Interaction of intense radiation with materials

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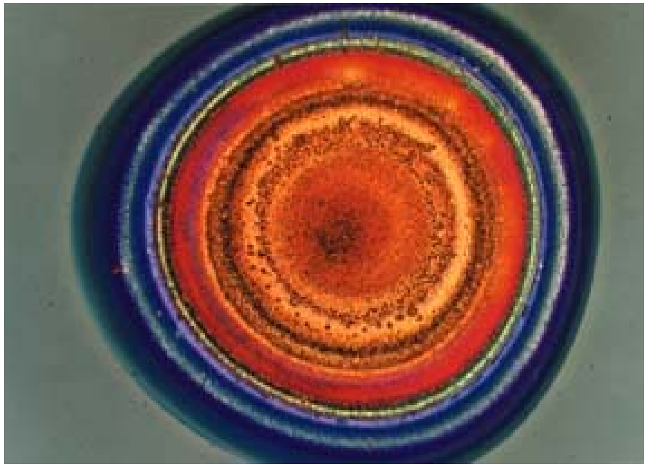
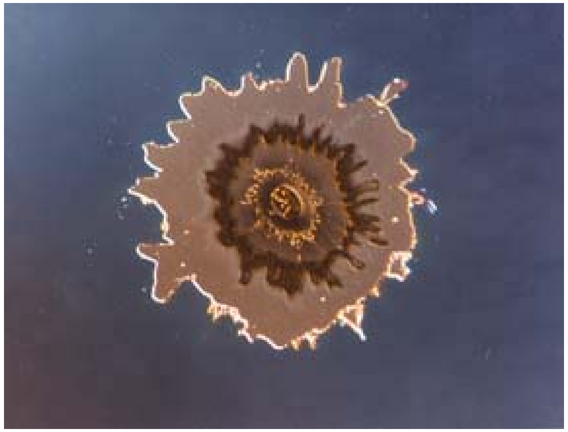
Laser Damage to Semiconductors

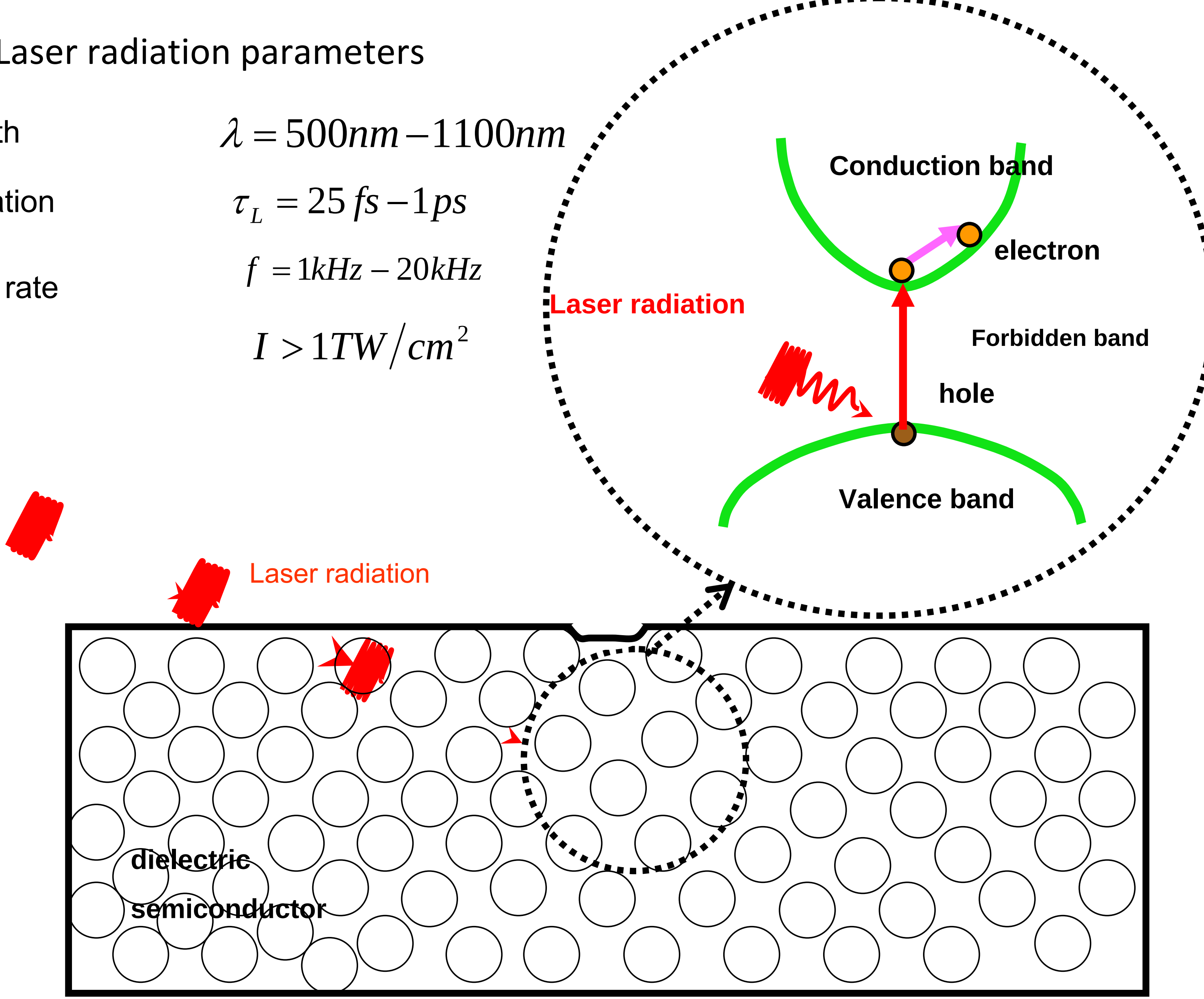




- The damage of materials can be described by a critical density of photo-excited electrons in the conduction band
- The critical density can be directly determined through observation of a total reflection of a laser from an electron plasma

Laser radiation parameters

Wavelength	$\lambda = 500nm - 1100nm$
Pulse duration	$\tau_L = 25\,fs - 1\,ps$
Repetition rate	$f = 1kHz - 20kHz$
Intensity	$I > 1TW/cm^2$



Investigated materials

Material	Laser wavelength λ	Laser pulse duration τ_L
SiO_2	1053 nm	25 fs - 300 fs
GaAs $GaAs/Al_xGa_{1-x}As$	763 nm $16\mu m - 22\mu m$	25 fs - 1 ps 1ps

- Short laser pulses –pulse durations $(\tau < 1ps)$ and intensity $(I > 1TW)$
- Not enough time for energy transfer to lattice
- Optical damage – due to a rapid electron production
- In contrast damage with long laser pulses $(\tau > 1ps)$

is due to thermal effects –melting and boiling

(i) Seed electrons in the material, made up initially of background conductionbandelectrons (CBE), are significantly increased in number via conventional photoionization channels (primarily multiphoton ionization (MPI)).

(ii) Heating of the free electrons occurs via inverse Bremsstrahlung in the laser field, as a result of multiple laser-assisted collisions with the material lattice.This is generally accompanied by a decline in the CBE population due to recombination and diffusion.

(iii) High-energy electrons, with energies exceeding the band gap, can collisionally promote more bound electrons into the conduction band. With sufficient electron density, this will lead to avalanche ionization (AVI) in the material. The transfer of electron plasma energy to the material lattice structure is responsible for the damage to the media.

- Laser Induced Breakdown (LIB) in bulk semiconductors- electron production in conduction band (CB) by combined

1. (coherent) excitation across the band-gap – single photon (narrow band-gap), multi-photon (wide band-gap)
2. (incoherent) inter-band transitions induced by collisional ionization with electrons that have acquired energy $E_{th} = E_G$ from the laser leading to avalanche

- critical electron density – the laser is completely reflected

- the laser fluence $F_{th} = \int I(t)dt \approx I_0\tau$ producing the critical electron density n_{cr} is the OBT (optical breakdown threshold).

- What are the mechanisms for energy gain – (CB electrons do not optically respond to the field w/o assistance from phonons and impurities)

1. for $\Omega\tau_p >> 1$ the average power gained from the laser leads to an energy drift of CB electrons to higher energies – this is a classical effect – joule heating
2. A free carrier absorption process via phonon assisted photon absorption of CB electrons

Classification of laser damage to semiconductors

•Optical – semiconductor gets opaque for $\Omega_L \geq \omega_p \propto n_c$

$$\Omega^2{}_L = \frac{e^2 n}{\varepsilon_0 \varepsilon_r(0) m^*{}_e}$$

$$n_c{}^{opt} = 1.3 \times 10^{23} cm^{-3}$$

- Electrical – by laser irradiation create N_I at T_m and produce big current under small bias

$N_I = \sqrt{N_C N_V} \exp\left(\frac{-E_G}{2k_B T}\right)$ thermally excited CE density at equilibrium

$$n_c{}^{elec} = 8.7 \times 10^{17} cm^{-3}$$

- Structural limit - the averaged kinetic energy per electron is high - chemical bonds unstable

$$\langle E_k \rangle = \frac{\int_0^{+\infty} E_k f_k dE_k}{\int_0^{+\infty} f_k dE_k} = E_G$$

Factors influencing laser damage to semiconductors

- Laser pulse width
- Peak intensity
- Semiconductor material properties
    - bandgap
    - Interband coupling
    - effective mass
    - phonon modes
    - lattice temperature
    - mobility

Theoretical model

$$H(t) = H_0(t) + H_I(t)$$

Total Hamiltonian

Non-interacting part

$$H_0(t) = \sum_{\vec{k}} E^e_{\vec{k}} \hat{a}^+_{\vec{k}}(t)\hat{a}_{\vec{k}}(t) + \sum_{\vec{q}} \hbar\omega_{\vec{q}} \hat{b}^+_{\vec{q}}(t)\hat{b}_{\vec{q}}(t)$$

