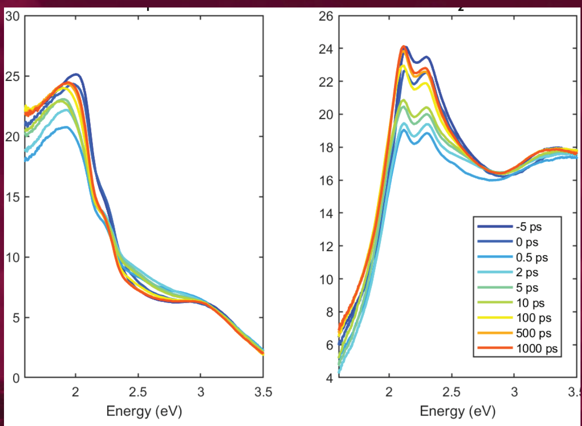
5 September 2024 ELI ALPS Szeged Hungary

FA9550-20-1-0135 AFOSR
FA9550-24-1-0061 AFOSR

Relaxation, Band Filling, and Screening in the Transient Dielectric Function of Ge Determined with Femtosecond Ellipsometry



Stefan Zollner

in collaboration with:

Carola Emminger, Carlos A. Armenta (NMSU)
Shirly Espinoza, Mateusz Rebarz, Martin Zahradnik,
Saul Vazquez-Miranda, Jakob Andreasson (ELI Beamlines)
Steffen Richter, Oliver Herrfurth, Rüdiger Schmidt-Grund
(Leipzig, Ilmenau)

NM STATE

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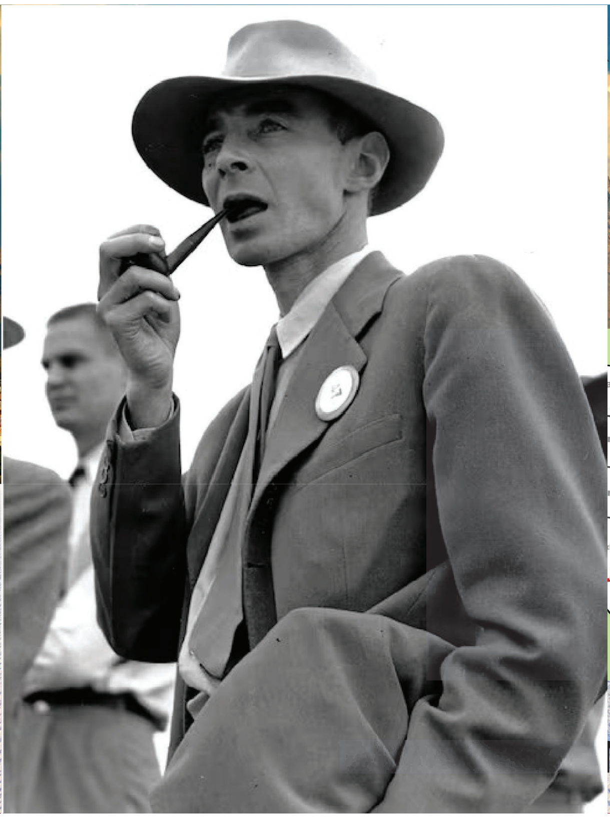
Biography
Regensburg/Stuttgart
Germany
Ames, IA
Motorola (Mesa, Tempe)
Arizona, 1997-2005
Freescale, IBM
New York, 91-92; 07-10
NMSU
Las Cruces, NM
Since 2010
Motorola, Freescale
Texas, 2005-2007
2

Where is Las Cruces, NM ???



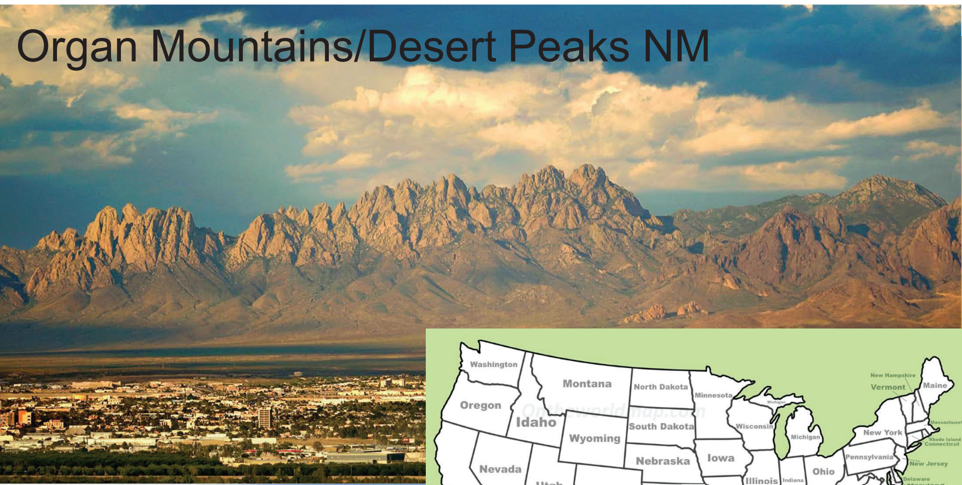
When I was a kid, I thought that **if I could find a way to combine physics with New Mexico, my life would be perfect.**

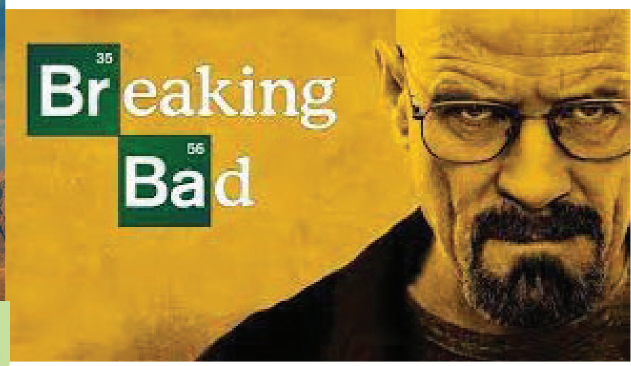
My two great loves are physics and New Mexico. It’s a pity they can’t be combined.

J. Robert Oppenheimer

Note: The NMSU Department of Physics was founded in 1934 by Prof. George Gardiner.

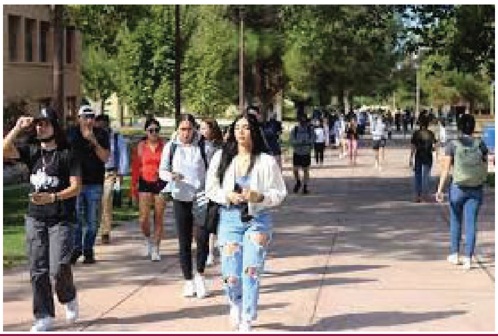
Where is Las Cruces, NM ???





Red or green chile peppers?

New Mexico State University, Las Cruces



Land grant institution, Carnegie R2 (soon to be R1)
Comprehensive: Arts and Sciences, Education, Business, Agriculture
Ph.D. programs in sciences, engineering, agriculture; Ag extension;
Chile Pepper Institute

12,700 students (11,000 UG, 1,700 GR), 1000 faculty

Minority-serving, Hispanic-serving (60% Hispanic/NA, 26% White)
Small-town setting (111,000)

Military-friendly institution (Army and Air Force ROTC programs)

Community engagement classification
(first-generation students, Pell grant recipients)

Physics: BS/BA, MS, PhD degrees. 67 UG and 39 GR students.
11 faculty (HE Nuclear and Materials Physics), **2.4 M$ expenditures.**
ABET-accredited BS in Physics and BS in Engineering Physics

Problem statement

(1) Achieve a **quantitative** understanding of **photon absorption** and **emission** processes.

- Our **qualitative** understanding of excitonic absorption is 50-100 years old (Einstein coefficients),
- But **insufficient** for modeling of detectors and emitters.

(2) How are optical processes affected by **high carrier concentrations** (screening)?

- High carrier densities can be achieved with
  - In situ doping or
  - **ultrafast (femtosecond) lasers** or
  - high temperatures (narrow-gap or gapless semiconductors)
- **Application:** CMOS-integrated mid-infrared camera (thermal imaging with a phone).
- Future: How are optical processes affected by an electric field (pin diode or thin layer)?

Application:
Midwave Infrared Detectors
Germanium-Tin Alloys

Intensity of Optical Absorption by Excitons

R. J. Elliott

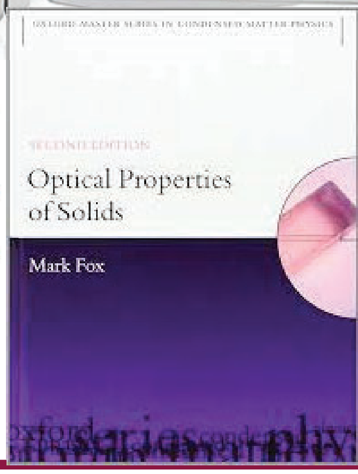
Phys. Rev. **108**, 1384 – Published 15 December 1957

Article | References | Citing Articles (1,780) | PDF | Export Citation

ABSTRACT

The intensity of optical absorption close to the edge in semiconductors is examined using band theory together with the effective-mass approximation for the excitons. Direct transitions which occur when the band extrema on either side of the forbidden gap are at the same **K**, give a line spectrum and a continuous absorption of characteristically different form and intensity, according as transitions between band states at the extrema are allowed or forbidden. If the extrema are at different **K** values, indirect transitions involving phonons occur, giving absorption proportional to $(\Delta E)^{\frac{1}{2}}$ for each exciton band, and to $(\Delta E)^2$ for the continuum. The experimental results on Cu_2O and Ge are in good qualitative agreement with direct forbidden and indirect transitions, respectively.

Received 9 April 1957



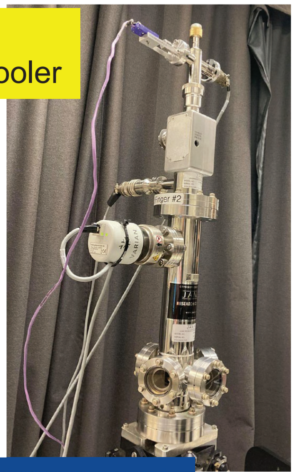
Ellipsometry at NMSU

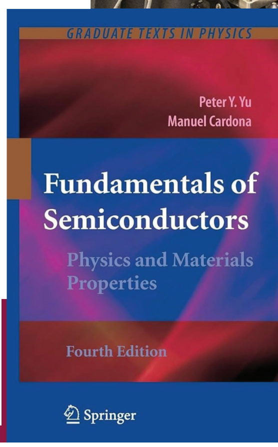
diamond windows
closed-cycle He cooler

Ellipsometry on anything (inorganic, 3D)

- Metals, insulators, semiconductors
- Mid-IR to vacuum UV (150 nm to 40 μm)
- **10 to 800 K, ultrafast ellipsometry**

Ellipsometry tells us a lot about materials quality (not necessarily what we want to know).





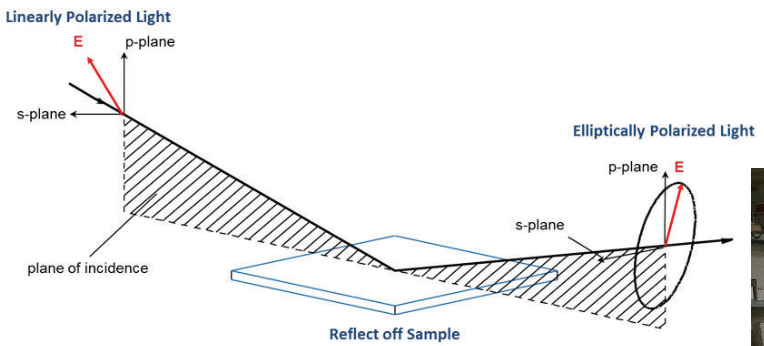
Optical critical points of thin-film $Ge_{1-y}Sn_y$ alloys: A comparative $Ge_{1-y}Sn_y$ / $Ge_{1-x}Si_x$ study VR D'costa, CS Cook, AG Birdwell, CL Littler, M Canonico, S Zollner, ... Physical Review B—Condensed Matter and Materials Physics 73 (12), 125207	440	2006
Growth and strain compensation effects in the ternary $Si_{1-x-y}Ge_xC_y$ alloy system K Eberl, SS Iyer, S Zollner, JC Tsang, FK LeGoues Applied physics letters 60 (24), 3033-3035	397	1992
Ge–Sn semiconductors for band-gap and lattice engineering M Bauer, J Taraci, J Tolle, AVG Chizmeshya, S Zollner, DJ Smith, ... Applied physics letters 81 (16), 2992-2994	335	2002

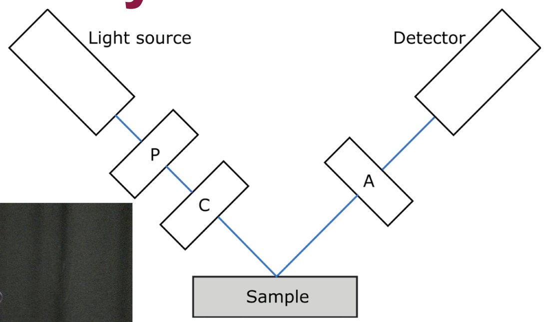
http://femto.nmsu.edu

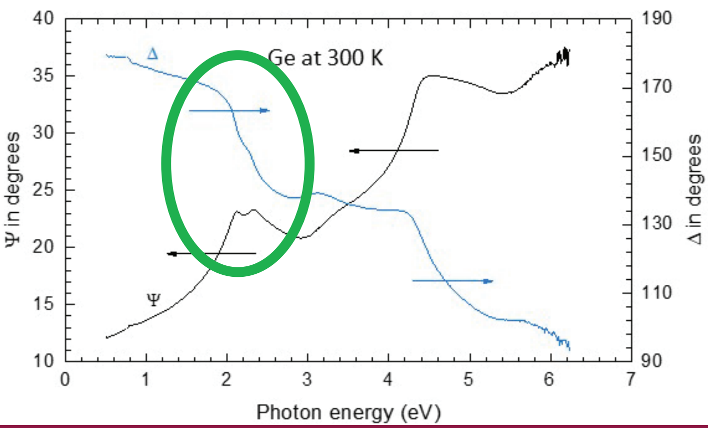
Bandwidth considerations

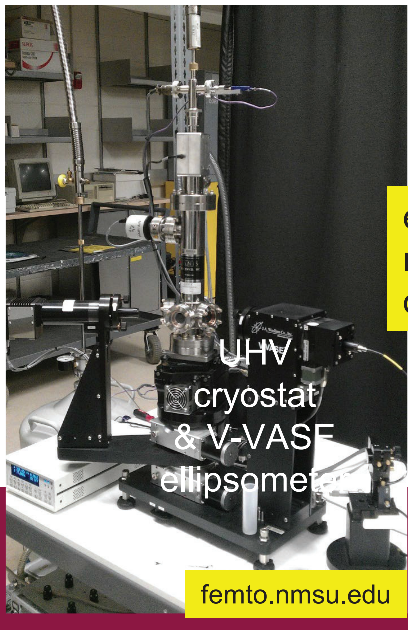
- **Heisenberg uncertainty principle:** $\Delta E \cdot \Delta t = \frac{\hbar}{2} = 330 \text{ meV} \cdot \text{fs}$
- **Attosecond spectroscopy:**
  Low spectral resolution: 33 eV for 10 as pulse duration (use x-ray pulses)
  High temporal resolution: Follow the real-space motion of electrons (and nuclei)
- **Femtosecond spectroscopy:**
  Better spectral resolution: 33 meV for 10 fs pulse length
  Minimal coherent artifacts (dephasing time smaller than pulse width)
  Temporal resolution insufficient to follow the real-space motion of electrons.
  Treat electrons and nuclei motion as **waves**: **Reciprocal space** (Brillouin zone of a crystal)
- **Molecular (or crystal) vibration spectroscopy (phonons):**
  Requires high spectral resolution (1 meV of better): use picosecond pulses
- **Electronic state (band structure) spectroscopy** (this work)**:**
  Requires moderate spectral resolution (10 meV): use 30 femtosecond pulses (or longer)

