Title	Monte Carlo study on ultrafast carrier dynamics and coherent oscillations in p-i-n diode structure under high electric fields
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Citation	
Issue Date	2004-09
Type	Thesis or Dissertation
Text version	none
URL	http://hdl.handle.net/10119/2167
Rights	
Description	Supervisor:片山　信一，材料科学研究科，博士

Monte Carlo study on ultrafast carrier dynamics and coherent oscillations in p-i-n diode structure under high electric fields

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1. Introduction

By recent development of technique in sub-micron semiconductor device fabrication and in generation of femtosecond optical laser pulses we are able to study carrier dynamics within sub-picosecond time regime (ultrafast carrier dynamics) and to perform a terahertz (THz) time-domain spectroscopy. The resulting information from the ultrafast carrier dynamics will give key ingredients for invention of electronic devices with higher maximum frequency of operation or higher logic switching speed and of the solid state THz radiation sources. The second one gives us new information of coherent collective oscillations in various solids. Understanding of ultrafast carrier dynamics as well as coherent oscillations will give a clear vision on scattering processes, or relaxation times of carriers. Under ultrafast photoexcitation, electrons and holes promote into non-equilibrium and non-stationary states exhibiting a non-linear i.e. non-ohmic conduction, so they are no longer characterized by a lattice temperature and they behave as hot carriers in ultrashort time regime. To reveal hot carrier dynamics from theoretical viewpoints, many studies have been carried out. They are either based on quantum-mechanical semiconductor Bloch equations or semiclassical Boltzmann equation. However, instead of solving approximately these equations, it has been proved that direct calculation by self-consistent ensemble Monte - Carlo method works well for hot carrier problems in sub-micron semiconductor devices in short time scale.

Recently Leitenstorfer et al have explored ultrafast carrier dynamics under high bias fields in GaAs and InP p-i-n diode by means of the broadband electro-optic sampling [1]. They have measured THz electromagnetic radiation emitted by photocarriers in intrinsic layer with the carrier density ~10^{14}cm^{-3}. The detected THz signals have provided information about drift overshoot velocities of both photo-excited electrons and holes as a function of time. The observed overshoot behavior has immediately attracted the attention in both theoretical and experimental works [2,3]. They have also reported an important contribution to their observed THz radiation from the coherent optical phonon oscillations. However, the intriguing observed oscillatory behavior in THz signal has not been theoretically analyzed yet.

2. Purpose, method and model

The purpose of the present research is to reveal the generation mechanism of THz radiation due to coherent longitudinal optical (LO) phonons in p-i-n diodes in connection with ultrafast carrier dynamics. We explore the ultrafast carrier dynamics in GaAs p-i-n diode structure under high electric field and calculate the THz transient from carrier movement by means of semiclassical self-consistent ensemble Monte Carlo (SC-EMC) method. The THz radiation due to coherent LO phonons is calculated by solving the proper equation for lattice oscillation.

Our model structure of GaAs p-i-n diode consists of p-type layer, insulating (i)-layer, and n-type layer as is shown in Fig. 1 in which each layer has thickness d_p, d_i, and d_n, respectively. The initial profile of self-consistent field is calculated by means of the drift-diffusion model [3] involving the impurity distributions before the irradiation of light pulses.

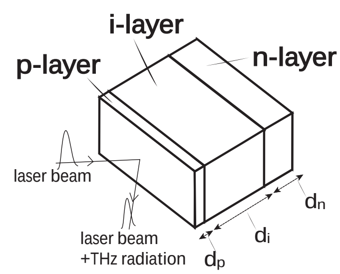

Fig. 1. Schematic view of GaAs p-i-n diode.

Since our main interest is in the THz radiation from the coherent LO phonon in GaAs p-i-n diodes, we focus on the equation of motion for coherent LO phonon oscillation as

$$\frac{d^2W}{dt^2} + \Gamma_p \frac{dW}{dt} + \omega_{LO}^2 W = \left[\frac{\varepsilon_s - \varepsilon_\infty}{4\pi\varepsilon_\infty^2}\right]^{1/2} \omega_{TO} \left(E_{ext} - 4\pi P_e(t)\right), \quad (1)$$