Interacting part

$$H_I(t) = \sum_{\vec{k},\vec{q}} C_{\vec{q}} \hat{a}^+_{\vec{k}+\vec{q}}(t)\hat{a}_{\vec{k}}(t)\left[\hat{b}_{\vec{q}}(t) + \hat{b}^+_{-\vec{q}}(t)\right] + \sum_{\vec{k}} F_{\vec{k}} \hat{a}^+_{\vec{k}}(t)\hat{d}^+_{-\vec{k}}(t) + F^*_{\vec{k}}\hat{d}_{-\vec{k}}(t)\hat{a}_{\vec{k}}(t)$$

Find solution for the Schrodinger equation

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = \frac{1}{2m^*}\left[\vec{p} + \frac{e}{c}\vec{A}(\vec{r},t)\right]^2 \psi(\vec{r},t)$$

for an electron in an intense field

$$\vec{A}(t) = \left(E_{L0}c/\Omega_L\right)\sin(\Omega_L t)\vec{e}_x$$

The electron annihilation operator in an intense field is given by:

$$\hat{c}_{\vec{k}}(t) = \hat{a}_{\vec{k}}(t)\exp\left[i\gamma_0 k_x\left(1-\cos\Omega_L t\right)\right]\exp\left[i\gamma_1\left(\sin(2\Omega_L t)-2\Omega_L t\right)\right]$$

$$\gamma_0 = eE_{L0} / m^* \Omega_L{}^2$$

mean traveling length of electron in one period of laser radiation

$$\gamma_1 = \left(eE_{L0}\right)^2 / 8\hbar m^* \Omega_L{}^3$$

induced energy due to the interaction of electrons with the laser field

Calculate electron-phonon interaction using the modified electron states- dynamic equation for the conduction-electron distribution function is obtained

$$\frac{\partial}{\partial t} n_{\vec{k}}^{e} = \left(1 - n_{\vec{k}}^{e}\right)\frac{2\pi}{\hbar}\sum_{\vec{q}\lambda}\left|C_{\vec{q}\lambda}\right|^{2}\left(e\left|\vec{q}.\vec{\mathrm{E}}(t)\right|/m^{*}\Omega_{L}^{2}\right)^{2}$$

$$\times\left[n_{\vec{k}-\vec{q}}^{e} N_{\vec{q}\lambda}^{ph}\delta\left(E_{\vec{k}} - E_{\vec{k}-\vec{q}} - \hbar\omega_{\vec{q}\lambda} - \hbar\Omega_{L}\right) + n_{\vec{k}+\vec{q}}^{e}\left(N_{q}^{ph} + 1\right)\delta\left(E_{\vec{k}} - E_{\vec{k}+\vec{q}} + \hbar\omega_{\vec{q}\lambda} + \hbar\Omega_{L}\right)\right]$$

$$- n_{\vec{k}}^{e}\frac{2\pi}{\hbar}\sum_{\vec{q}\lambda}\left|C_{\vec{q}\lambda}\right|^{2}\left(e\left|\vec{q}.\vec{\mathrm{E}}(t)\right|/m^{*}\Omega_{L}^{2}\right)^{2}$$

$$\left[\left(1 - n_{\vec{k}+\vec{q}}^{e}\right)N_{\vec{q}\lambda}^{ph}\delta\left(E_{\vec{k}+\vec{q}} - E_{\vec{k}} - \hbar\omega_{\vec{q}\lambda} - \hbar\Omega_{L}\right) + \left(1 - n_{\vec{k}-\vec{q}}^{e}\right)\left(N_{\vec{q}\lambda}^{ph} + 1\right)\delta\left(E_{\vec{k}-\vec{q}} - E_{\vec{k}} + \hbar\omega_{\vec{q}\lambda} + \hbar\Omega_{L}\right)\right]$$

1, Expand for small phonon and photon energies relative to electron energies

2. Include local fluctuation of electron kinetic energy due to laser field or free carrier absorption of photons for $\Omega_{L}\tau_{p} >> 1$

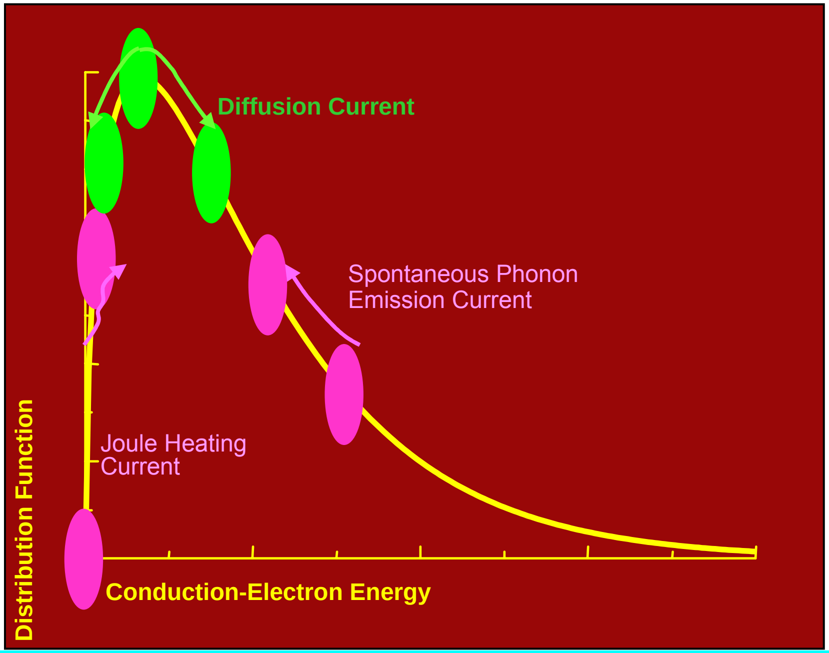
3. Include impact ionization and Auger recombination as second-order two-particle Coulomb scattering processes

4. Include one-photon stimulated interband absorption of photons

Energy loss to phonons term

$$\frac{\partial f^{e}(E,t)}{\partial t} + V(E,t)\frac{\partial f^{e}(E,t)}{\partial E} - D(E,t)\frac{\partial^{2} f^{e}(E,t)}{\partial \left(E_{k}^{e}\right)^{2}} = A(E,t)\, f^{e} + S(E,t)$$

Terms:
Photon ionization
Impact ionization
Auger recombination



- **The distribution function is a product of the density-of-states and the state-occupation probability**
- **Electrons can flow to higher energies by gaining power from an incident pulsed laser field**
- **Electrons can also flow to lower energies by emitting spontaneous phonons**
- **The competition between different currents in the energy space can be described by a Fokker-Planck equation**

Local fluctuation of electron kinetic energy is included in the kinetic Fokker-Planck equation under the condition

$$\Omega_L \tau_p >> 1$$

$\left\langle \mathrm{E}_L(t) \right\rangle_t = 0$ but $\left\langle \mathrm{E}_L^2(t) \right\rangle_t \neq 0$ where $\mathrm{E}_L(t) = \mathrm{E}_{0L} \cos(\Omega_L t)$

$$V(E,t) = V_T(E) + \frac{1}{3}\sigma(\Omega_L)\mathrm{E}_{0L}^2 + A_T(E)\frac{\tau_p}{3}\sigma(\Omega_L)\mathrm{E}_{0L}^2$$

$$D(E,t) = D_T(E) + \frac{2}{3}\sigma(\Omega_L)\mathrm{E}_{0L}^2 E + V_T(E)\frac{\tau_p}{3}\sigma(\Omega_L)\mathrm{E}_{0L}^2$$

$\sigma_c(\Omega_L) = e^2\tau_e / m_e^* \left(1 + \Omega_L^2 \tau_p^2\right)$ Drude ac conductivity

ensemble-average relaxation time

Free carrier absorption of photons

$$\Omega_L \tau_p >> 1$$

$$V(E,t) = V_T(E) + V_F(E)$$

$$D(E,t) = D_T(E) + D_F(E)$$

$$A(E,t) = A_T(E) + A_F(E)$$

$$A_T\left(E_{\vec{k}}\right) = \frac{2\pi}{\hbar}\sum_{\vec{q}\lambda}\left|C_{\vec{q}\lambda}\right|^2 \times\left[N_{\vec{q}\lambda}^{ph}\delta\left(E_{\vec{k}} - E_{\vec{k}-\vec{q}} - \hbar\omega_{\vec{q}\lambda}\right) - \left(N_{\vec{q}\lambda}^{ph} + 1\right)\delta\left(E_{\vec{k}} - E_{\vec{k}+\vec{q}} + \hbar\omega_{\vec{q}\lambda}\right)\right]$$

$$V_T\left(E_{\vec{k}}\right) = \frac{2\pi}{\hbar}\sum_{\vec{q}\lambda}\left|C_{\vec{q}\lambda}\right|^2 \hbar\omega_{\vec{q}\lambda} \times\left[N_{\vec{q}\lambda}^{ph}\delta\left(E_{\vec{k}} - E_{\vec{k}-\vec{q}} - \hbar\omega_{\vec{q}\lambda}\right) - \left(N_{\vec{q}\lambda}^{ph} + 1\right)\delta\left(E_{\vec{k}} - E_{\vec{k}+\vec{q}} + \hbar\omega_{\vec{q}\lambda}\right)\right]$$

$$D_T\left(E_{\vec{k}}\right) = \frac{\pi}{\hbar}\sum_{\vec{q}\lambda}\left|C_{\vec{q}\lambda}\right|^2 \left(\hbar\omega_{\vec{q}\lambda}\right)^2 \times\left[N_{\vec{q}\lambda}^{ph}\delta\left(E_{\vec{k}} - E_{\vec{k}+\vec{q}} - \hbar\omega_{\vec{q}\lambda}\right) - \left(N_{\vec{q}\lambda}^{ph} + 1\right)\delta\left(E_{\vec{k}} - E_{\vec{k}+\vec{q}} + \hbar\omega_{\vec{q}\lambda}\right)\right]$$

dependence on magnitude and frequency of the field

$$V_F = \frac{2\pi}{\hbar}\sum_{\vec{q}\lambda}\left|C_{\vec{q}\lambda}\right|^2\left(e\left|\vec{q}.\vec{\mathrm{E}}(t)\right|/m^*\Omega_L^2\right)^2$$
$$\times N_{\vec{q}\lambda}^{ph}\left(E_k - E_{k-q}\right)\left[\delta\left(E_{\vec{k}} - E_{\vec{k}-\vec{q}} - \hbar\omega_{\vec{q}\lambda} + \hbar\Omega_L\right) + \delta\left(E_{\vec{k}} - E_{\vec{k}-\vec{q}} - \hbar\omega_{\vec{q}\lambda} - \hbar\Omega_L\right)\right]$$
$$+\left(N_{\vec{q}\lambda}^{ph} + 1\right)\left(E_k - E_{k-q}\right)\left[\delta\left(E_{\vec{k}} - E_{\vec{k}+\vec{q}} + \hbar\omega_{\vec{q}\lambda} + \hbar\Omega_L\right) + \delta\left(E_{\vec{k}} - E_{\vec{k}+\vec{q}} + \hbar\omega_{\vec{q}\lambda} - \hbar\Omega_L\right)\right]$$