Spectroscopic ellipsometry







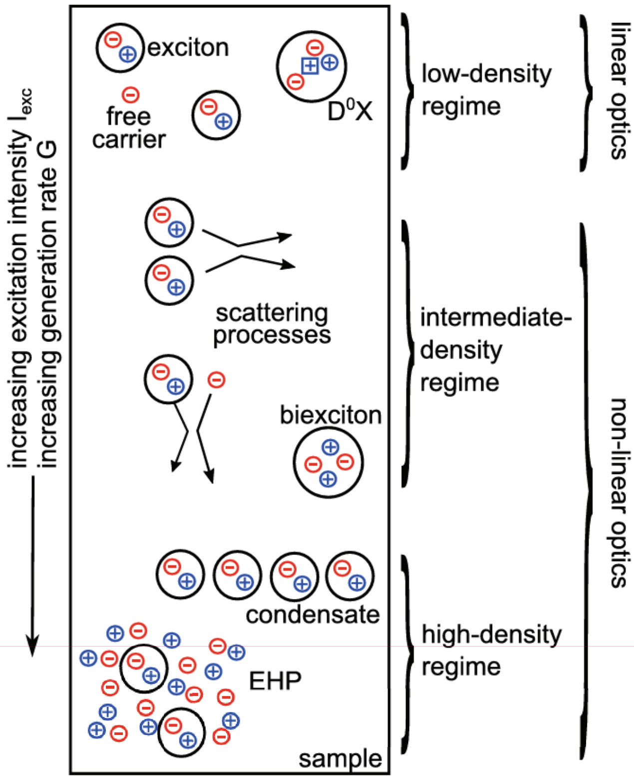


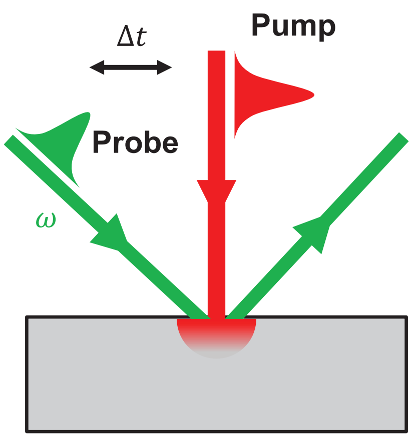
ellipsometric angles ψ, Δ
refractive index n+ik
dielectric function ε

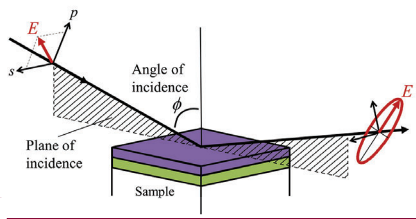
$$\rho = \frac{r_p}{r_s} = \tan\Psi\, e^{i\Delta}$$

Tompkins & Hilfiker, Spectroscopic Ellipsometry (2016)

Femtosecond Pump-Probe Ellipsometry





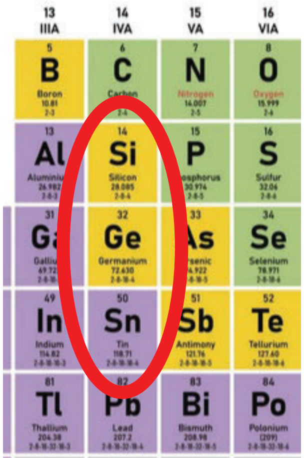


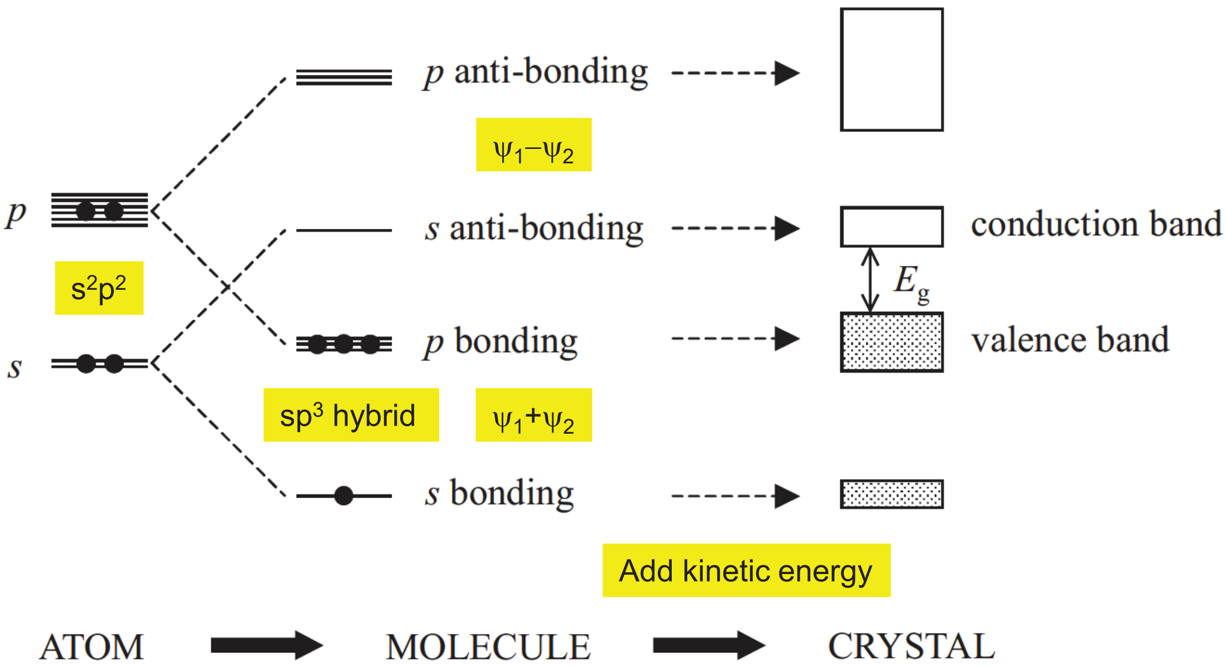
Non-linear effects in germanium induced by photoexcited carriers:

- Screening (many-body)
- Carrier-carrier scattering.
- Carrier-phonon scattering.
- Intervalley scattering.
- Momentum and energy relaxation of hot carriers.

H. Kalt, Semiconductor Optics 2 (2024).
Tompkins & Hilfiker, Spectroscopic Ellipsometry (2016)

Ge Band structure: where did this come from?





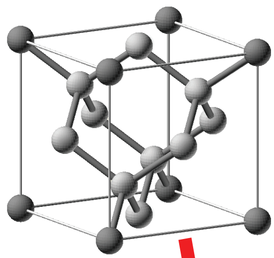
Darwin shift

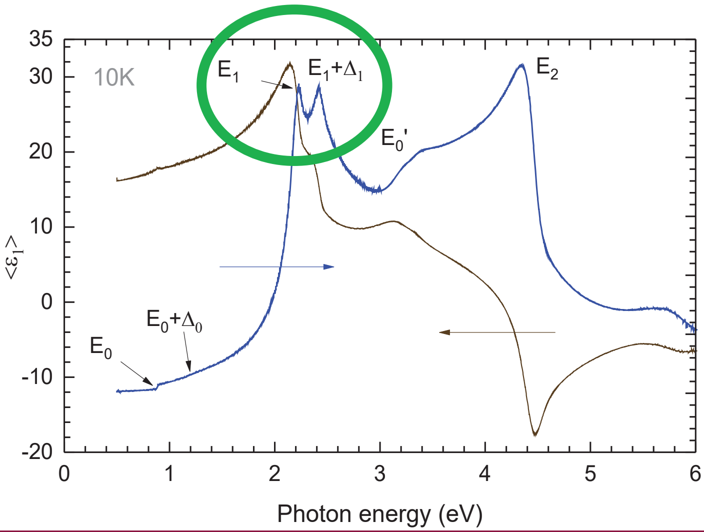
Works well for Ge, GaAs, etc.

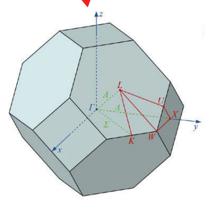
Fox, Chapter 3

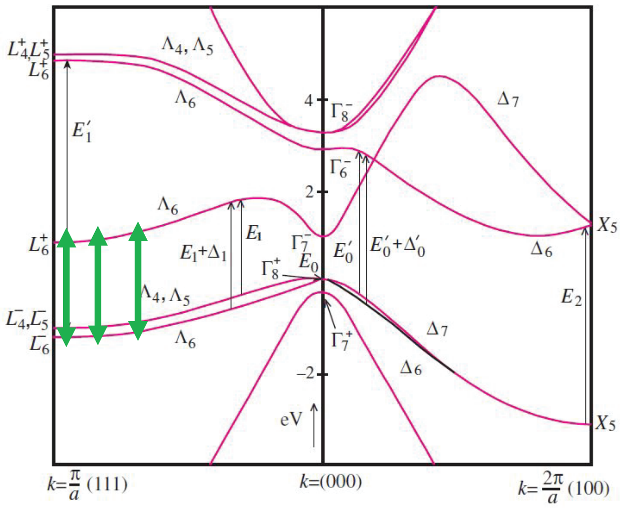
Critical points in the dielectric function of Ge

- Peaks in the dielectric function
- Due to interband transitions from valence to conduction band (electron-hole pairs)



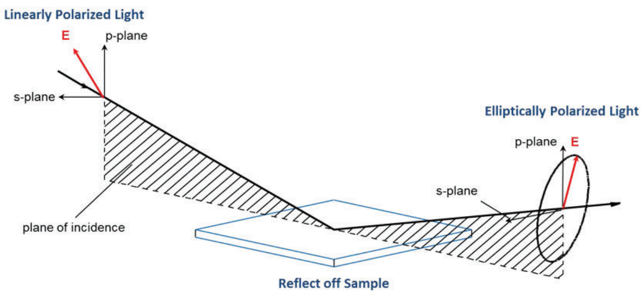


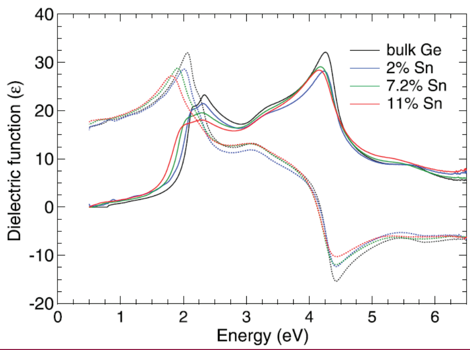




$$\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{n,\vec{k}}(\vec{r})$$

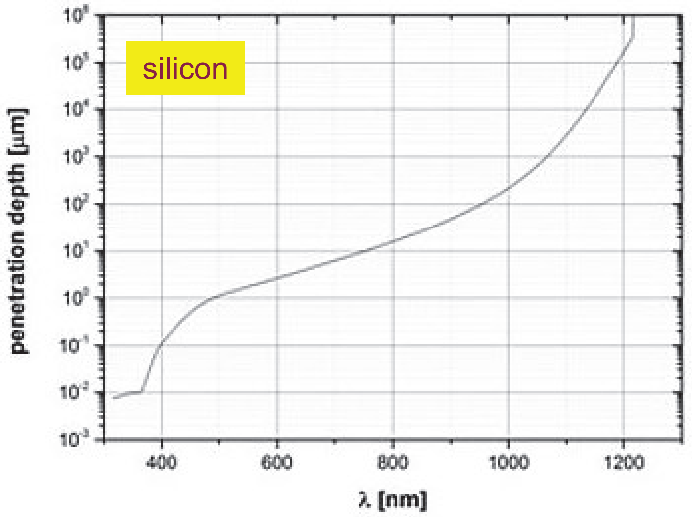
Penetration depth





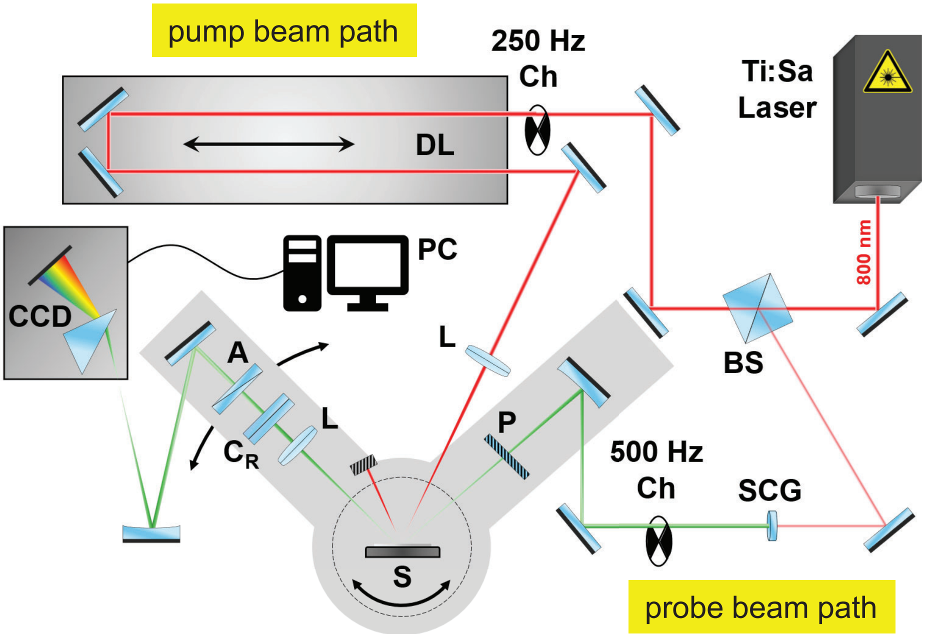
The penetration depth is the inverse of the absorption coefficient (measured with spectroscopic ellipsometry).