where $W = (NM_r)^{1/2}(u_+ - u_-)$ is the displacement field of lattice, N and M_r being the number of unit cells per unit volume and the reduced mass of ion pair, $u_{+(-)}$ the displacement of cation (anion), and ω_{LO} (ω_{TO}) and Γ_p denote the frequency of the LO (TO) phonon and damping constant, respectively. The static and high frequency dielectric constants are given by ε_s and ε_∞. As a driving force of lattice vibration, we introduce a self-consistent field which consists of the external bias field E_{ext} and the transient electronic polarization P_e. In the present case, the latter transient electronic polarization comes from the ballistic separation of electrons and holes so that the velocity overshoots of electron and hole dominate the $P_e(t)$ within a very short time regime. This may be evaluated by

$$P_e(t) = e\int_{-\infty}^{t} N_{ex}(t')v_{e-h}(t')dt', \qquad (2)$$

where $N_{ex}(t)$ and $v_{e-h}(t)$ denote the photoexcited electron-hole pair density and the relative velocity $v_{e-h}(t) = v_e(t) - v_h(t)$ at time t, v_e and v_h being the electron and hole drift velocity, respectively. The total dynamical electric polarization is estimated by considering the lattice polarization in addition to $P_e(t)$. The lattice part is given by $P_L(t) = Ne_T^* W(t)/(NM_r)^{1/2}$, e_T^* being the transverse effective charge. Thus the electric field of THz radiation is proportional to the electronic and ionic accelerations as

$$E_{THz}(t+\frac{r}{c}) \propto \frac{d^2P_e}{dt^2} + \frac{d^2P_L}{dt^2}. \qquad (3)$$

We estimate the electric field of THz radiation according to the above formula based on semi-classical simulation of $P_e(t)$ and $P_L(t)$, and analyze the experimental data.

3. Results and discussion

By means of SC-EMC method, we have simulated the dynamics of carriers injected inside the GaAs p-i-n diode assuming an irradiation of the laser pulse with 12-fs duration at center energy 1.49 eV as shown in Fig. 1. We assume that $d_p = d_n$ = 20 nm, d_i = 500 nm and N_A = 1x10^{19} cm^{-3}, N_D =5x10^{17} cm^{-3} (the concentrations of acceptors and donors) and N_{ex} = 5 × 10^{14} cm^{-3} (the photoexcited carrier density) after 1 ps. In the simulation of $v_{e-h}(t)$ and $W(t)$, the time-step, mesh size and number of particles in p-i-n device structure are assumed to be 0.25 fs, 10 Å and 4x10^4, respectively.

In Fig. 2(a), we plot v_{e-h} at E_{ext} = 24, 62 and 130 kV/cm. It is evident that the velocity overshoot of carriers takes place clearly. In Fig. 2(b), the total pair-density and the occupations of carrier density in Γ and L valley at 130 kV/cm are plotted as a function of time. Since the electron velocity overshoot in GaAs is produced by the competition between the high-field acceleration and Γ –L intervalley scattering, we can imagine the physical reason of velocity overshoot explicitly from Fig. 2.

The calculated THz signals due to the electronic polarization and coherent LO phonon oscillation are depicted by plotting the second time derivative of P_e and P_L, i.e. d^2P_e/dt^2 and d^2P_L/dt^2 for E_{ext} = 24, 62 and 130 kV/cm in Figs. 3 (a) and (b).

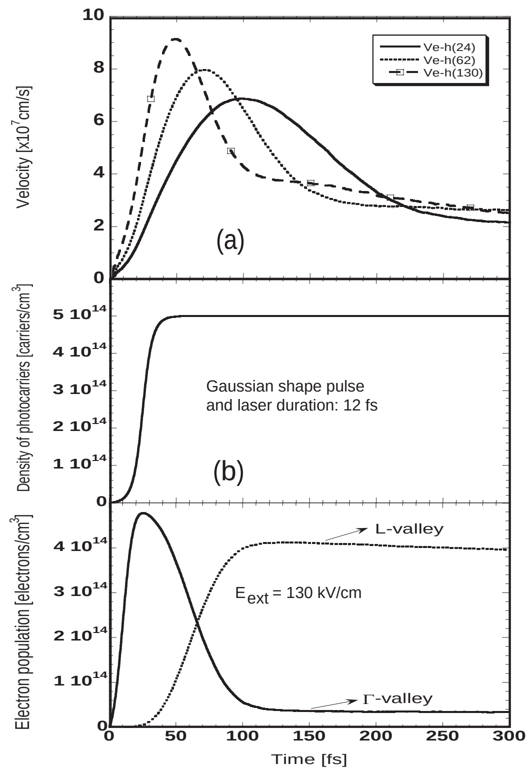

Fig.2. (a) Relative velocity of electrons and holes v_{e-h} versus time for E_{ext} = 24, 62 and 130 kV/cm; (b) density of photoexcited carriers and time evolution of electron population in valleys.