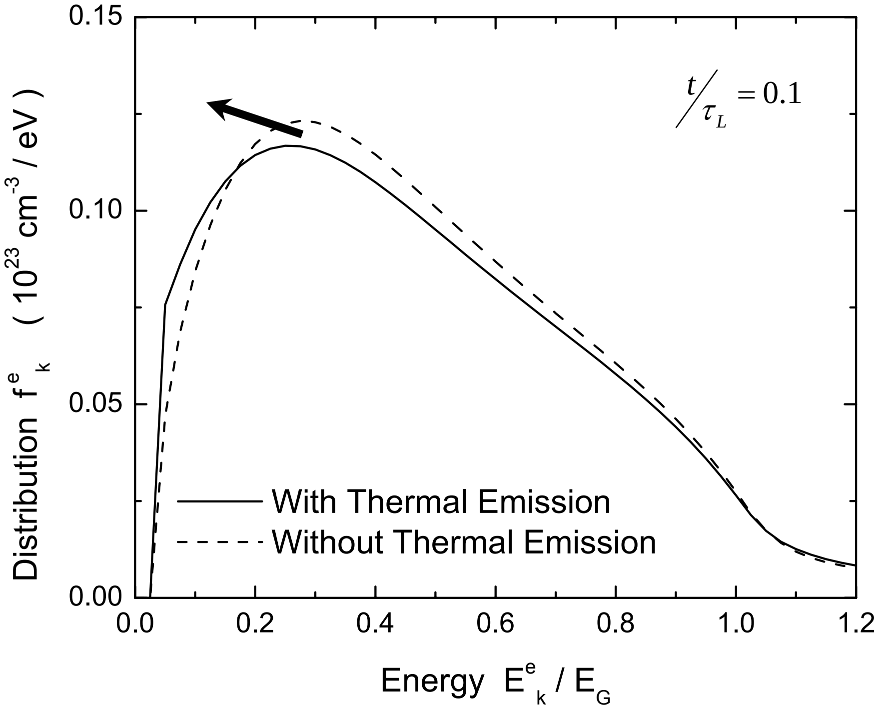
$$D_F = \frac{\pi}{4\hbar}\sum_{\vec{q}\lambda}\left|C_{\vec{q}\lambda}\right|^2\left(e\left|\vec{q}.\vec{\mathrm{E}}(t)\right|/m^*\Omega_L^2\right)^2$$
$$\times N_{\vec{q}\lambda}^{ph}\left(E_k - E_{k-q}\right)^2\left[\delta\left(E_{\vec{k}} - E_{\vec{k}-\vec{q}} - \hbar\omega_{\vec{q}\lambda} + \hbar\Omega_L\right) + \delta\left(E_{\vec{k}} - E_{\vec{k}-\vec{q}} - \hbar\omega_{\vec{q}\lambda} - \hbar\Omega_L\right)\right]$$
$$+\left(N_{\vec{q}\lambda}^{ph} + 1\right)\left(E_k - E_{k-q}\right)^2\left[\delta\left(E_{\vec{k}} - E_{\vec{k}+\vec{q}} + \hbar\omega_{\vec{q}\lambda} + \hbar\Omega_L\right) + \delta\left(E_{\vec{k}} - E_{\vec{k}+\vec{q}} + \hbar\omega_{\vec{q}\lambda} - \hbar\Omega_L\right)\right]$$

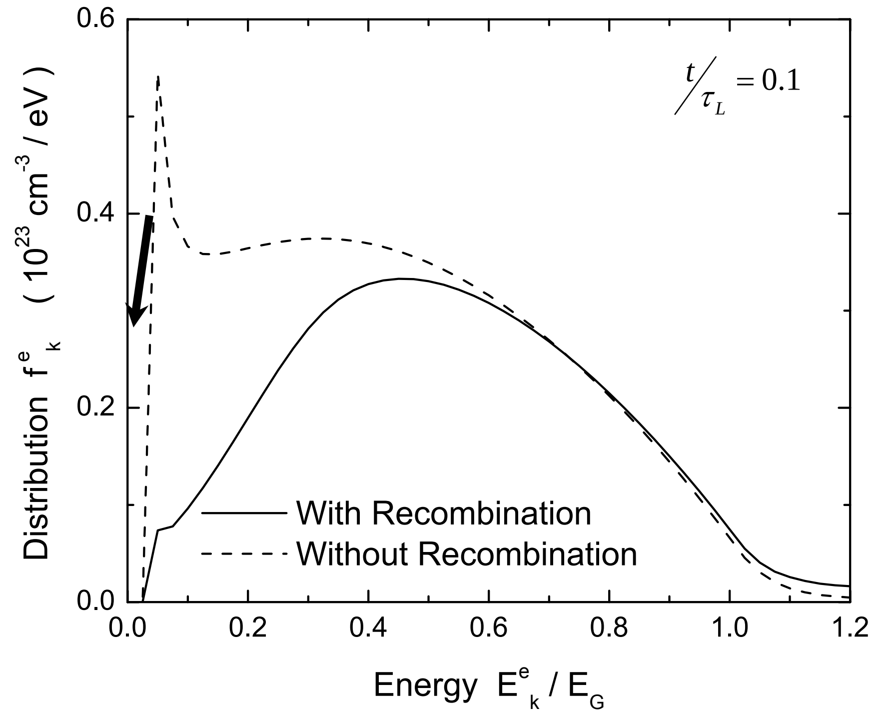
Single photon excitation

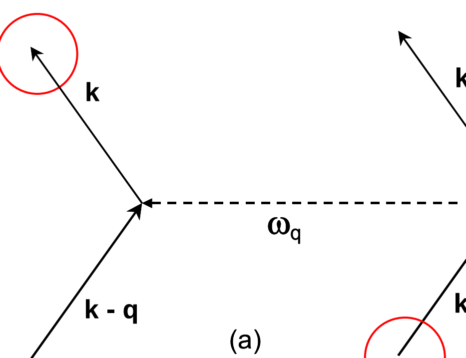
$$S_{abs} \propto \frac{2\pi}{\hbar}\left|F_k\right|^2\left[\frac{2F_k/\pi}{\left(\hbar\Omega_L - E_k^e - E_k^h - E_G\right)^2 + 4\left|F_k\right|^2}\right]$$

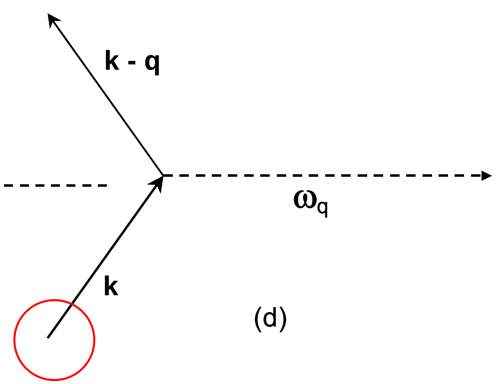
$$\left|F_k\right|^2 \approx \frac{e^2\mathrm{E}_{0L}^2}{m_0\Omega_L}\left[\left(\frac{m_0}{m_e^*} - 1\right)\frac{E_G\left(E_G + \Delta_0\right)}{2\left(E_G + 2\Delta_0/3\right)}\right]$$

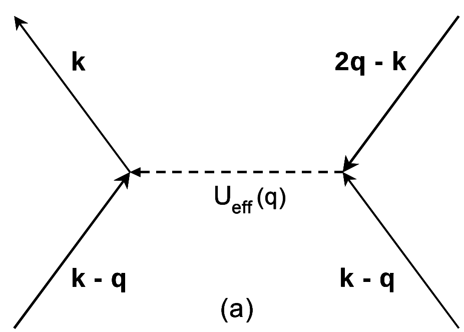
Effects of thermal emission and recombination