Below the direct band gap (0.8 eV for Ge, 3.4 eV for Si), the penetration depth is very large (many micrometers).
The penetration depth is smallest at the E_2 peak in the UV, about 10 nm.



tunable ε: Sn content

Experimental setup: pump-probe ellipsometry



Ch: Chopper (500 Hz, 250 Hz)

A: Analyzer

P: Polarizer

C_R: Rotating Compensator

L: Lens

S: Sample

DL: Delay Line
(~6.67 ns pump-probe delay, 3 fs resolution)

BS: Beam Splitter

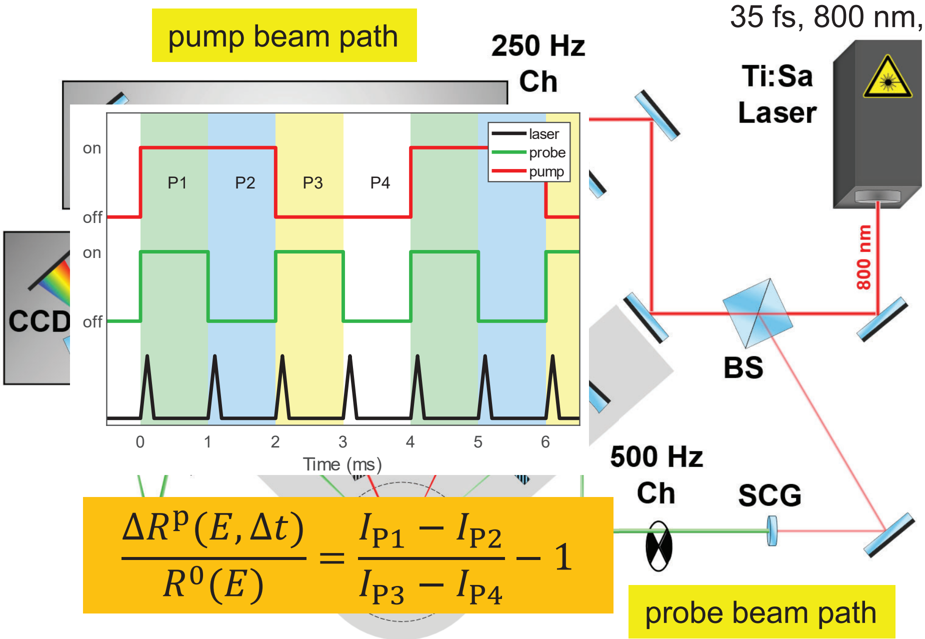
SCG: Super-continuum Generation

CCD: Charge-coupled device detector

S. Richter, Rev. Sci. Instrum. **92**, 033104 (2021).
S. Espinoza, Appl. Phys. Lett. **115**, 052105 (2019).

Experimental setup: pump-probe ellipsometry

35 fs, 800 nm, 1 kHz



$$\frac{\Delta R^{\mathrm{p}}(E,\Delta t)}{R^{0}(E)} = \frac{I_{\mathrm{P1}} - I_{\mathrm{P2}}}{I_{\mathrm{P3}} - I_{\mathrm{P4}}} - 1$$

Ch: Chopper (500 Hz, 250 Hz)

A: Analyzer

P: Polarizer

C_R: Rotating Compensator

L: Lens

S: Sample

DL: Delay Line
(~6.67 ns pump-probe delay, 3 fs resolution)

BS: Beam Splitter

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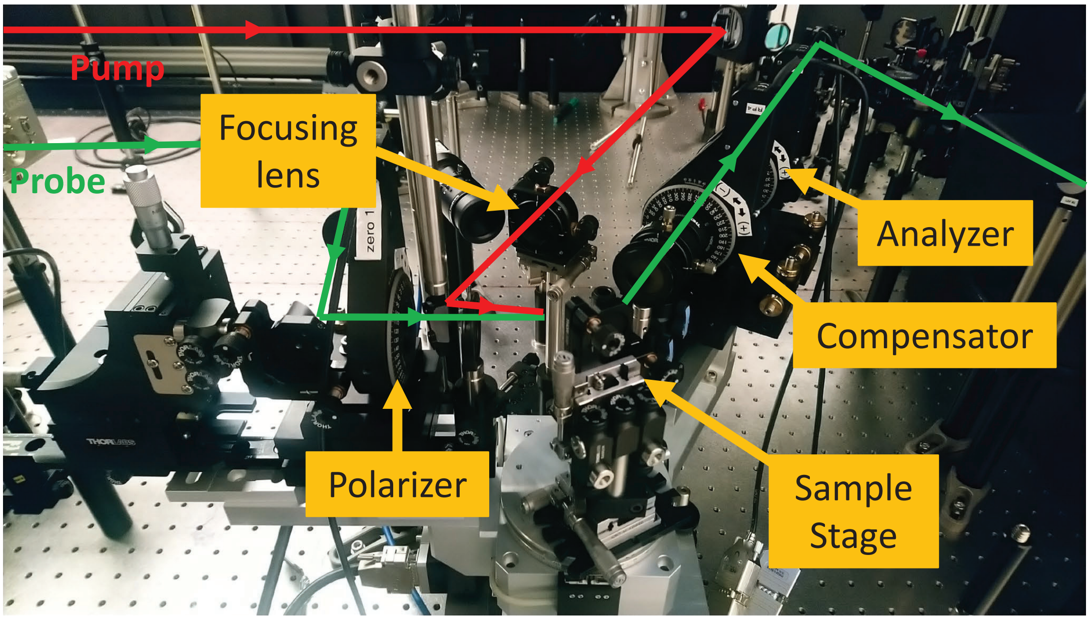
CCD: Charge-coupled device detector

S. Richter, Rev. Sci. Instrum. **92**, 033104 (2021).
S. Espinoza, Appl. Phys. Lett. **115**, 052105 (2019).

Set-up: Femtosecond pump-probe ellipsometry



Rotating compensator ellipsometer:

Compensator was rotated in steps of 10° for a total of 55-65 angles.

Probe beam of 350-750 nm at 60° incidence angle.

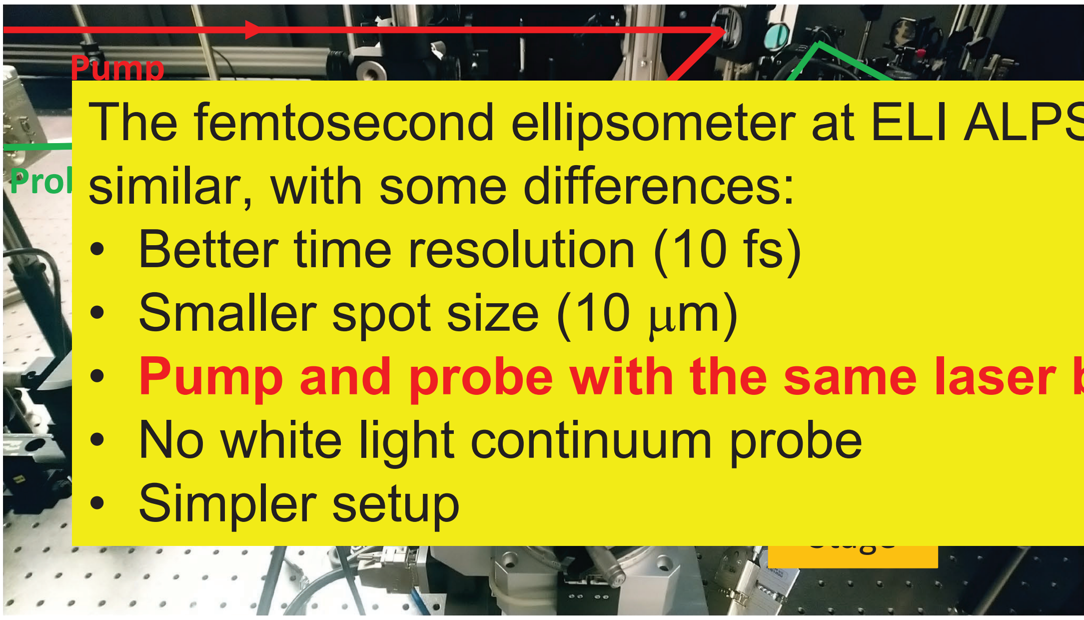
P-polarized pump beam: 35 fs pulses of 800 nm wavelength at 1 kHz repetition rate.

Delay time from -10 to 50 ps.

Time resolution of about 500 fs.

Espinoza et al., APL **115**, 052105 (2019).

Femtosecond pump-probe ellipsometry at ELI ALPS



The femtosecond ellipsometer at ELI ALPS is similar, with some differences:

- Better time resolution (10 fs)
- Smaller spot size (10 μm)
- **Pump and probe with the same laser beam**
- No white light continuum probe
- Simpler setup

Rotating compensator ellipsometer:

r was rotated in steps
otal of 55-65 angles.

of 350-750 nm at 60°
gle.

pump beam: 35 fs
) nm wavelength at 1
n rate.

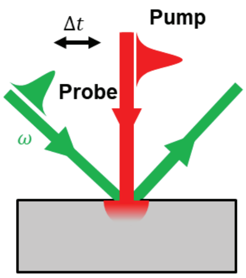
om -10 to 50 ps.

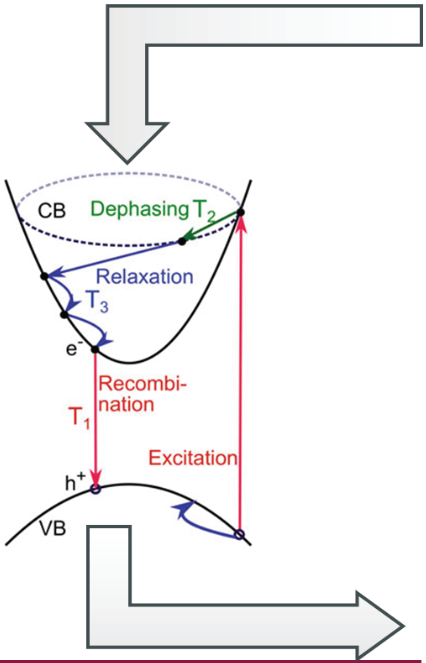
Time resolution of about 500 fs.

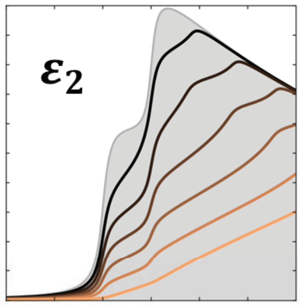
Espinoza et al., APL **115**, 052105 (2019).

Outline

- Introduction:
- Experimental set up and procedure.
- Pump-pulse absorption and charge carrier density.
- Raw data.
- Ultrafast dynamics:
- Scattering processes and carrier statistics.
- Preliminary results.
- Modeling additional absorption processes.
- Conclusion & future work

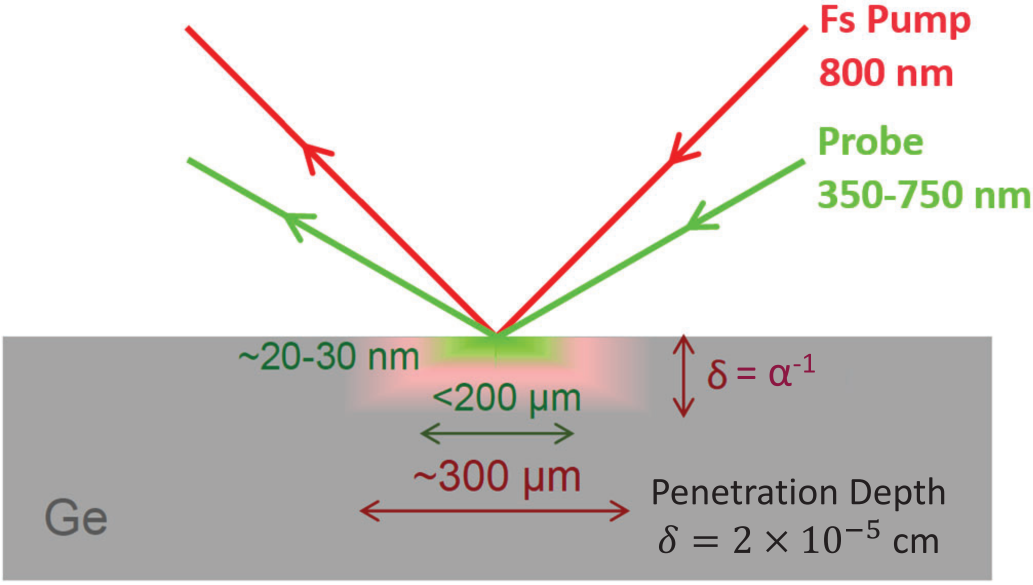






H. Kalt, Semiconductor Optics 2 (2024).

Absorption of pump energy: charge carrier density



Number of Incident Photons

$$N = \frac{E_{\text{pulse}}}{E_{\text{photon}}} = \frac{P/f}{\omega\hbar}$$

Absorbed Photons

$$N_{\text{absorbed}} = (1 - R_{\text{P}}(\theta, \lambda))N$$

Charge Carrier Density

$$\frac{N_{\text{absorbed}}}{V} = \frac{N_{\text{absorbed}}}{A\delta}$$

Probed volume is smaller than excited (pumped) volume

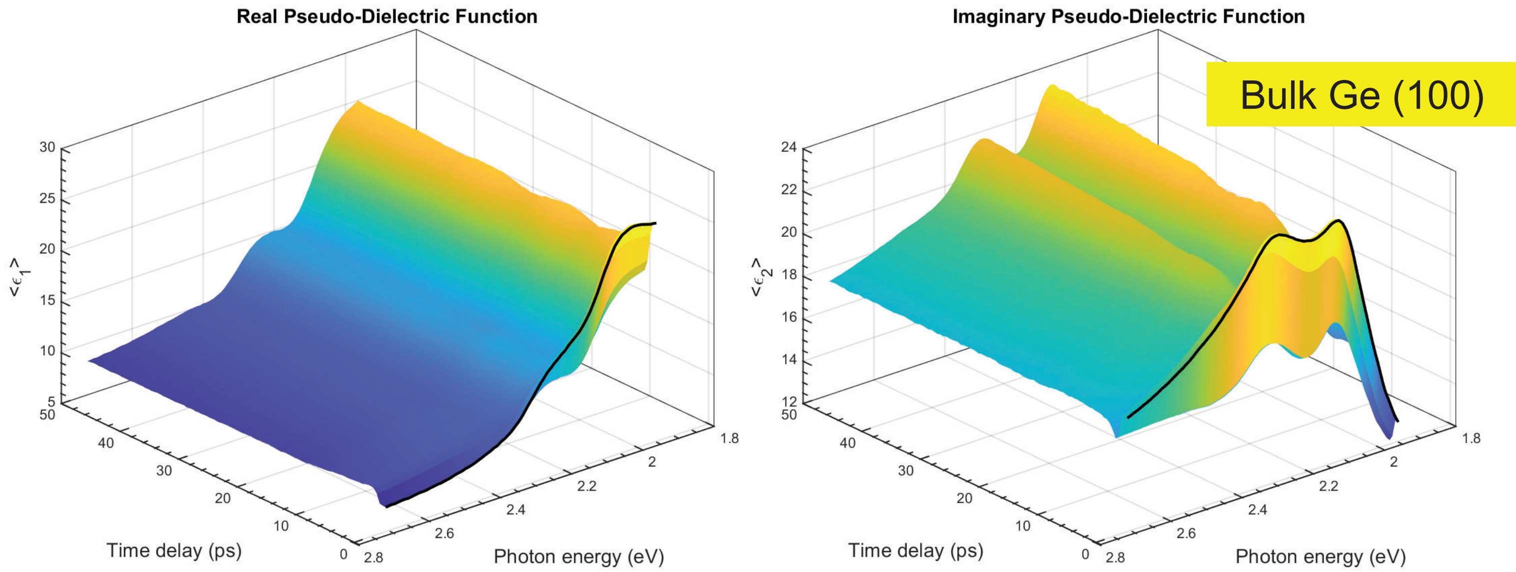
Absorption of pump energy: charge carrier density

Charge Carrier Density						
(Orientation) Pump Intensity	Bulk Ge (111)	Bulk Ge (110)	Bulk Ge (100)	nDoped Ge film*	GeSn Film (10% Sn)	GeSn Film (18% Sn)
Pump Power (mW) **Pulse Energy (μJ)**	13	14	3	2.5	2	5
Pump Beam Diameter (μm)	295	295	180	261	269	517
Charge Carrier Density (cm^{-3})	3.42×10^{21}	3.69×10^{21}	3.16×10^{21}	5.93×10^{20}	7.62×10^{20}	1.31×10^{20}

Excitation density just below the damage threshold.
Carrier concentration of 3×10^{21} cm^{-3} is not physical.
The absorption is already bleached by the pump pulse.

