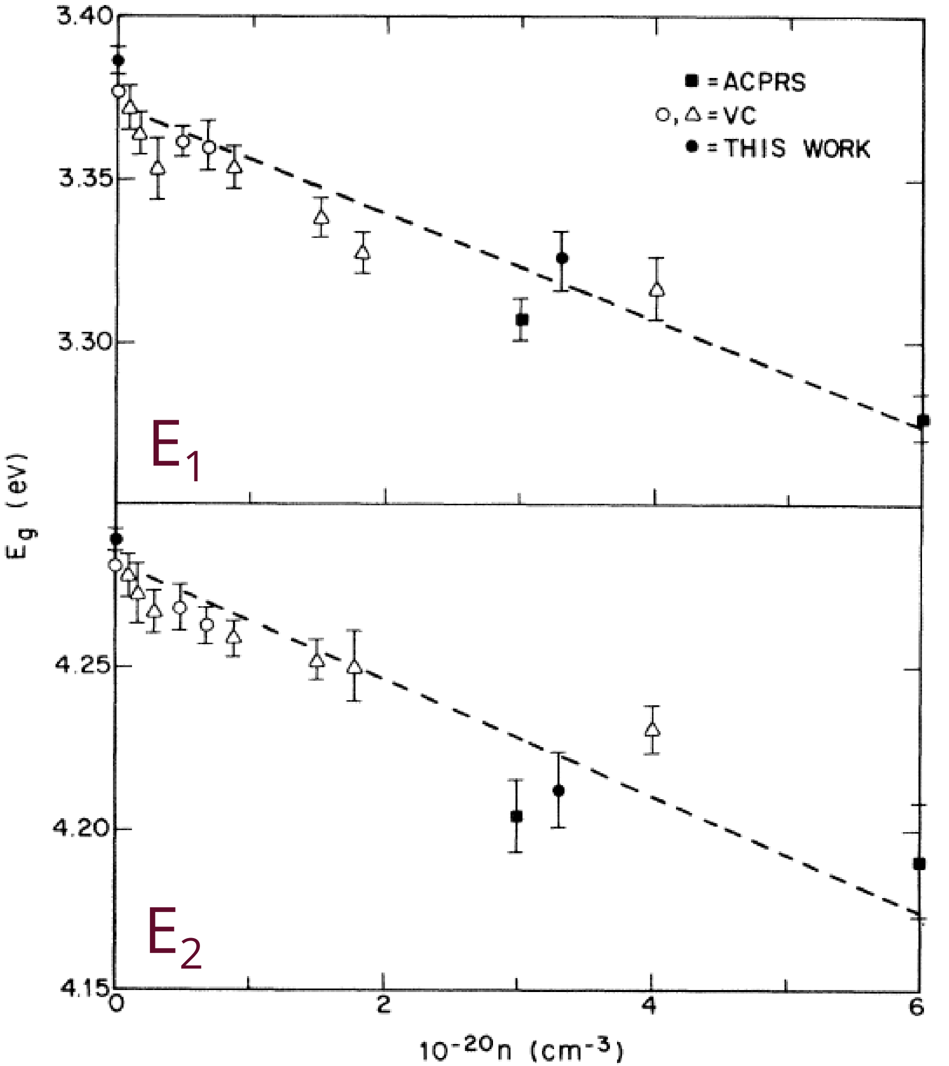
C. Haas, Phys. Rev. **125**, 1965 (1962). Near-gap IR absorption
J. Menendez et al., 2015 APS March meeting

Band gap collapse in Si



Is this collapse due to free carriers or due impurity scattering (Viña-like)?

Linear dependence of redshift with dopant density suggests impurity scattering.

E_1 and E_2 show the same trend. Band gap renormalization should depend on the valley contributing to the CP.

D.E. Aspnes, A.A. Studna, and E. Kinsbron, PRB **29**, 768 (1984).