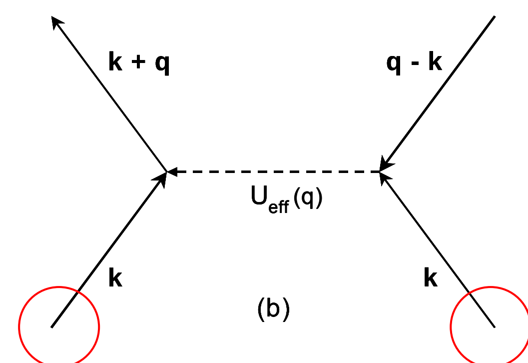












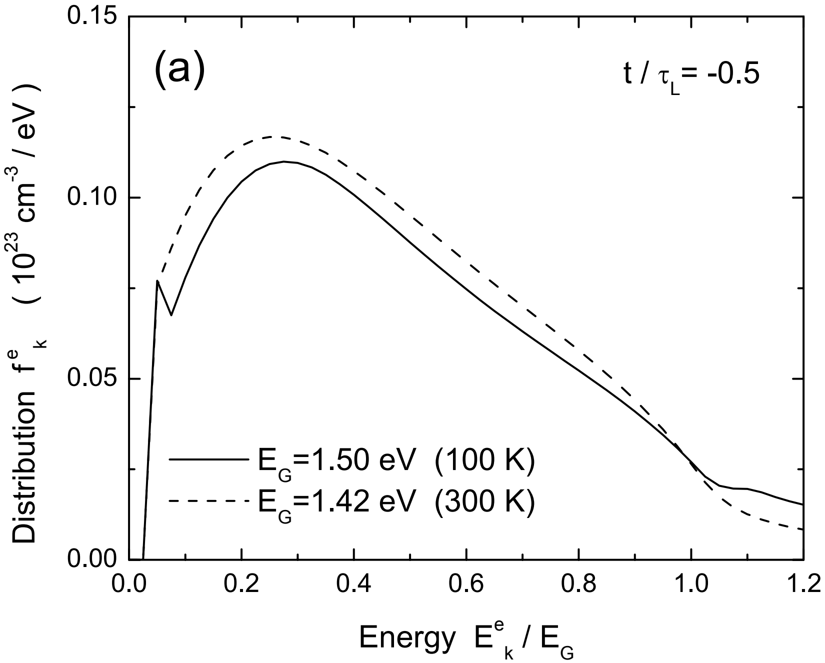
scattering-in

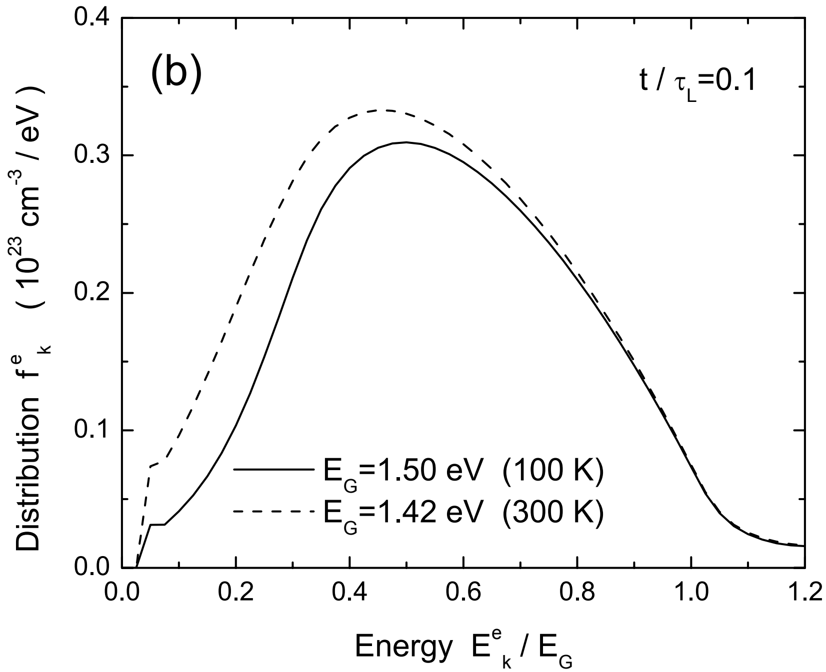
scattering-out

scattering-in

scattering-out

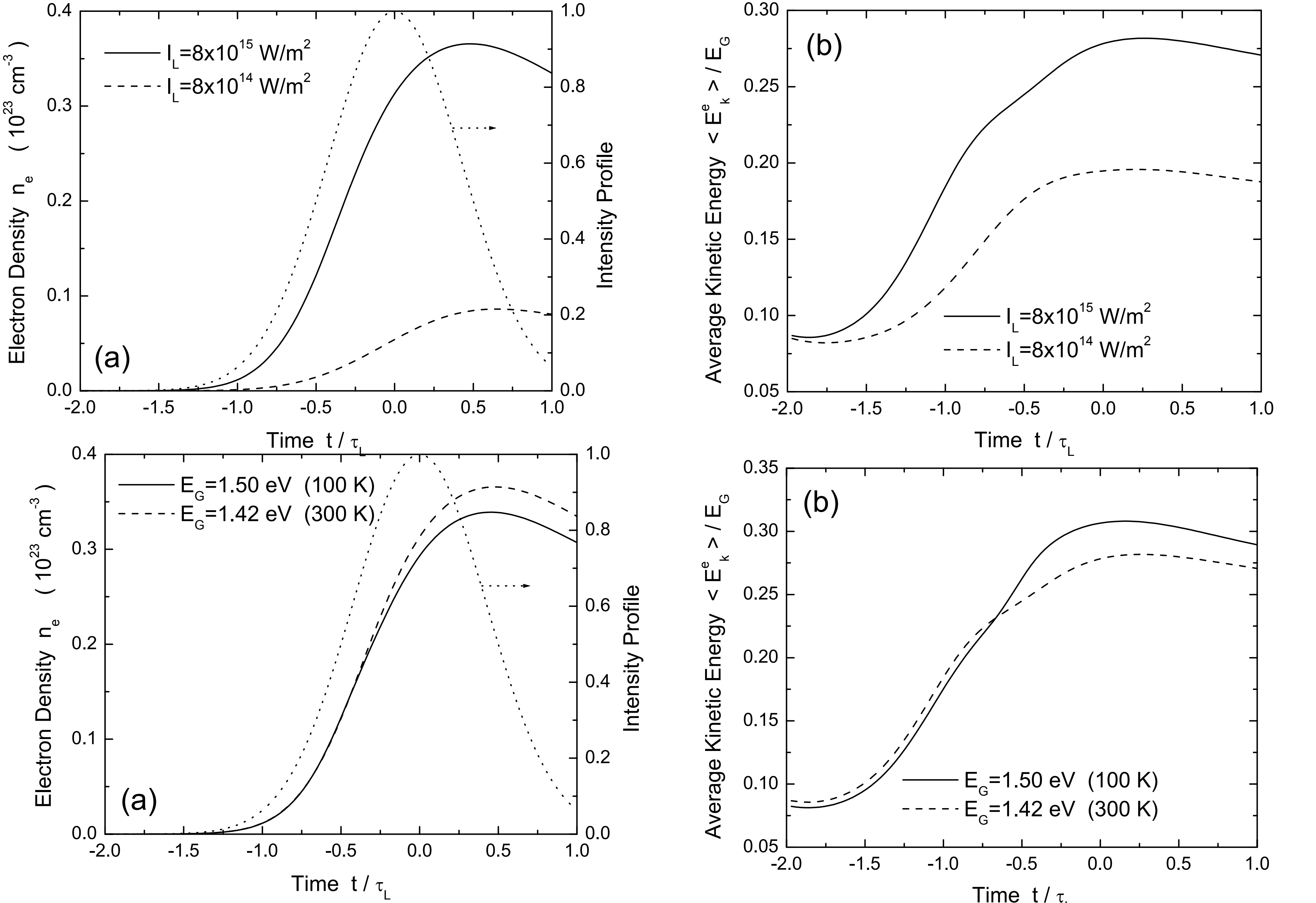
Effects of lattice temperature



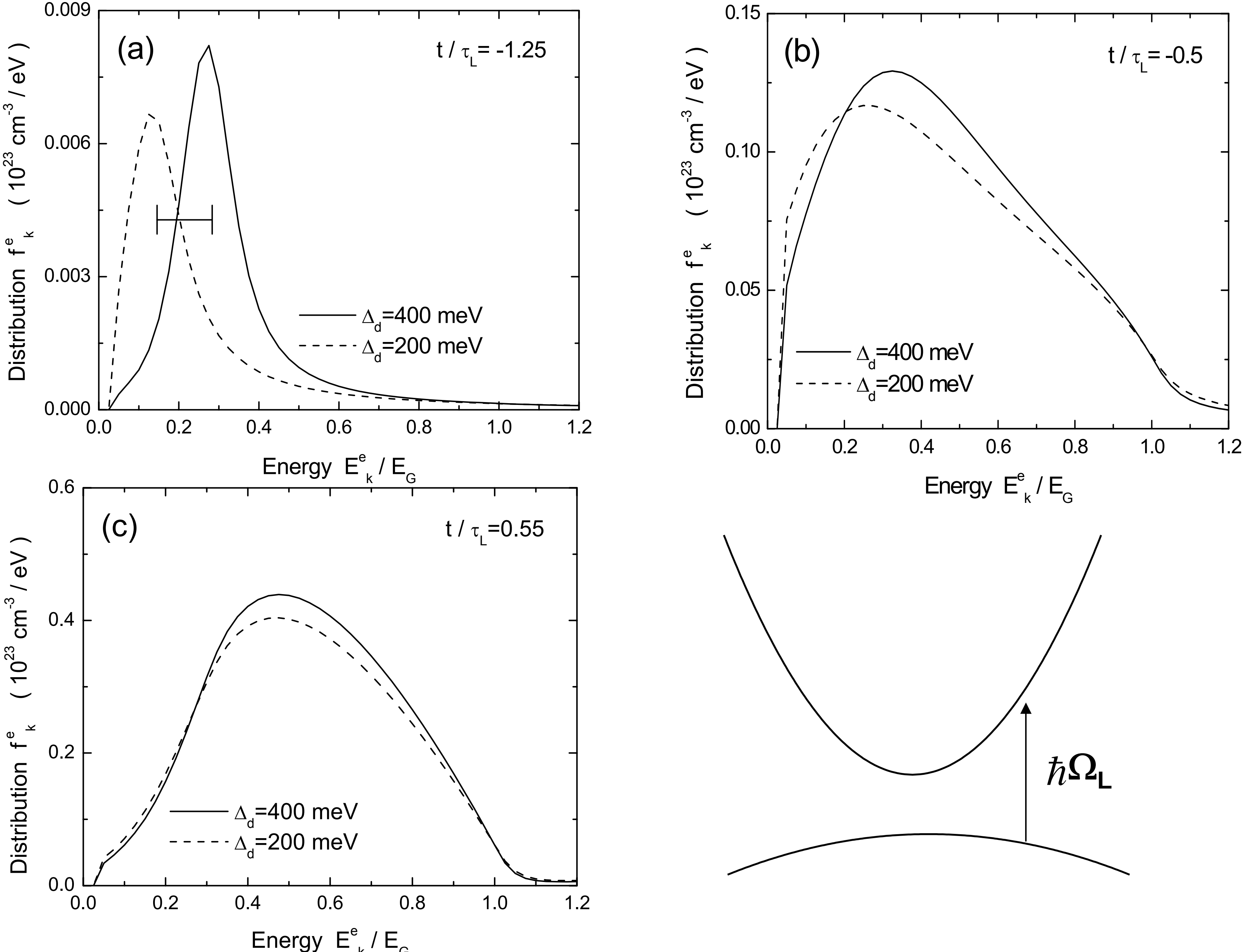


T. Apostolova et. al. Phys. Rev. B 66, 075208 (2002)

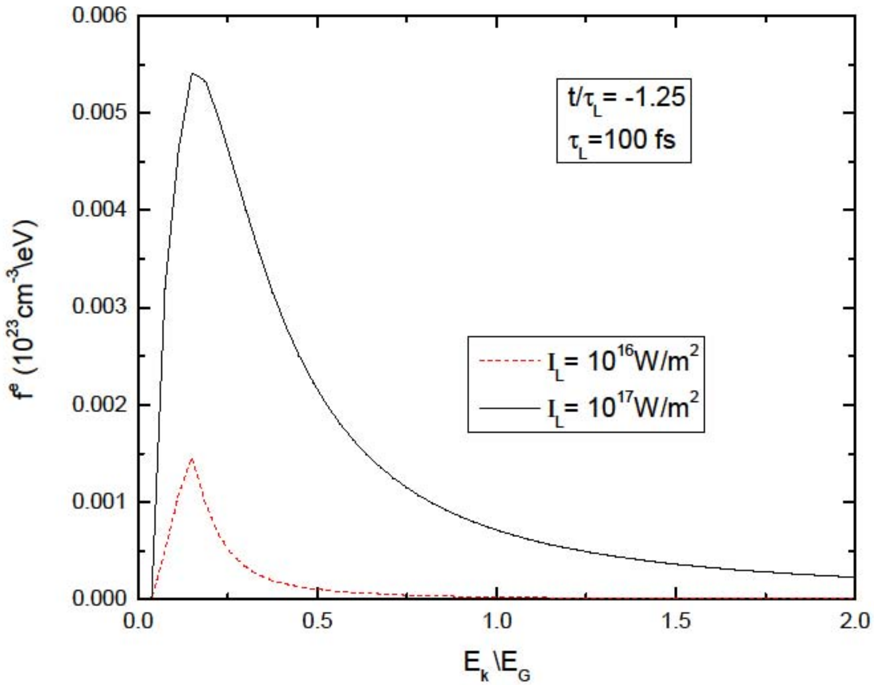
Time dependence of the electron density and average kinetic energy for different intensities and different bandgap widths