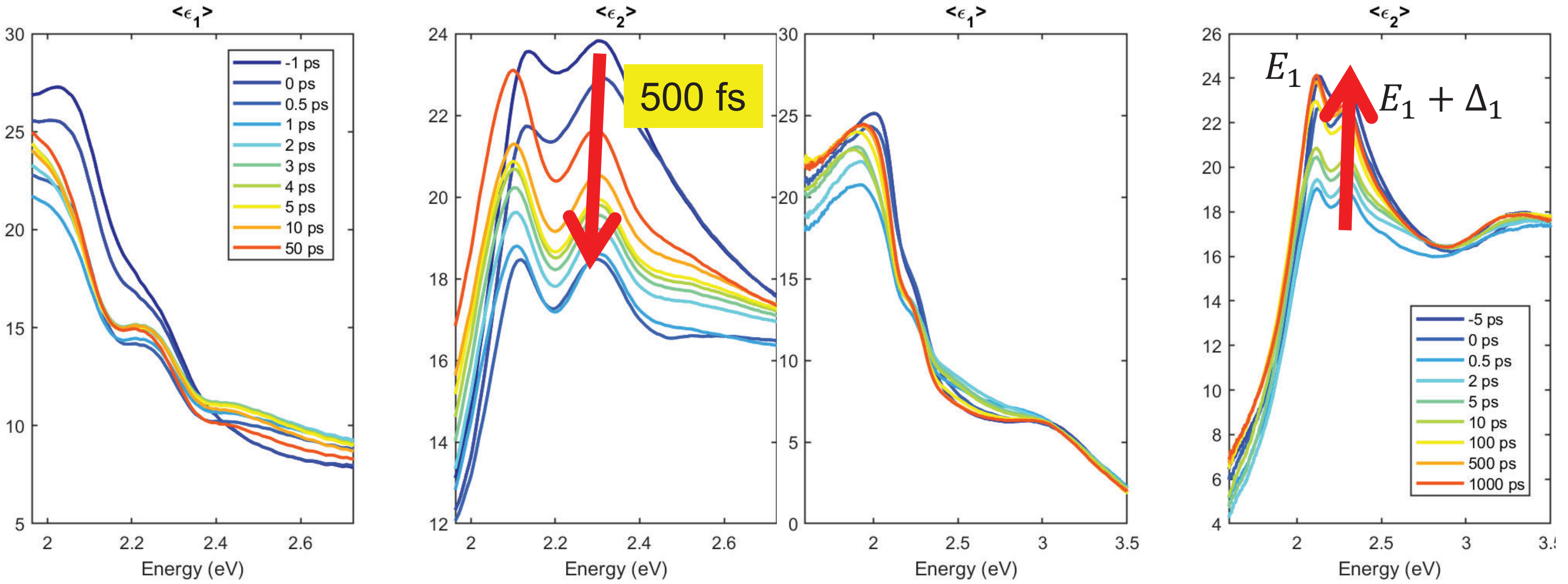
* Doping: $n=1.05 \times 10^{20}$ cm^{-3}

Pseudo-dielectric constant as function of delay time



Rapid decrease of ε followed by recovery.
More pronounced in imaginary part (KK consistent).

Pseudo-dielectric constant as function of delay time



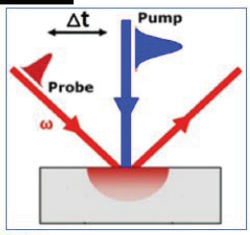
Rapid decrease of ε within first 500 fs.

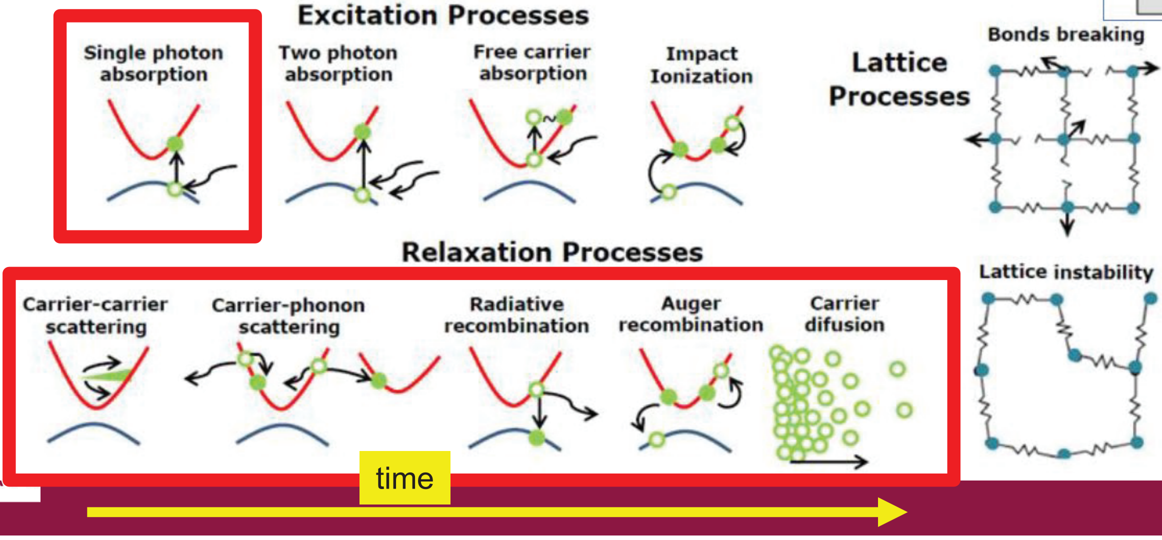
Recovery takes 1 ns or longer.

What is happening on these time scales ?

[redacted]

Shirly Espinoza



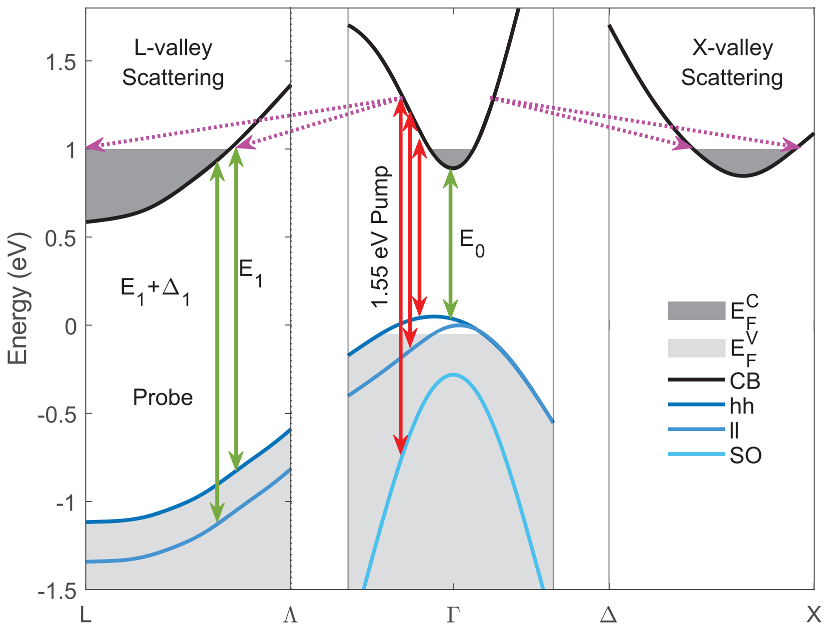


Excitation density below damage threshold.

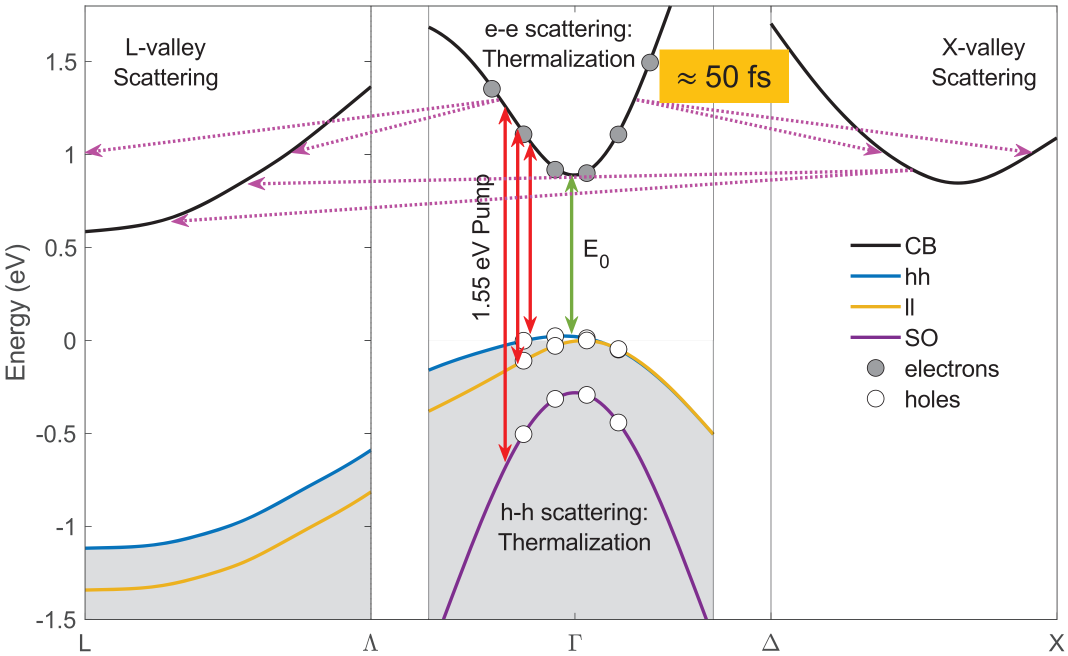
Interband transitions in Ge

- Generation of hot electrons in the Γ-valley with excess energy ε (≈0.7 eV).
- Momentum relaxation and thermalization of hot electrons (<100 fs).
- Energy relaxation by intervalley scattering (GaAs: Γ to X: 50 fs).
- Optical functions change as a function of the density and energy of the electrons.
- Many-body phenomena affect the band transition energy:

$$\Delta E = \Delta E_{\text{str}} + \Delta E_{\text{BM}} + \Delta E_{\text{BGR}}$$



Carrier relaxation (<100 fs): Energy transfer to lattice



$$\varepsilon = \frac{\hbar\omega_{\text{pump}} - E_0}{1 + m_e/m_h}$$

Plasma temperature:

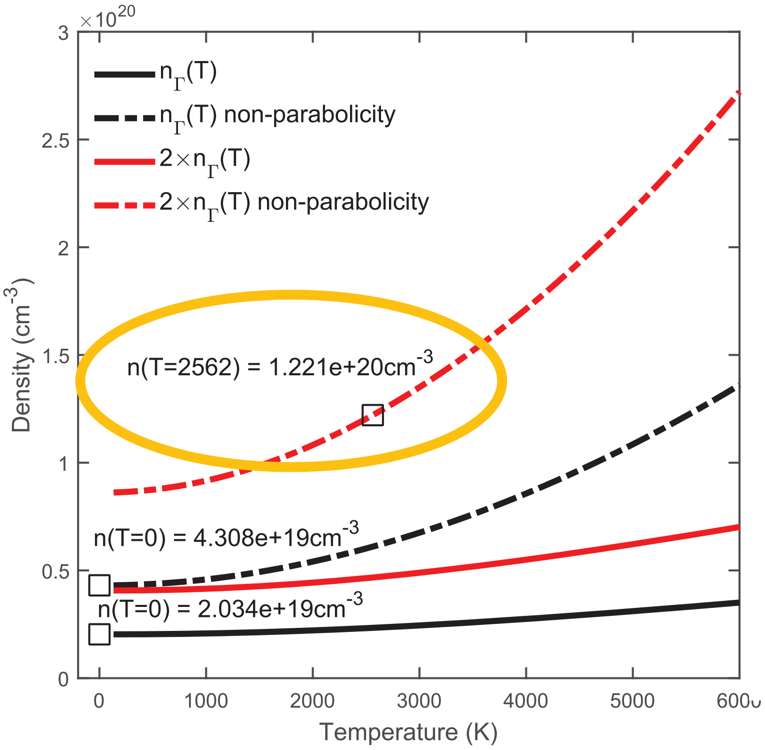
$$T_C \approx \frac{\varepsilon}{3k_B}$$

ε=0.7 eV
T=2500 K

Intervalley scattering is more efficient than intravalley scattering.

Stefan Zollner, Sudha Gopalan, and Manuel Cardona, Effective **deformation potentials** in the description of time-resolved and hot-electron luminescence, Solid-State Commun. **76**, 877-879 (1990)

Electron concentration from density of states



To avoid bleaching of the absorption, the chemical potential μ cannot be larger than the excess electron energy ε. Assume

$\mu = \varepsilon + E_0$

$$n_\Gamma(T) = \frac{1}{4}\left(\frac{2m_{e,\Gamma}k_B T}{\pi\hbar^2}\right)^{3/2} F_{1/2}\left(\frac{\varepsilon}{k_B T}\right)$$

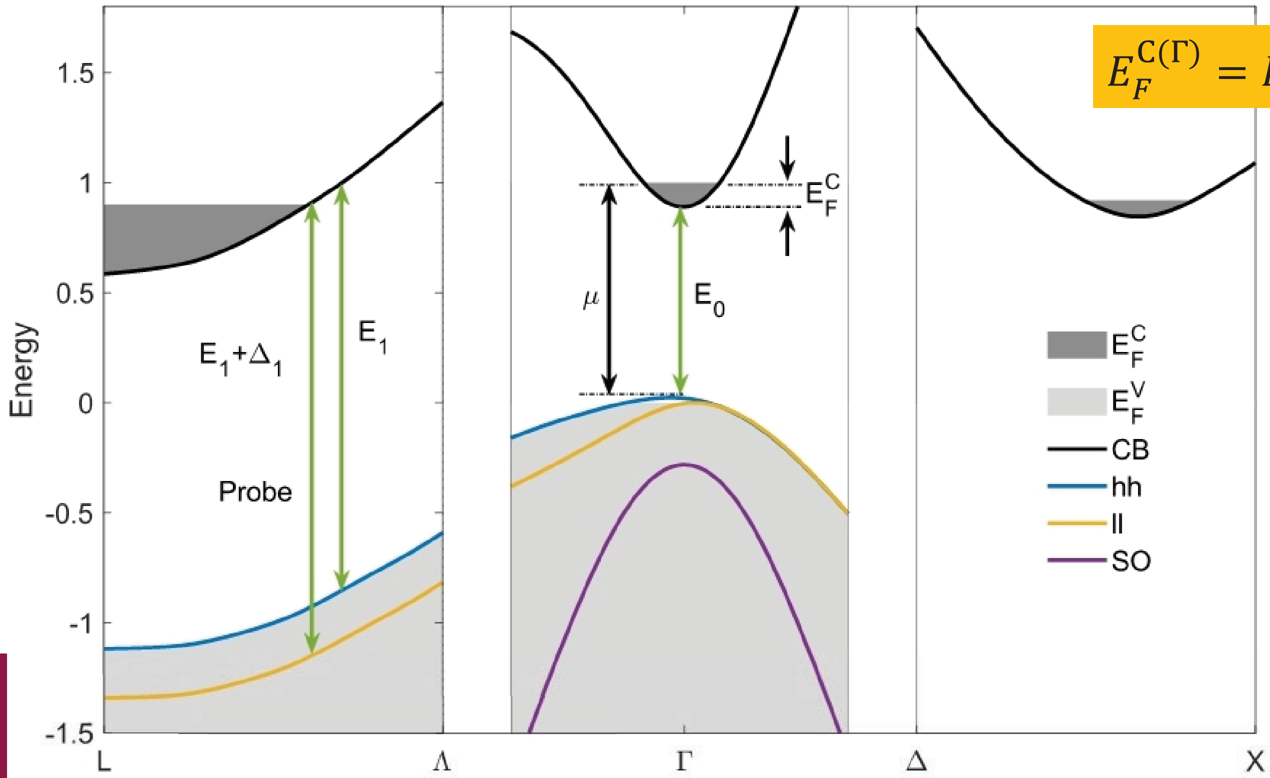
Calculate maximum electron concentration with Fermi-Dirac statistics:

n cannot be more than 10^{20} cm^{-3}.

High above the Mott density (10^{17} cm^{-3}).

Consider density of states with conduction band non-parabolicity from k.p theory.

Thermal equilibrium between valleys (>500 fs)



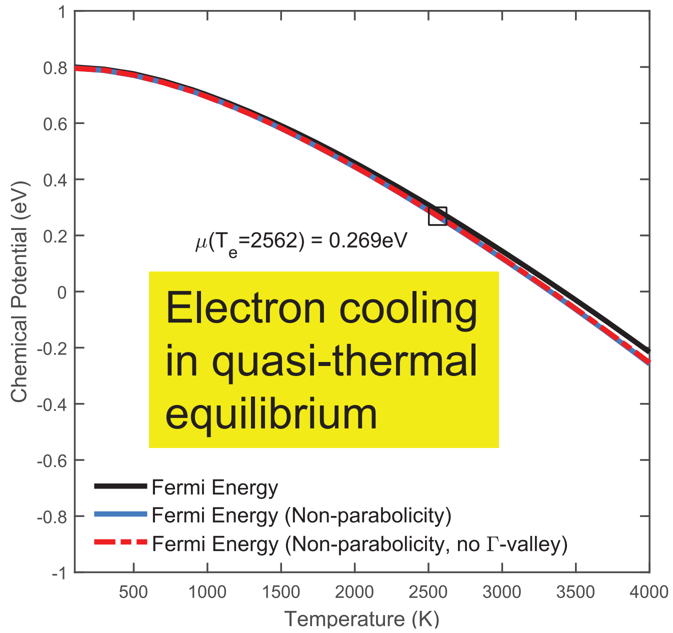
$$E_F^{C(\Gamma)} = E_F^{C(L)} = E_F^{C(X)}$$

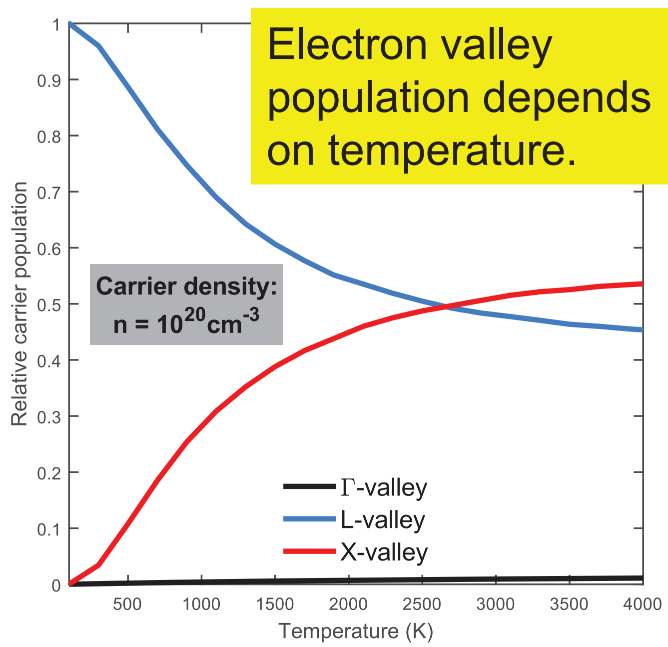
Hot-electron plasma
T<2500 K

High above the Mott density

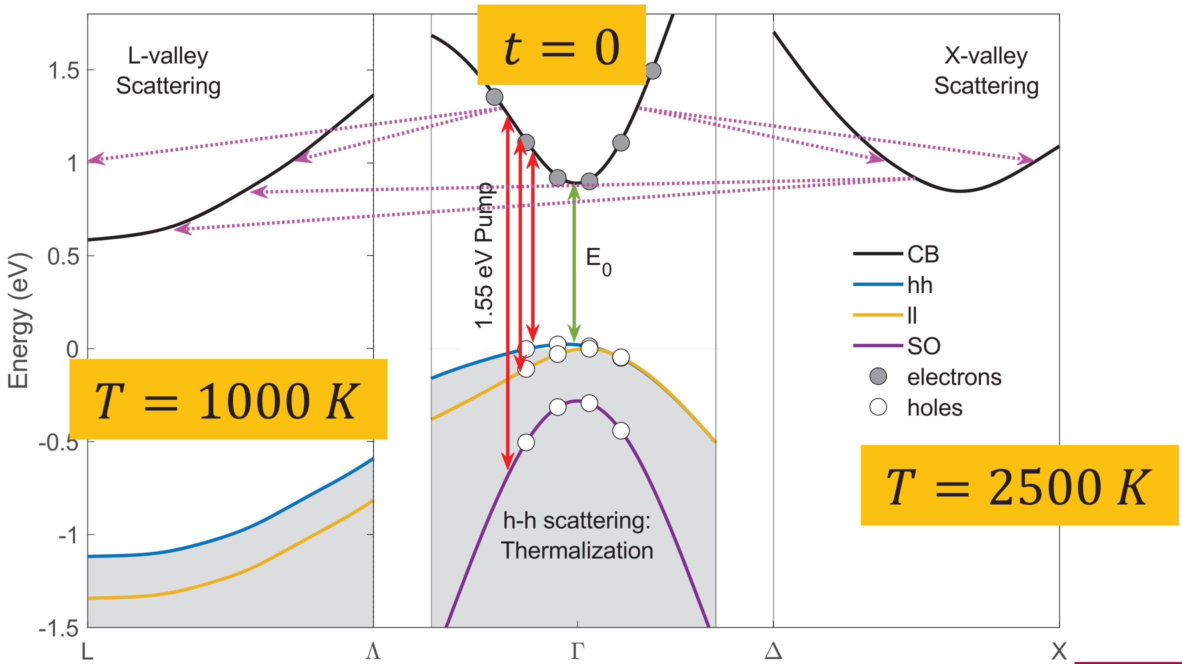
Plasma cools by intervalley scattering.

Electrons cooling by intervalley scattering (>500 fs)

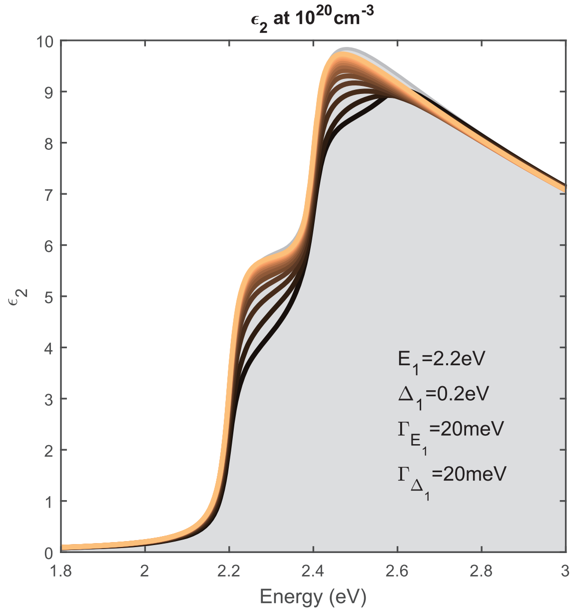


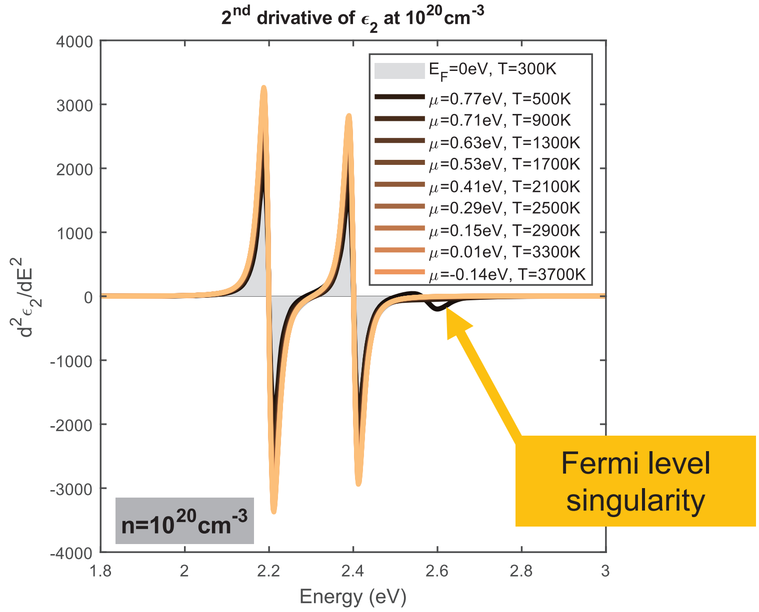


Electrons cooling by intervalley scattering (>500 fs)



Band-filling model for transient dielectric function





$$\varepsilon_2(E) = \frac{2e^2\bar{P}^2\mu_\perp}{3\pi\varepsilon_0 m^2 E^2} H(E-E_1) \int_{-k_{\max}}^{k_{\max}} 1 - f[E_c(E, k_z^2)]dk_z$$

Xu, JAP **125**, 085704 (2019).
Xu, PRL **118**, 267402 (2017).

Band-filling model for transient dielectric function

$$\varepsilon_2(E) = \frac{2e^2\bar{P}^2\mu_\perp}{3\pi\varepsilon_0 m^2 E^2} H(E - E_1) \int_{-k_{\max}}^{k_{\max}} 1 - f[E_c(E, k_z^2)]dk_z$$

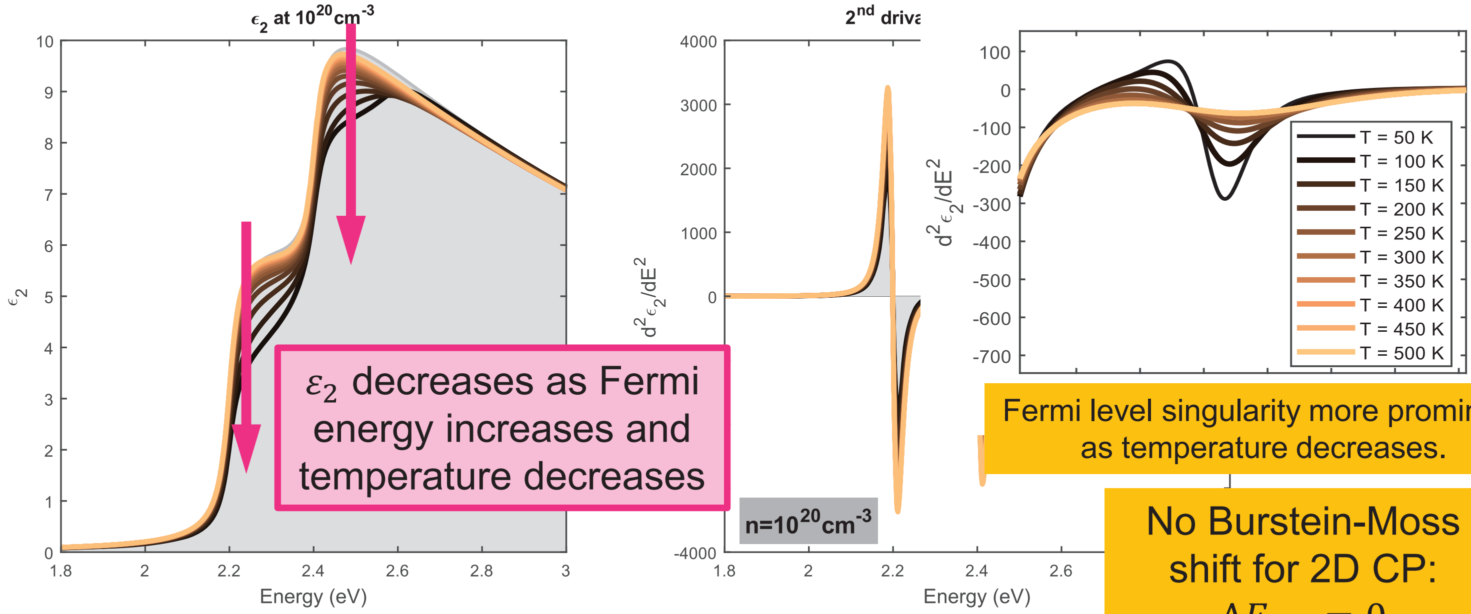
Introduce broadening Γ of interband transitions.
Integration over Fermi-Dirac distribution yields Fermi integral $F_{-1/2}$.

$$\varepsilon_2(E, \Gamma, \mu, T) = \frac{1}{\pi}\mathrm{Im}\left\{\ln\left[\frac{2(E_1 - i\Gamma - \mathrm{E})}{E_1 - i\Gamma}\right]\right\} \frac{4k_{\max} e^2 \bar{P}^2 \mu_\perp^{(E_1)}}{3\pi\varepsilon_0 m^2 E^2} \left\{1 - \left(\frac{k_T}{2k_{\max}}\right) F_{-1/2}\left[\frac{\mu - (E - E_1)\frac{\mu_\perp}{m_\perp}}{k_B T}\right]\right\}$$

Fixed parameters: Band gap E_1, momentum matrix element P, effective masses m_i, μ_i
Adjustable parameters: Broadening Γ, chemical potential μ, temperature T, wave vector range k_{max}

Xu, JAP **125**, 085704 (2019).
Xu, PRL **118**, 267402 (2017).