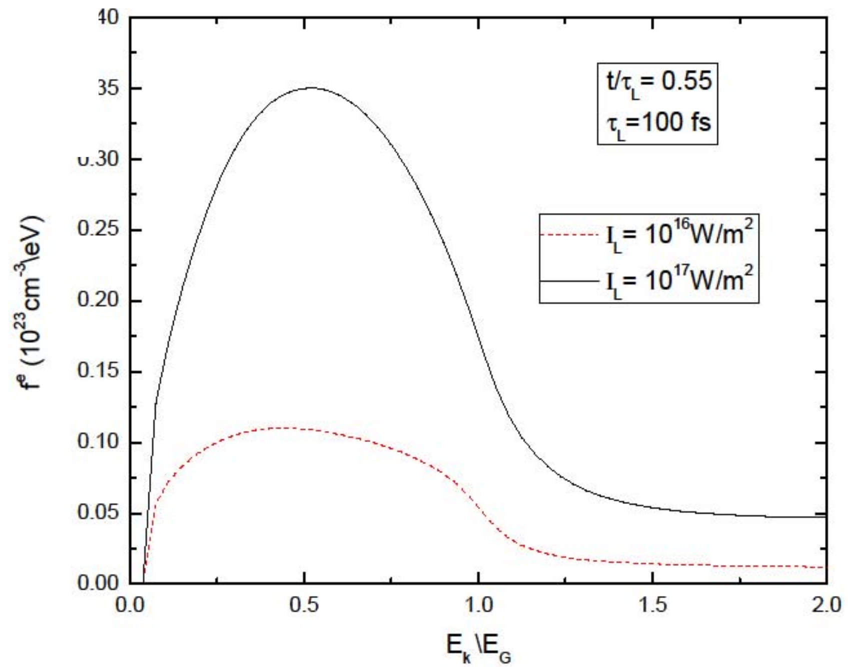


Effects of detuning

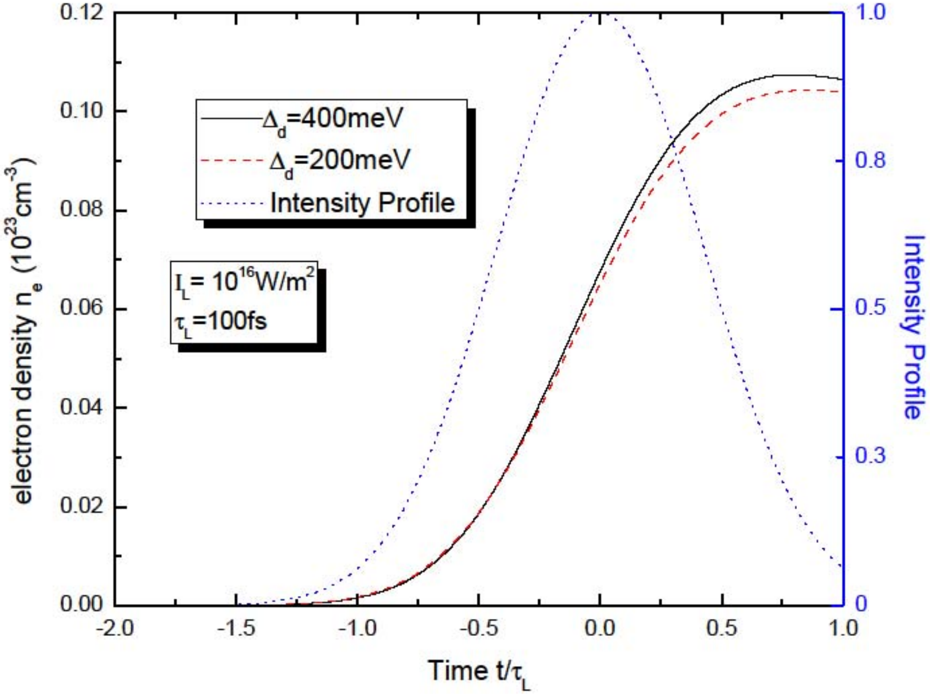


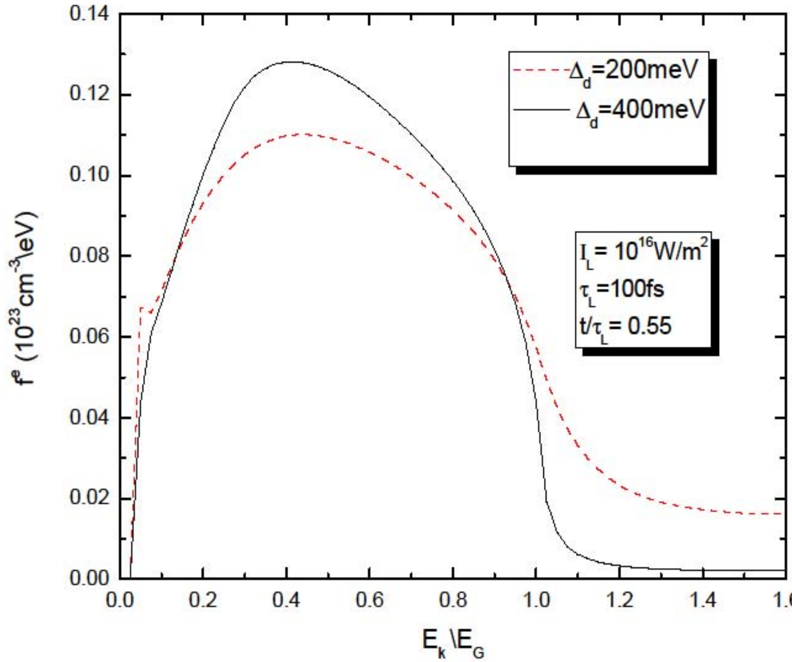
Effects of laser intensity – 100fs



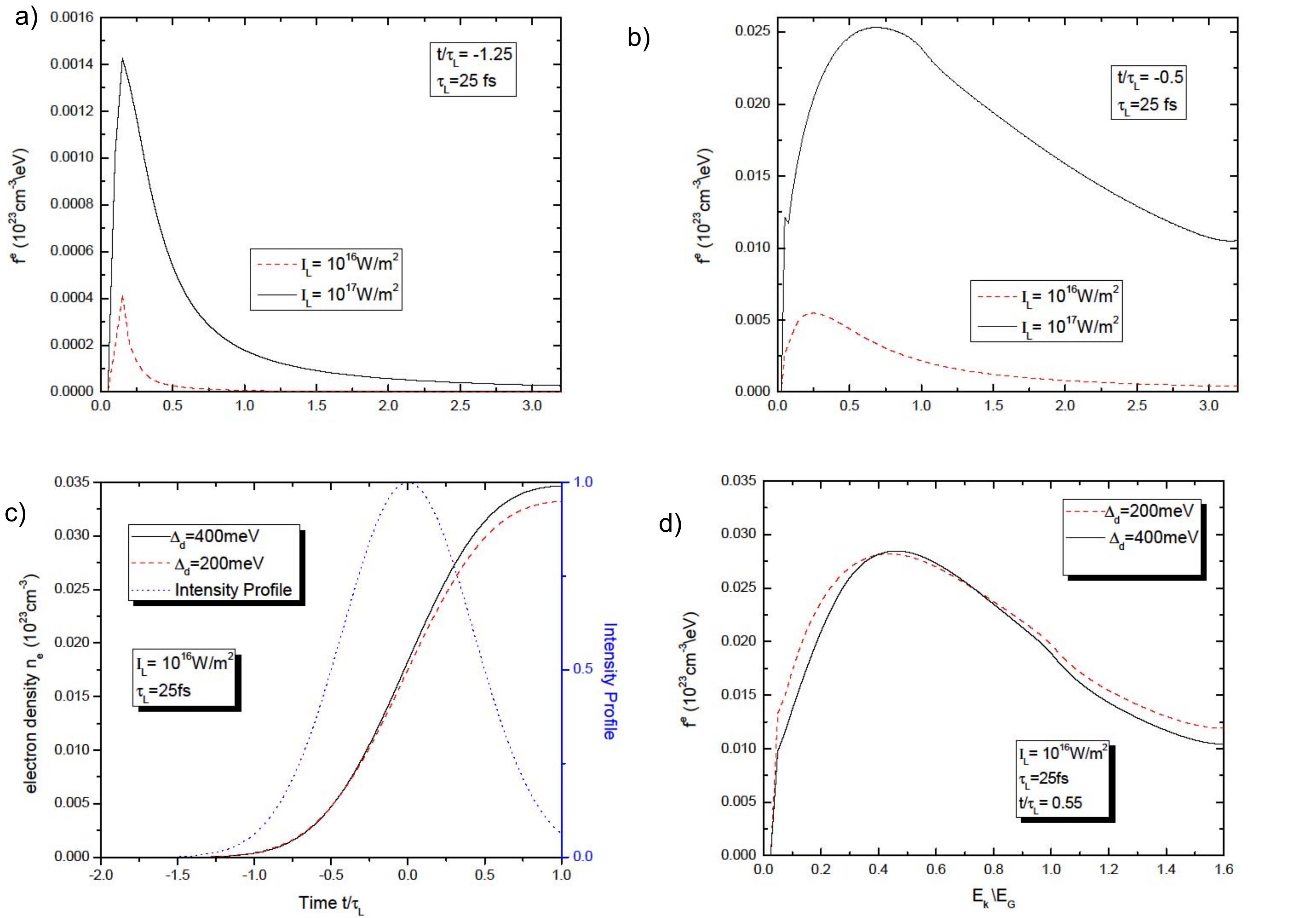


Effects of laser detuning– 100fs



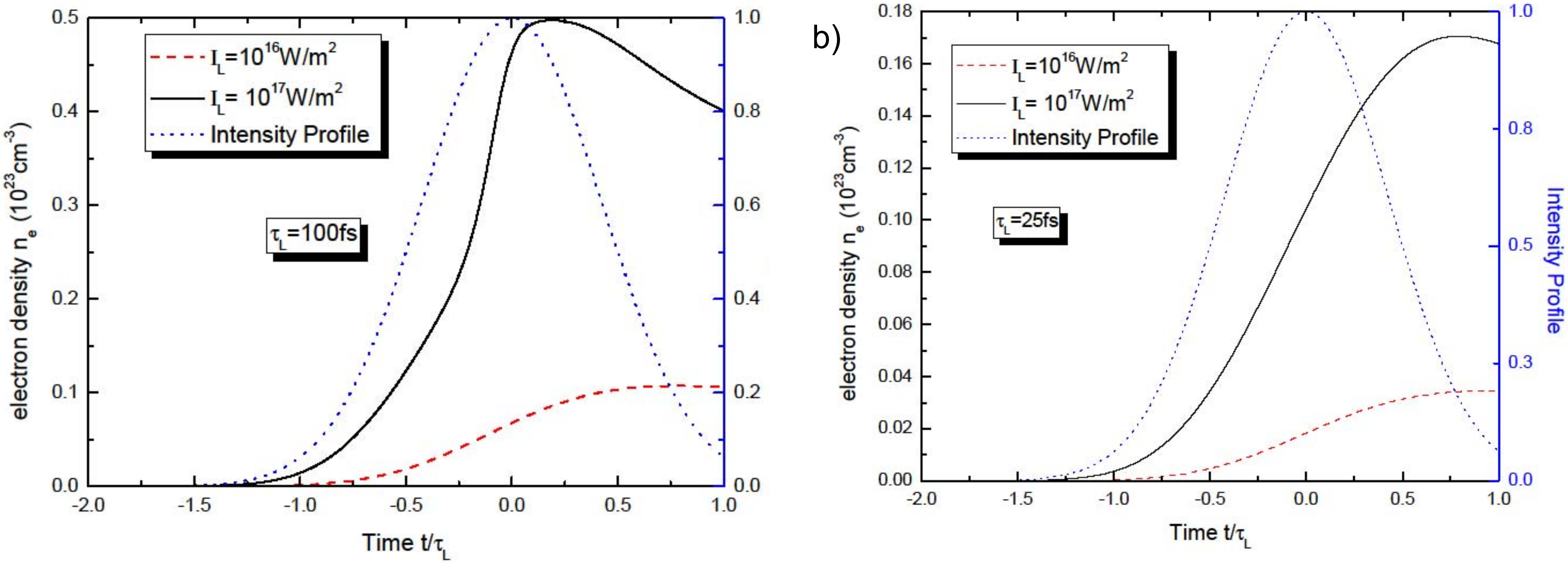


Effects of laser intensity and detuning– 25fs



Effects of laser intensity on electron density – 100fs, 25fs

a)
b)



Comparison of electron density as a function of scaled time for higher and lower laser intensity for pulse duration of 100fs (a) and 25fs (b)

- For laser field of $I_L = 8\times10^{15} W/m^2$ and $\tau_L = 1ps$

irradiating GaAs the calculations show that:

$$8.7\times10^{17} cm^{-3} = n^{elec}{}_{cr} < n_e < n^{opt}{}_e = 1.3\times10^{23} cm^{-3}$$

- For the chosen parameters the semiconductor GaAs is electrically damaged but not optically damaged.

- The average conduction electron kinetic energy is smaller than the bandgap energy $\langle E^e{}_k \rangle < E_G$ at all times which means that for the given parameters of the laser field the semiconductor GaAs is structurally stable.

Spatially uniform infrared field interacting with GaAs in a dc field with the polarization of the infrared field parallel and perpendicular to the dc field

The equation for the center of mass motion of electrons is built after a quantum statistical average is taken to obtain a classical frictional force. The "frictional" force acting on the drifting electrons is due to the phonon and impurity scattering of the conduction electrons.

Equation of motion of electrons center of mass

Number and effective mass of conduction electrons.

Friction force

$$N_e m^* \frac{d}{dt}\vec{u}_0(t) = N_e e\vec{E}_{dc} + F_p[\vec{u}_d(t)]$$

Drift velocity of the center of mass of electrons

$$\vec{u}_d = \vec{u}_0 - \left(\frac{e}{m^*\Omega_L}\right)\vec{E}_L(t)\cos\Omega_L t$$

Dependence on the dc field amplitude, and on the infrared field amplitude and frequency

$$F_p[\vec{u}_d(t)] = -2\pi\sum_{\vec{k}}\sum_{\vec{q},\lambda}\left|C_{\vec{q},\lambda}\right|^2\vec{q}\sum_{M=-\infty}^{\infty} J^2_{|M|}\left(e\left|\vec{q}.E_L(t)\right|/m^*\Omega_L\right)\left(2N^{ph}_{\vec{q},\lambda}+1\right)\times$$
$$\left(f_{\vec{k}+\vec{q}} - f_{\vec{k}}\right)\delta\left(\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}} + \hbar\omega_{\vec{q},\lambda} + \hbar\vec{q}.\vec{u}_0 - M\hbar\Omega_L\right)$$

Doppler shift in energy

D. Huang, **T. Apostolova** et. al. Phys. Rev. B 69, 075214 (2004) D. Huang, P. M. Alsing, **T. Apostolova** et. al. Phys. Rev. B **71**, 045204, 2005

Boltzmann scattering equation for the relative electron motion

$$\frac{d}{dt} f_{\vec{k}} = W_{\vec{k}}^{(in)}\left(1 - f_{\vec{k}}\right) - W_{\vec{k}}^{(out)} f_{\vec{k}}$$

Dependence on the infrared laser field amplitude and frequency

$$W_k^{(in)} = \frac{2\pi}{\hbar}^{2} \sum_{\vec{q}\lambda} \left|C_{\vec{q}\lambda}\right|^2 f_{\vec{k}+\vec{q}} \sum_{M=-\infty}^{\infty} J^2_{|M|}\left(e\left|\vec{q}.\vec{E}_L(t)\right|/m*\Omega_L\right) \times$$

$$\left\{N^{ph}_{\vec{q},\lambda}\delta\left(\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}} - \hbar\omega_{\vec{q},\lambda} + \hbar\vec{q}.\vec{u}_0 - M\hbar\Omega_L\right) + \left(N^{ph}_{\vec{q},\lambda} + 1\right)\delta\left(\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}} + \hbar\omega_{\vec{q},\lambda} + \hbar\vec{q}.\vec{u}_0 - M\hbar\Omega_L\right)\right\}$$

Doppler shift in energy

Doppler shift in energy

$$W_k^{(out)} = \frac{2\pi}{\hbar}^{2} \sum_{\vec{q}\lambda} \left|C_{\vec{q}\lambda}\right|^2 \left(1 - f_{\vec{k}+\vec{q}}\right) \sum_{M=-\infty}^{\infty} J^2_{|M|}\left(e\left|\vec{q}.\vec{E}_L(t)\right|/m*\Omega_L\right) \times$$