Band-filling model for transient dielectric function



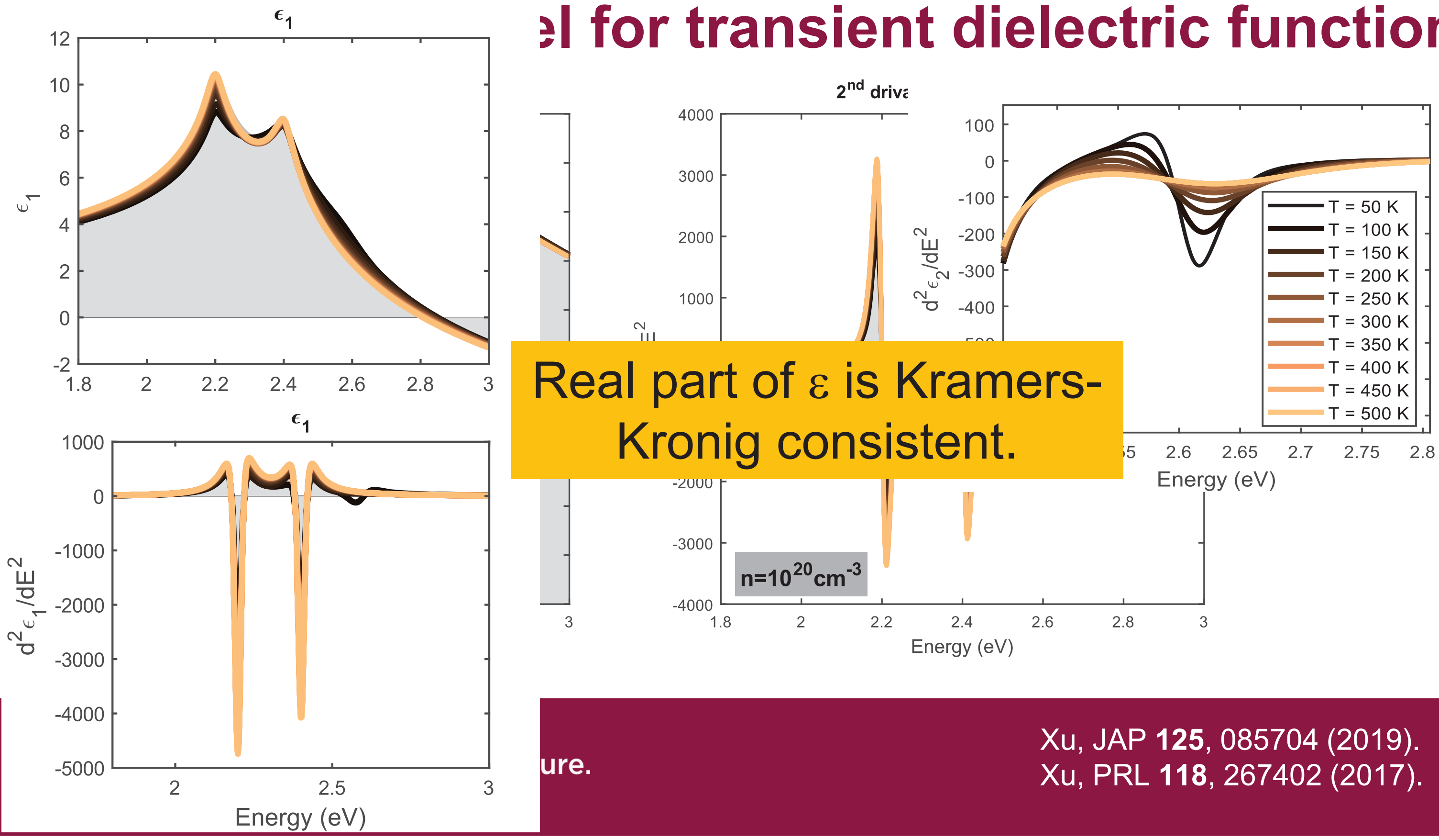
Fermi level singularity more prominent as temperature decreases.

No Burstein-Moss shift for 2D CP: $\Delta E_{\mathrm{BM}} = 0$

$$\varepsilon_2(E) = \frac{8e^2\bar{P}^2\mu_\perp}{3m^2E^2} H(E - E_1) \int_{-k_{\max}}^{k_{\max}} 1 - f[E_c(E, k_z^2)]\, dk_z$$

Xu, JAP **125**, 085704 (2019).
Xu, PRL **118**, 267402 (2017).

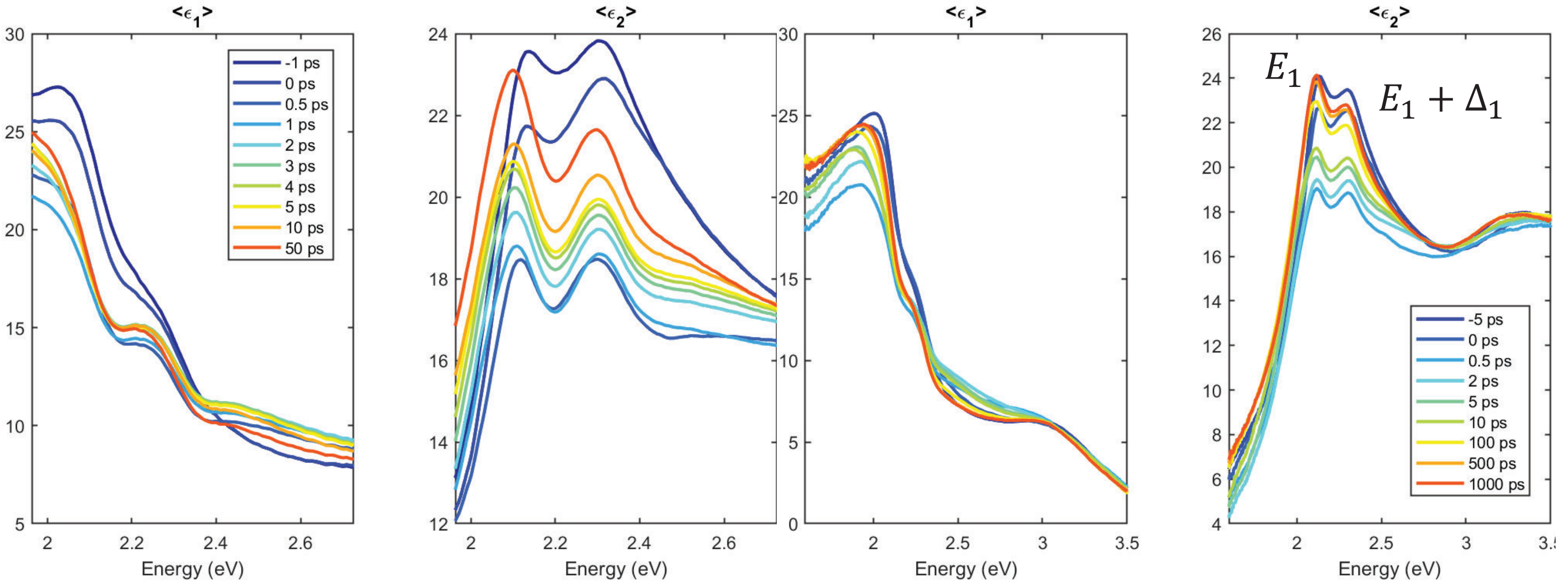
el for transient dielectric function



ure.

Xu, JAP **125**, 085704 (2019).
Xu, PRL **118**, 267402 (2017).

Pseudo-dielectric constant as function of delay time



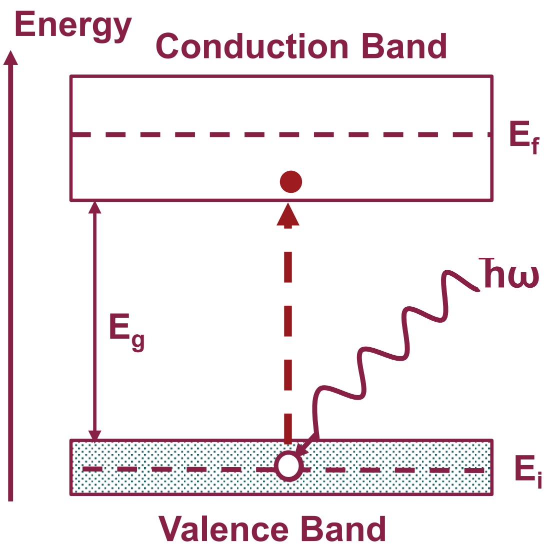
No quantitative agreement.
Need to include excitonic effects.

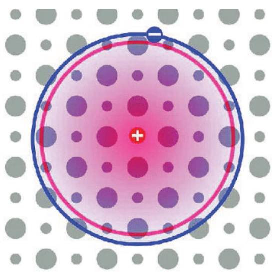
What have we learnt so far ?

- Calculated electron-hole concentration (about 10^{20} cm^{-3}) from Fermi-Dirac statistics.
- Electrons initially in Γ-valley, very hot electron plasma (2500 K)
- Within 50 fs, most electrons (>50%) scatter to the X-valley (large density of states).
- Electrons cool by intervalley scattering.
  When T<1000 K, most electrons are in the L-valley
  L-electrons are observable by bleaching the absorption of the probe pulse.
- Theory predicts a reduction of ε_2 due to band filling (Pauli blocking) by about 20%.
- **A reduction by 25% is observed in the experiment, but the amplitude and line shape are wrong.**

- **What is missing?**
- L-valley absorption is enhanced by excitons.
- Excitonic (Sommerfeld) enhancement is screened by high electron density.
- Next, we need to talk about **excitons**.

Exciton concept: Bound Electron-Hole Pair





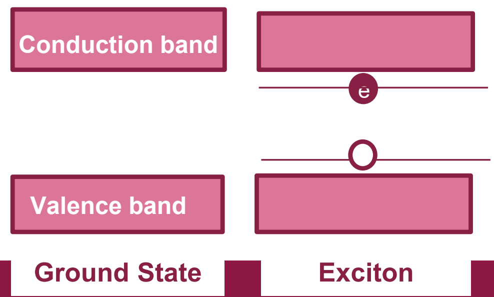
Excitons in semiconductors

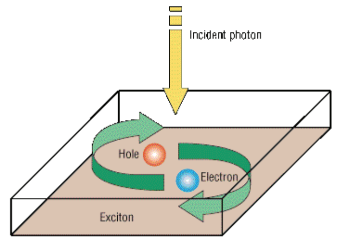
	Excitonic Radius(Å)	Lattice Constant(Å)	Excitonic Binding Energy (meV) *R*
GaAs	130	5.6532	4.2
$SrTiO_3$	62.5	3.9050	20
GaP	50	5.4505	21
ZnO	20	a=3.2500, c=5.2040	60

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

Bohr model for exciton

Semiconductor Picture

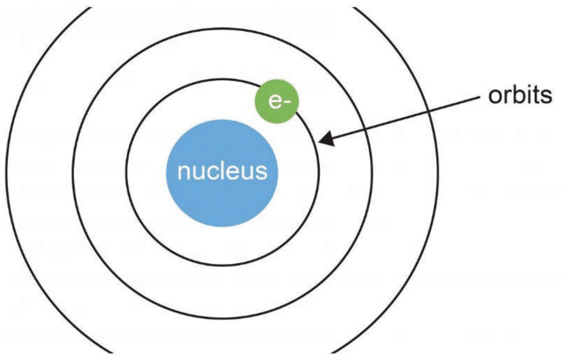




hape the Future.

Fox, Chapter 4

Bohr model for free excitons



Electron and hole form a bound state with binding energy.

$$E(n) = -\frac{\mu}{m_0}\frac{1}{\varepsilon_r^2}\frac{R_H}{n^2} = -\frac{R}{n^2}$$

R_H=13.6 eV Rydberg energy.
QM mechanical treatment easy.

1. Reduced electron/hole mass (**optical mass**) $\frac{1}{\mu} = \frac{1}{m_e} + \frac{1}{m_h}$
2. **Static screening** with static dielectric constant ε_r.
3. **Exciton radius**: $a_n = \frac{m_0}{\mu}\varepsilon_r n^2 a_H$

   a_H=0.53 Å
4. Excitons **stable** if *R*>>kT ????
5. Exciton **momentum** is zero.
6. **Exciton enhancement important even if R<<kT.**

Sommerfeld enhancement

Excitonic Rydberg energy

$$R = \frac{\mu}{m_0 \varepsilon_r^2} R_H$$

Discrete states

$$E_n = E_g - \frac{1}{n^2} R_X$$

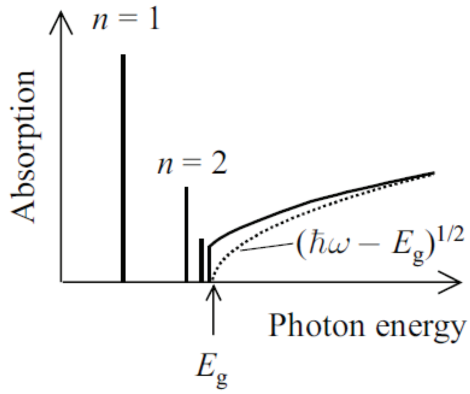
Discrete absorption

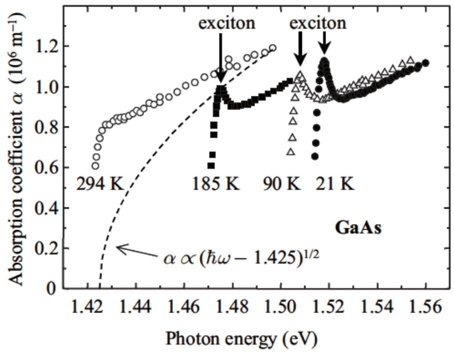
$$\varepsilon_2(E) = \frac{8\pi |P|^2 \mu^3}{3\omega^2 (4\pi\varepsilon_0)^3 \varepsilon_r^3} \sum_{n=1}^{\infty} \frac{1}{n^3} \delta(E - E_n)$$

Continuum absorption

$$\varepsilon_2(E) = \frac{2|P|^2 (2\mu)^{3/2} \sqrt{E - E_0}}{3\omega^2} \frac{\xi e^{\xi}}{\sinh \xi}$$

$$\xi = \pi \sqrt{R/_{E - E_0}}$$





Use Bohr wave functions to calculate ε_2.
Toyozawa discusses broadening.