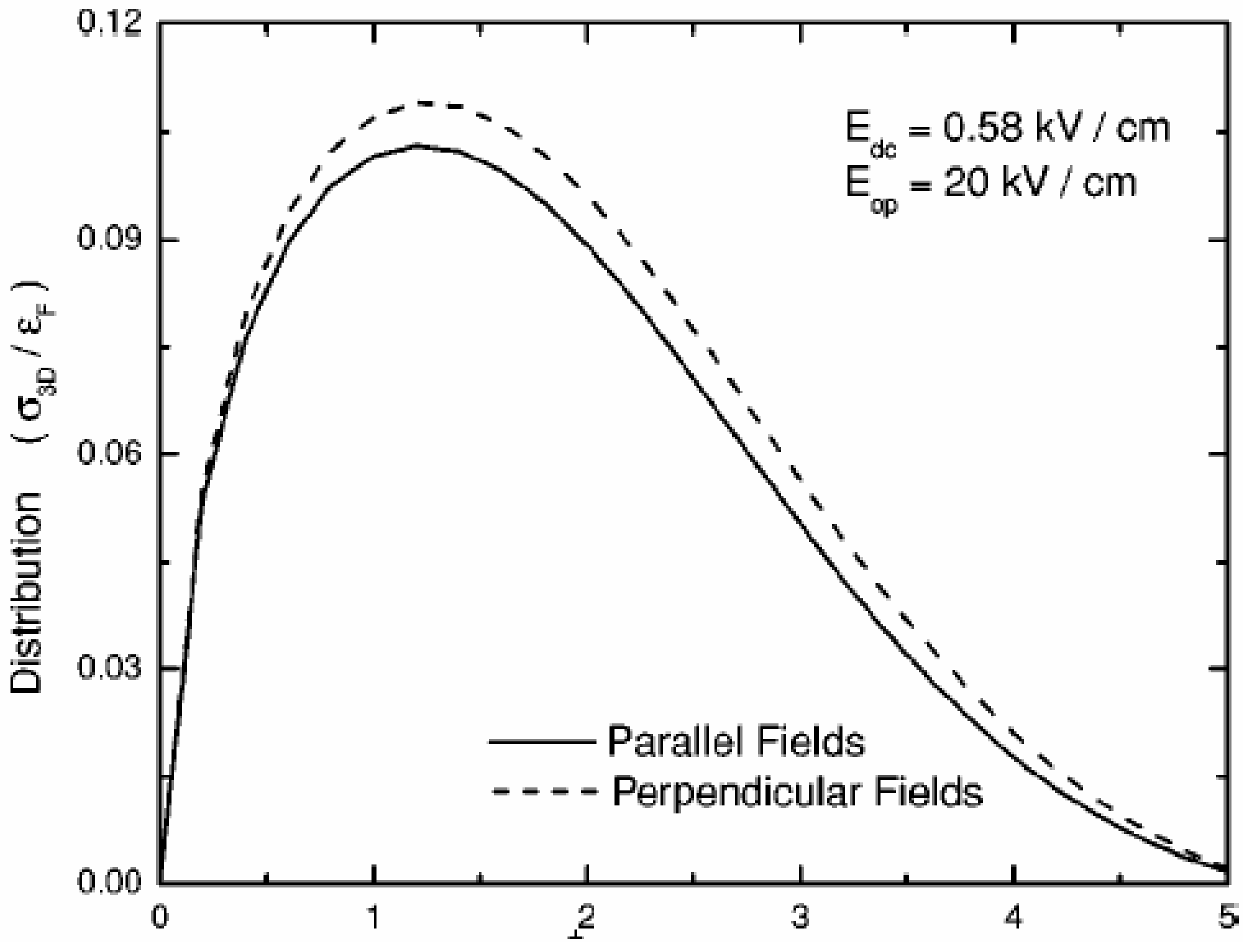
$$\left\{N^{ph}_{\vec{q},\lambda}\delta\left(\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}} + \hbar\omega_{\vec{q},\lambda} + \hbar\vec{q}.\vec{u}_0 - M\hbar\Omega_L\right) + \left(N^{ph}_{\vec{q},\lambda} + 1\right)\delta\left(\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}} - \hbar\omega_{\vec{q},\lambda} + \hbar\vec{q}.\vec{u}_0 - M\hbar\Omega_L\right)\right\}$$

Photon absorption with phonon assistance

When $\varepsilon_F >> \hbar\omega_{q\lambda}, \hbar\Omega_L, \hbar\vec{q}.\vec{u}_0$ we expand the Boltzmann equation and solve a Fokker-Planck type equation.

anisotropic scattering of electrons with phonons and impurities

Results for GaAs - **electron energy distribution function dependence on the infrared field polarization in respect to the dc field**



$\varepsilon_{k_\parallel} = \hbar^2 k_\parallel^2 / 2m^*$

$\sigma_{3D} = 1 \times 10^{18}\, cm^{-3}$

$\varepsilon_{k_\perp} = \hbar^2 k_\perp^2 / 2m^*$, =0

D. Huang, **T. Apostolova** et. al. Phys. Rev. B 69, 075214 (2004)

Boltzmann scattering equation – impurity and phonon- assisted photon absorption and Coulomb electron scattering for a doped GaAs semiconductor

$$\frac{\partial}{\partial t} n_{\vec{k}}^{e} = W_{k}^{(in)(\alpha)} \left(1 - n_{\vec{k}}^{e}\right) - W_{k}^{(in)(\alpha)} n_{\vec{k}}^{e} \qquad \alpha = (im),(ph),(c)$$

$$W_{k}^{(in)(ph)} = \frac{2\pi}{\hbar} \sum_{\vec{q}\lambda} \left|C_{\vec{q}\lambda}\right|^{2} J_{|M|}^{2} \left(e\left|\vec{q}.\vec{\mathrm{E}}(t)\right| / \sqrt{2} m^{*} \Omega_{L}^{2}\right)^{2}$$
$$\times [n_{\vec{k}-\vec{q}} N_{\vec{q}\lambda}^{ph} \delta\left(E_{\vec{k}} - E_{\vec{k}-\vec{q}} - \hbar\omega_{\vec{q}\lambda} - M\hbar\Omega_{L}\right)$$
$$+ n_{\vec{k}+\vec{q}} \left(N_{\vec{q}\lambda}^{ph} + 1\right) \delta\left(E_{\vec{k}} - E_{\vec{k}+\vec{q}} + \hbar\omega_{\vec{q}\lambda} + M\hbar\Omega_{L}\right)]$$

$$\left|C_{q\lambda}\right|^{2} = \left(\frac{\hbar\omega_{LO}}{2V}\right)\left(\frac{1}{\varepsilon_{\infty}} - \frac{1}{\varepsilon_{0}}\right)\frac{e^{2}}{\varepsilon_{0}\left(q^{2} + Q_{s}^{2}\right)}$$

$$W_k^{(in)(im)} = n_I \sum_{\vec{q}} \left|U^{(im)}(q)\right|^2 J_{|M|}^2 \left(e\left|\vec{q}.\vec{\mathrm{E}}(t)\right| / \sqrt{2} m^* \Omega_L^2 \right)^2$$

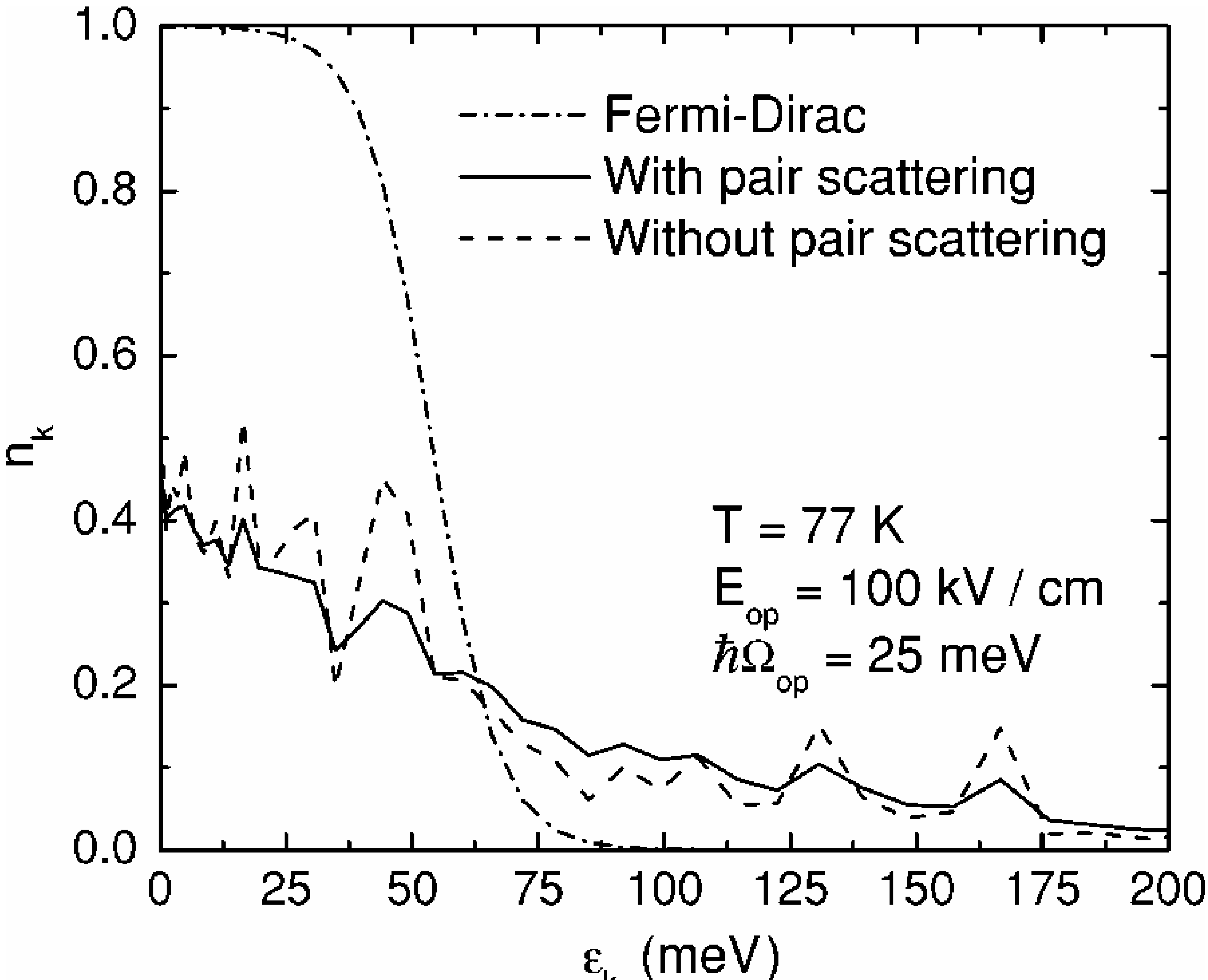
$$\times [n_{\vec{k}-\vec{q}} \delta\left(E_{\vec{k}} - E_{\vec{k}-\vec{q}} - M\hbar\Omega_L\right)$$

$$+ n_{\vec{k}+\vec{q}} \delta\left(E_{\vec{k}} - E_{\vec{k}+\vec{q}} + M\hbar\Omega_L\right)]$$

$$\left|U^{(im)}(q)\right| = \frac{Ze^2}{\varepsilon_0 \varepsilon_r \left(q^2 + Q_s^2\right)}$$

$$W_k^{(in)(c)} = \frac{2\pi}{\hbar} \sum_{\vec{k}',\vec{q}} \left|V^{(c)}(q)\right|^2 \left(1 - n_{\vec{k}'}\right) n_{\vec{k}-\vec{q}} n_{\vec{k}'+\vec{q}} \times \delta\left(E_{\vec{k}} - E_{\vec{k}'} - E_{\vec{k}-\vec{q}} - E_{\vec{k}'+\vec{q}}\right)$$

$$\left|V^{(c)}(q)\right| = \frac{e^2}{\varepsilon_0 \varepsilon_r \left(q^2 + Q_s^2\right) V}$$