R. J. Elliott, Phys. Rev. **108**, 1384 (1957)
Yu & Cardona; Fox, Chapter 4

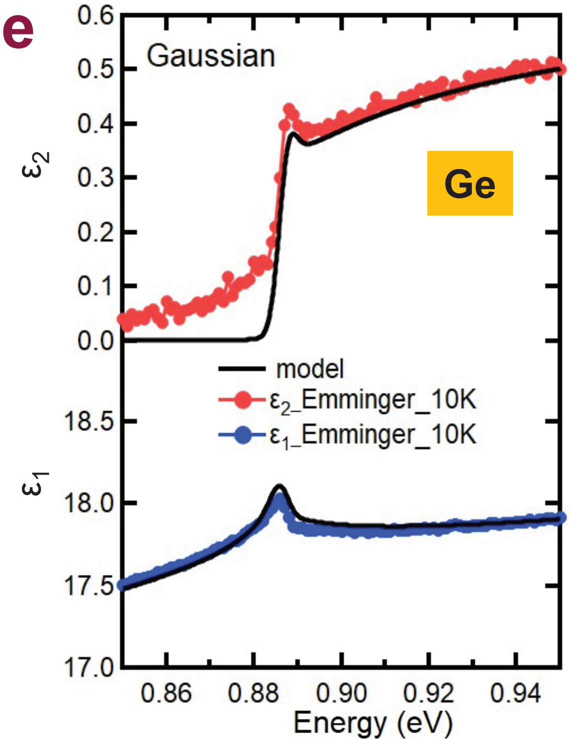
Elliott-Tanguy theory applied to Ge

- **Fixed parameters:**
- Electron and hole masses (temperature dependent)
- Excitonic binding energy R
- Amplitude A (derived from matrix element P)

- **Adjustable parameters:**
- Broadening Γ: 2.3 meV
- Band gap E_0
- Linear background A_1 and B_1 (contribution from E_1 to real part of ε)

Quantitative agreement

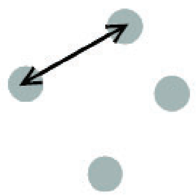
- **Problems:**
- Broadening below the gap (band tail, oxide correction)



Carola Emminger *et al.*, JAP **131**, 165701 (2022).

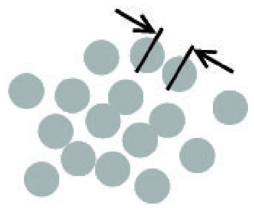
Condensation of excitons at high density

Exciton gas



(a) Low density
Separation $\gg$ diameter

Electron-hole liquid



(b) High density
Separation $\approx$ diameter

Mott transition (insulator-metal) when electron separation equals exciton radius.

Electron separation d for density N

$$d = \sqrt[3]{\frac{3}{4\pi n}} \qquad r_s = \frac{d}{a_X} \qquad \text{dimensionless}$$

Mott transition occurs at r_s near 1.
GaAs: $n=10^{17}$ cm^{-3}.

Biexciton, triexciton molecule formation.
Electron-hole droplets. Bose-Einstein condensation.

Excitons in doped or excited semiconductors

Need to include exciton screening due to doping.
Yukawa potential: Schrödinger equation not solvable.
Use Hulthen potential as an approximation

Coulomb $V(r) = -k\frac{1}{r}$ $\qquad k = \frac{e^2}{4\pi\varepsilon_0\varepsilon_r}$

Yukawa $V(r) = -k\frac{\exp(-r/\lambda_D)}{r}$ $\qquad \lambda_D = \sqrt{\frac{\varepsilon_r\varepsilon_0 k_B T}{ne^2}} = \frac{1}{k_D}$

Debye screening length

Hulthen $V(r) = -k\frac{2/ga_X}{\exp\left(\frac{2r}{ga_X}\right) - 1}$ $\qquad g = \frac{\lambda_D}{a_X}$

Unscreened: g=∞
Fully screened: g=0
Mott criterion: g=1

Hulthen exciton

e Future.

C. Tanguy, Phys. Rev. **60,** 10660 (1999).
Banyai & Koch, Z. Phys. B **63**, 283 (1986).

Tanguy: Dielectric function of screened excitons

Bound exciton states (finite number):

$$A=\frac{\hbar^2 e^2}{6\pi\varepsilon_0 m_0^2}\left(\frac{2\mu}{\hbar^2}\right)^{3/2}|P|^2$$

$$\varepsilon_2(\omega)=\frac{2\pi A\sqrt{R}}{E^2}\sum_{n=1}^{n^2<g}2R\frac{1}{n}\left(\frac{1}{n^2}-\frac{n^2}{g^2}\right)\delta\left[E-E_0+\frac{R}{n^2}\left(1-\frac{n^2}{g}\right)^2\right]$$

Reduced Rydberg energy

exciton continuum:

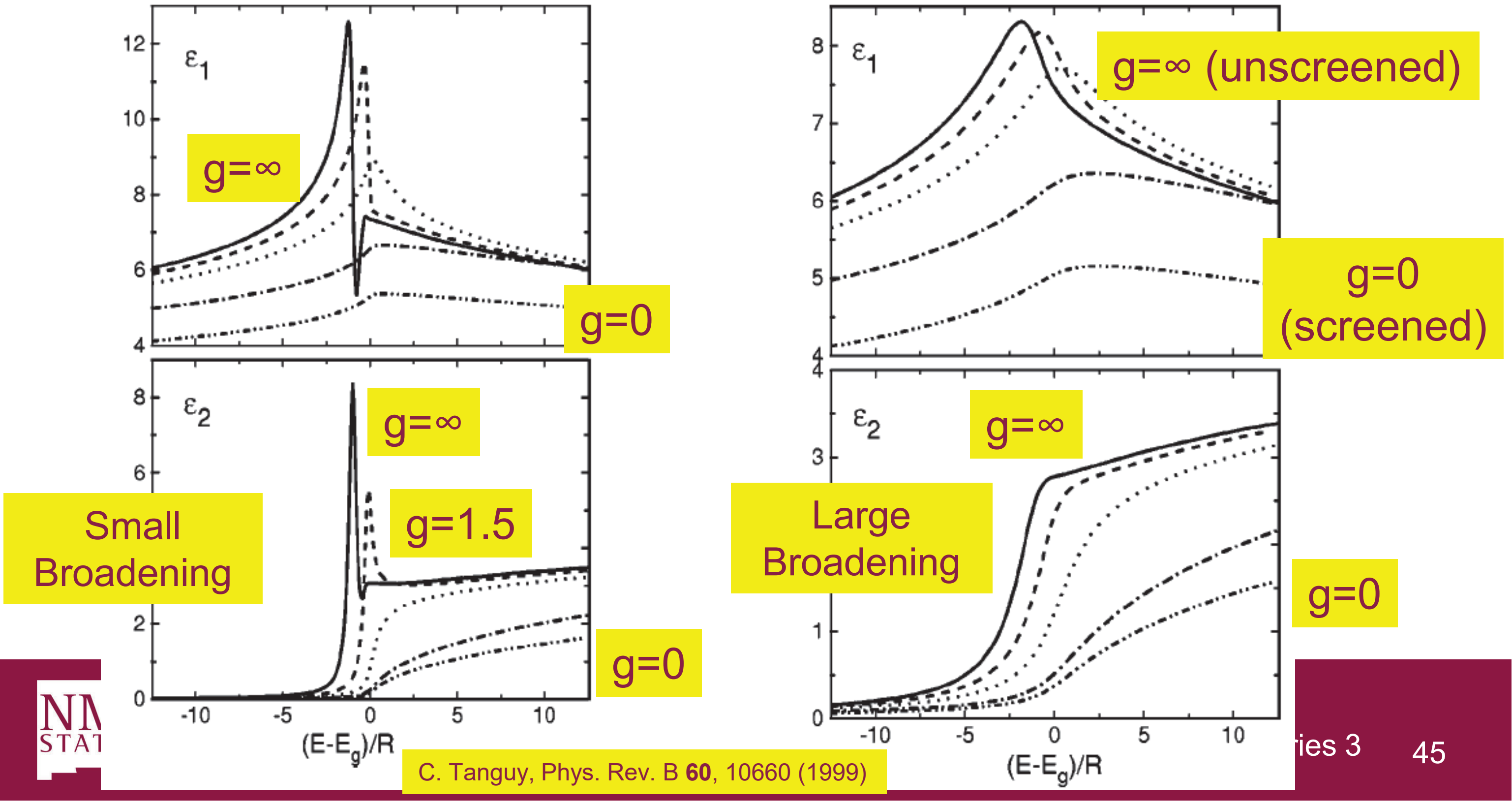
$$\varepsilon_2(\omega)=\frac{2\pi A\sqrt{R}}{E^2}\frac{\sinh\pi g k}{\cosh(\pi g k)-\cosh\left(\pi g\sqrt{k^2-\frac{4}{g}}\right)}\theta(E-E_0)$$

$$k=\pi\sqrt{(E-E_0)/R}$$

Need to introduce Lorentzian broadening and perform numerical KK transform.

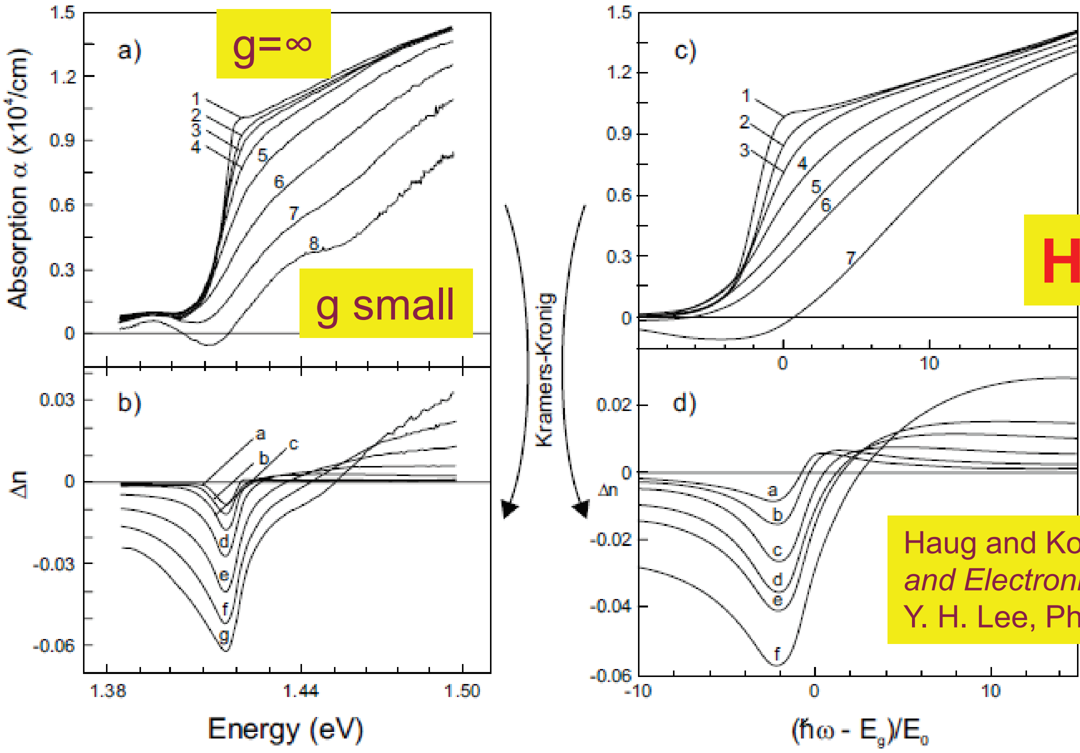
C. Tanguy, Phys. Rev. B **60**, 10660 (1999)

Tanguy: Dielectric function of screened excitons



C. Tanguy, Phys. Rev. B **60**, 10660 (1999)

Excitons in laser-excited GaAs



GaAs 300 K

High laser excitation

Hulthen exciton

Haug and Koch, *Quantum Theory of Optical and Electronic Properties of Semiconductors*

Y. H. Lee, Phys. Rev. Lett **57**, 2446 (1986)

Two-dimensional Bohr problem

$$H = -\frac{\hbar^2}{2\mu_\perp}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) - \frac{\hbar^2}{2\mu_\parallel}\frac{\partial^2}{\partial z^2} - \frac{e^2}{\varepsilon_r r}$$

Assume that $\mu_\parallel$ is infinite (separate term).
Use cylindrical coordinates.
Separate radial and polar variables.
Similar Laguerre solution as 3D Bohr problem.