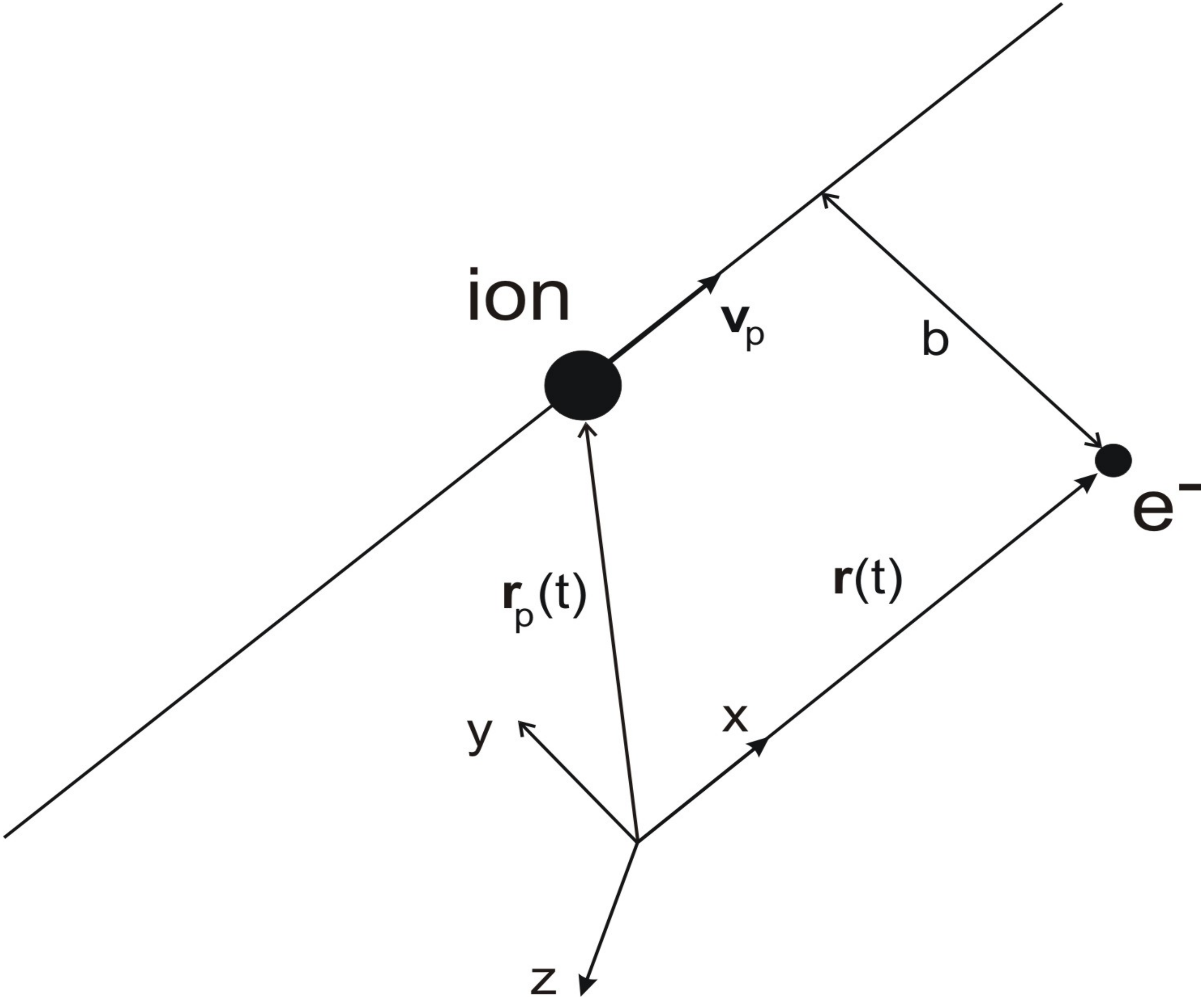
D. Huang, P. Alsing, **T. Apostolova** et. al. Phys. Rev. B 71, 195205 (2005)

Electron dynamics in ion-semiconductor interaction

•After investigating the electron dynamics in semiconductors on a femtosecond time scale in such a physical processes as irradiation by an intense ultrashort laser pulse we would like to adapt the technique to the passage of a highly charged ion. Same time scales of interaction

•For projectile kinetic energies of 1 keV or greater, we consider only constant-velocity, straight-line trajectories for the projectile.

•In terms of three-dimensional Cartesian coordinates, we define the reaction to occur in the x-y plane with the beam directed along $\vec{e}_x$ and the impact parameter b along $\vec{e}_y$ defining the straight-line trajectory to be



ion
$\mathbf{v}_p$
b
e^-
$\mathbf{r}_p(t)$
$\mathbf{r}(t)$
y
x
z

•**We use the same Hamiltonian as before**

$$H(t) = H_0(t) + H_I(t)$$

but instead solve a different Schrodinger equation

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \frac{\vec{p}^2}{2m^*}\psi(\vec{r},t) + V_p(\vec{r},t)\psi(\vec{r},t)$$

$$V_p(\vec{r},t) = -\frac{Ze^2}{4\pi\varepsilon_0 \left|\vec{r} - \vec{r}_p(t)\right|}$$

L.Plagne et. al. Phys. Rev. B 61, (2000),

J.C.Wells, et. al. Phys. Rev. B 54, (1996),

$$\vec{r}_p(t) = (v_p t, b, 0)$$

with velocity of projectile v_p

$$\psi\left(\vec{r},t\right)=\frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}f(t)$$

$$f(t)=f(0)e^{\frac{i}{\hbar}\frac{Ze^2}{4\pi\varepsilon_0 v_p}\ln(t+\sqrt{t^2+a^2})}e^{-\frac{i}{\hbar}\frac{Ze^2}{4\pi\varepsilon_0 v_p}\ln(a)}$$

$$a=\frac{b}{v_p};\ c=\frac{Ze^2}{4\pi\varepsilon_0 v_p}$$

$$f(t)=f(0)e^{\frac{i}{\hbar}c\ln(t+\sqrt{t^2+a^2})}e^{-\frac{i}{\hbar}c\ln(a)}$$

$$c\ln(t+\sqrt{t^2+a^2})=c\ln a+c\frac{t}{a}-c\frac{t^3}{6a^3}+c\frac{3t^5}{40a^5}-\ldots\ldots$$

$$c\ln(t+\sqrt{t^2+a^2})\approx c\ln a+c\frac{t}{a}$$

Looking closely at the problem parameters for justification of the approx.

The electron annihilation operator in the ion potential is given by:

$$\hat{c}_{\vec{k}}(t) = \hat{a}_{\vec{k}}(t)\exp\left[\frac{i}{\hbar}c\ln\left(t+\sqrt{t^2+a^2}\right)\right]\exp\left[-\frac{i}{\hbar}c\ln(a)\right]$$

Boltzmann scattering equation

$$\frac{\partial}{\partial t}n_{\vec{k}}^{e} = W_{k}^{(in)(\alpha)}\left(1-n_{\vec{k}}^{e}\right) - W_{k}^{(in)(\alpha)}n_{\vec{k}}^{e} \qquad \alpha = (im),(ph),(c)$$

$$W_{k}^{(in)(ph)} = \frac{2\pi}{\hbar}\sum_{\vec{q}\lambda}\left|C_{\vec{q}\lambda}\right|^2$$
$$\times[n_{\vec{k}-\vec{q}}N_{\vec{q}\lambda}^{ph}\delta\left(E_{\vec{k}}-E_{\vec{k}-\vec{q}}-\hbar\omega_{\vec{q}\lambda}+Ze^2/b4\pi\varepsilon_0\right)$$
$$+n_{\vec{k}+\vec{q}}\left(N_{\vec{q}\lambda}^{ph}+1\right)\delta\left(E_{\vec{k}}-E_{\vec{k}+\vec{q}}+\hbar\omega_{\vec{q}\lambda}+Ze^2/b4\pi\varepsilon_0\right)]$$

$$W_{k}^{(in)(im)} = n_I \sum_{\vec{q}} \left| U^{(im)}(q) \right|^2 J_{|M|}^2 \left(e \left| \vec{q}.\vec{\mathrm{E}}(t) \right| \Big/ \sqrt{2} m^* \Omega_L^2 \right)^2$$

$$\times [n_{\vec{k}-\vec{q}} \delta \left(E_{\vec{k}} - E_{\vec{k}-\vec{q}} + Ze^2 / b4\pi\varepsilon_0 \right) +$$

$$+ n_{\vec{k}+\vec{q}} \delta \left(E_{\vec{k}} - E_{\vec{k}+\vec{q}} + Ze^2 / b4\pi\varepsilon_0 \right)]$$

Preliminary conclusions

- The effect of the potential of the incident ion is reflected in the phonon and impurity assisted electron transitions through modifying (“renormalizing”) the scattering of electrons with phonons and impurities
- This method can offer unique ability to study the change in the collision dynamics when a single projectile characteristic is modified.
- The same numerical code as with the excitation with a laser field is used and numerical results for the interaction with an ion projectile are underway

Thank you for your attention!