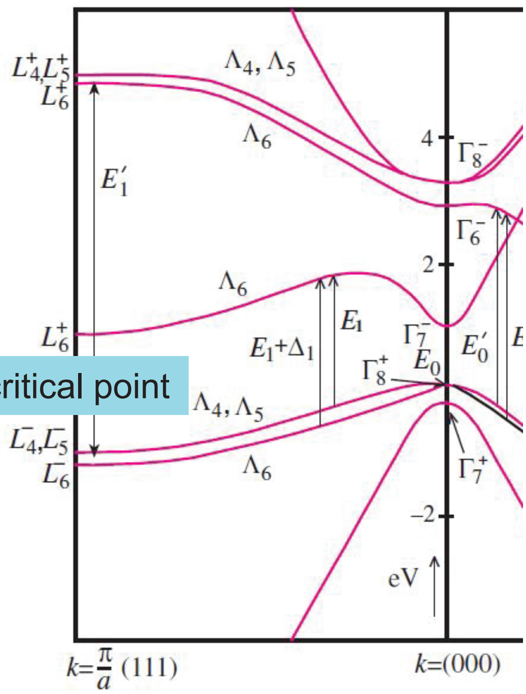
$$a_X = \frac{4\pi\varepsilon_0\varepsilon_r\hbar^2 m_0}{\mu_\perp \mu e^2}$$

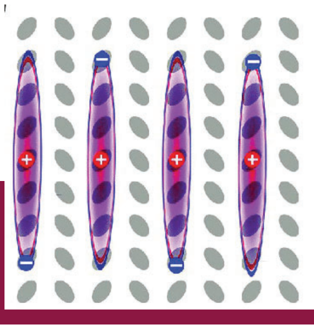
$$R = \frac{\mu_\perp e^4}{2\hbar^2 m_0 (4\pi\varepsilon_0\varepsilon_r)^2}$$

$$E_n = -\frac{R}{\left(n-\frac{1}{2}\right)^2}, \qquad n = 1,2,\ldots$$

Half-integral quantum numbers

2D critical point





M. Shinada and S. Sugano, J. Phys. Soc. Jpn. **21**, 1936 (1966).

Two-dimensional saddle-point excitons (E_1, $E_1+\Delta_1$)

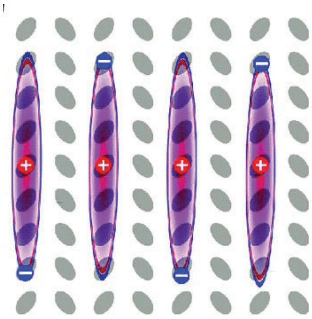
$$\varepsilon(E) = \frac{A}{(E+i\Gamma)^2}\{g[\xi(E+i\Gamma)] + g[\xi(-E-i\Gamma)] - 2g[\xi(0)]\}$$

$$g(\xi) = 2\ln(\xi) - 2\psi(\frac{1}{2} - \xi)$$

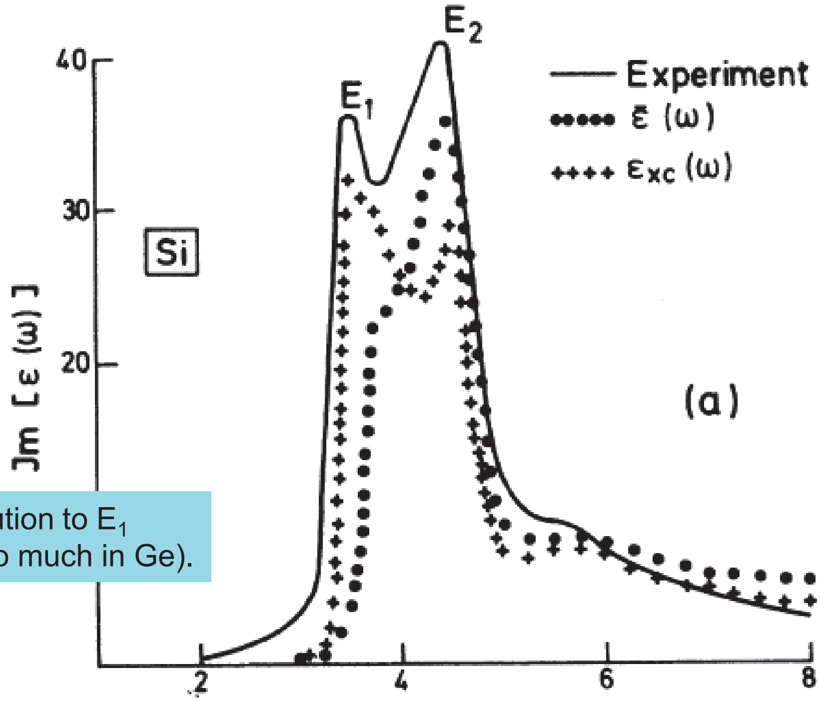
$$\psi(z) = \frac{d\ln\Gamma(z)}{dz}$$

$$\xi(z) = \sqrt{R/E_0 - z}$$

$$A = \frac{\mu e^2}{3\pi\varepsilon_0 m_0^2}|P|^2$$



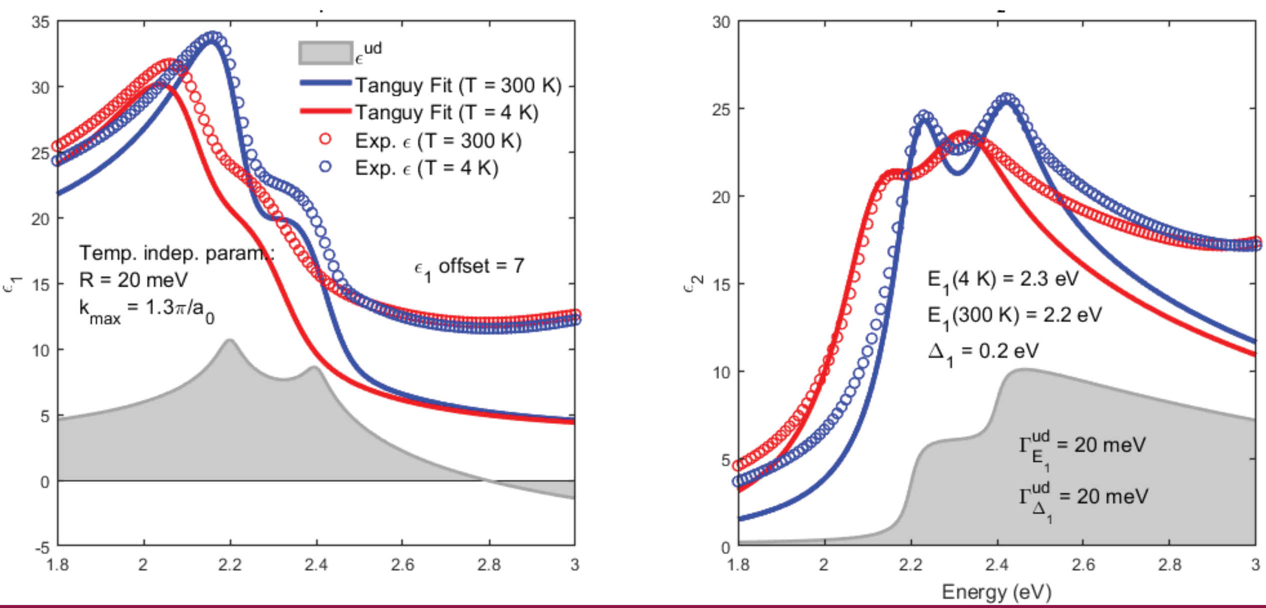
Strong excitonic contribution to E_1 critical point in Si (mot so much in Ge).



B. Velicky and J. Sak, phys. status solidi **16**, 147 (1966)
C. Tanguy, Solid State Commun. **98**, 65 (1996)
W. Hanke and L.J. Sham, Phys. Rev. B **21**, 4656 (1980)

Comparison with experimental data

$$\varepsilon(E, E_1, \Gamma, R, k_{\max}) = \frac{k_{\max} e^2 \bar{P}^2 \mu_\perp^{(E_1)}}{3\varepsilon_0 m^2 \pi (E + i\Gamma)^2} \left\{ g_a\left[\sqrt{\frac{R}{E_1 - (E + i\Gamma)}}\right] + g_a\left[\sqrt{\frac{R}{E_1 - (-E - i\Gamma)}}\right] - 2g_a\left[\sqrt{\frac{R}{E_1 - (0)}}\right] \right\}$$



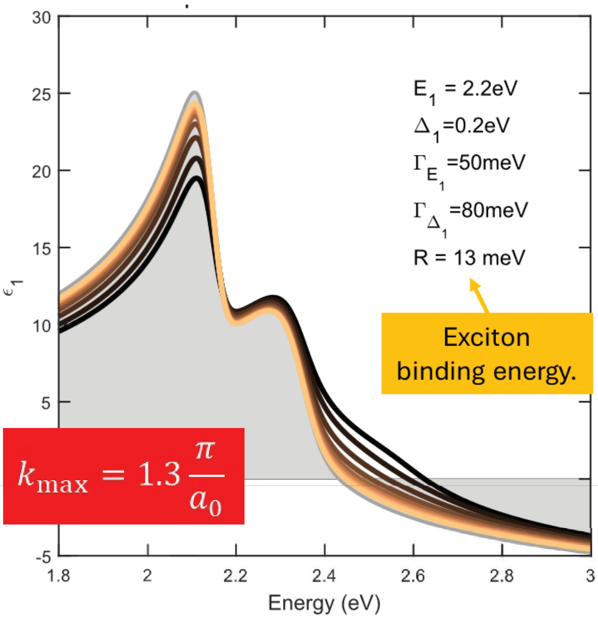
Experimental data:

Emminger (5 K), JVST B **38**, 012202 (2020).

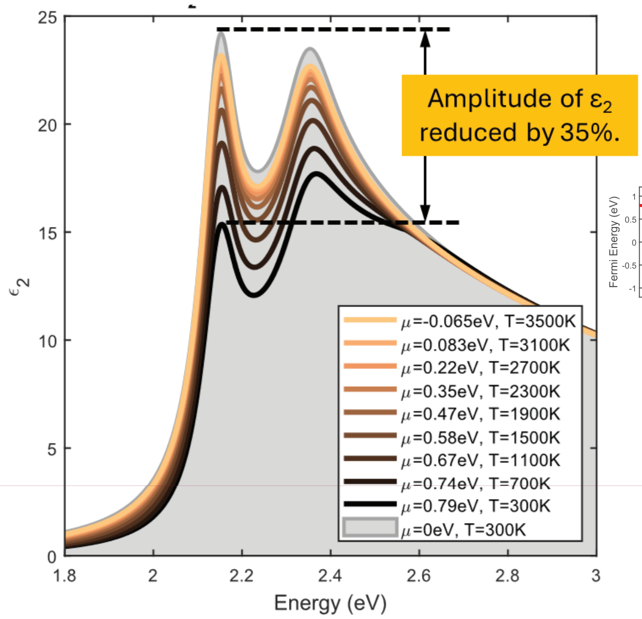
Nunley (300 K), JVST B **34**, 061205 (2016)

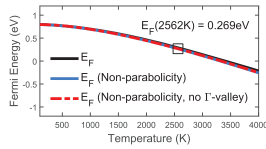
2D excitons with band filling (E_1, $E_1+\Delta_1$)

$$\varepsilon_2(E) = \frac{e^2 \mu_\perp^{(E_1)} \bar{P}^2}{6\varepsilon_0 m^2 \pi} \mathrm{Im}\left\{\frac{\{g_a[\xi(E+i\Gamma)] + g_a[\xi(-E-i\Gamma)] - 2g_a[\xi(0)]\}}{(E+i\Gamma)^2}\right\} \int_{-k_{\max}}^{k_{\max}} \{1 - f[E_c(E, k_z^2)]\} dk_z$$

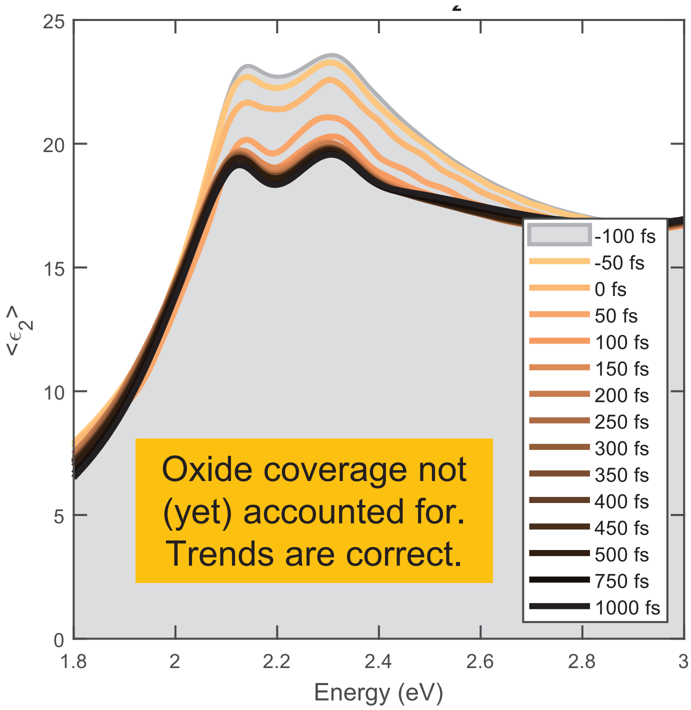


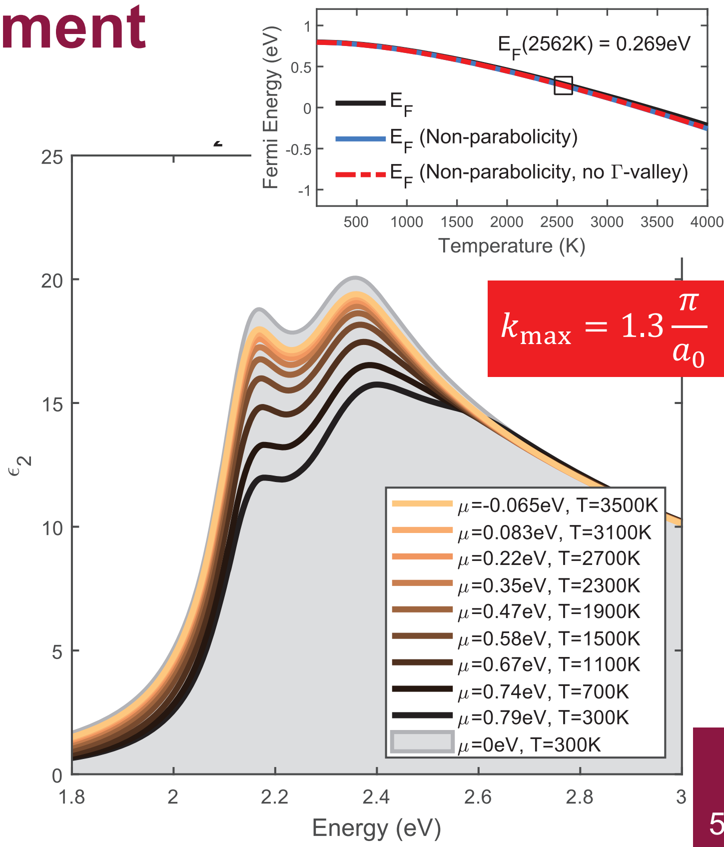
$$k_{\max} = 1.3\,\frac{\pi}{a_0}$$





Comparison with experiment





$$k_{\max} = 1.3\,\frac{\pi}{a_0}$$

Conclusions

- Calculated electron-hole concentration (about 10^{20} cm^{-3}) from Fermi-Dirac statistics.
- Electrons initially in Γ-valley, very hot electron plasma (2500 K)
- Within 50 fs, most electrons (>50%) scatter to the X-valley (large density of states).
- Electrons cool by intervalley scattering.
  When T<1000 K, most electrons are in the L-valley
  L-electrons are observable by bleaching the absorption of the probe pulse.
- Theory predicts a reduction of ε_2 due to band filling (Pauli blocking) by about 20%.
- **A reduction by 25% is observed in the experiment, but the amplitude and line shape are wrong.**
- **Low-density dielectric function can be modeled by 2D-excitons.**
- **Band filling effects are in good agreement with transient dielectric function.**

- **What is missing?**
- Excitonic (Sommerfeld) enhancement is screened by high electron density (TBD).

Thank you!

Questions?

Many students contributed to this project.

http://femto.nmsu.edu