It is quite interesting that a significant enhancement of amplitude and phase shift take place when E_{ext} is increased. To understand these, we rely on the following analysis in which the velocity overshoot of carriers is regarded as one cycle oscillation of v_{e-h}. Thus we put $v_{e-h}(t) = A(1-\cos(\omega_0 t))$ in eq.(2) where $\omega_0 = 2\pi/T_0$, T_0 being the period of oscillatory velocity overshoot. This means that the time at maximum of velocity is $T_0/2$. We derive analytical expression of $P_L(t)$ by solving eq.(1), so this result is referred to as analytical model 1. For understanding the oscillatory behavior of v_{e-h}, we also calculate $P_L(t)$ for constant v_{e-h} = A (analytical model 2) which is the average of $v_{e-h}(t)$ over T_0. In Figs. 4(a) and (b), we compare our numerical results with ones obtained by analytical form for $E_{ext} = 24$ and 130 kV/cm. The solid, dashed and dot-dashed lines indicate our numerical and analytical (model 1 and 2) results, respectively. By fitting $v_{e-h}(t)$ = $A(1-\cos(\omega_0 t))$ with our simulated results as shown in the inset, we find $A = 3.5\times10^7$ cm/s, $T_0 = 190$ fs at

24 kV/cm, and $A = 4.55\times 10^7$ cm/s, $T_0 = 96$ fs at 130 kV/cm. In Fig. 4(b), we can see the prominent enhancement of oscillatory amplitude due to the resonance between proper oscillation of lattice and one cycle oscillation of v_{e-h} by $T \approx T_0$.

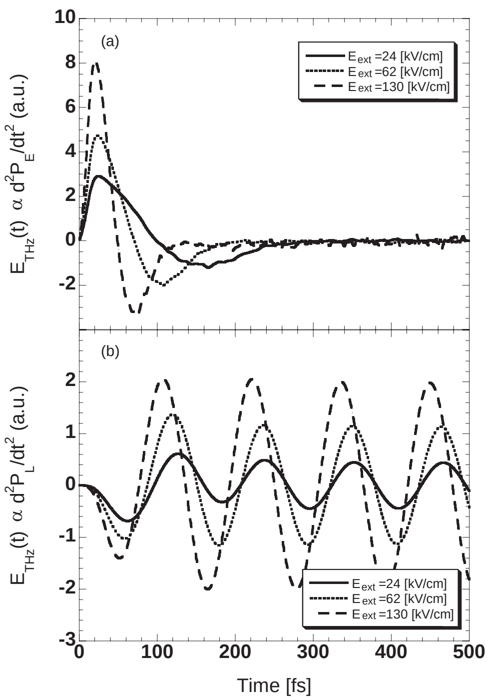

Fig. 3. THz signal due to electronic polarization (a) and coherent phonons (b) at E_{ext} = 24, 62, and 130 kV/cm.

Further we predicted the saturation and phase change of the THz signal due to coherent LO phonon with the high electric fields above 150 kV/cm. By fitting the data with $C(E_{ext})\cos(\omega_{LO}(t-t_0)-\Phi(E_{ext}))$, we plotted $C(E_{ext})$ and $\Delta\Phi(E_{ext}) = \Phi(E_{ext}) - \Phi(E_{ext}=70\,kV/cm)$ as a function of bias field E_{ext} in Fig. 5 by choosing t_0 = 115 fs. It is seen from this figure that a saturation of THz radiation occurs above 150 kV/cm, and there is no change of phase of oscillation above 200 kV/cm. As long as we concern the generation mechanism discussed here, the velocity overshoot limits the amplitude of THz radiation because the magnitude of overshoot is determined by the competition between the field acceleration and valley transfer from Γ-valley to L-valleys.

4. Conclusion

We have succeeded in calculating THz radiation due to coherent LO phonons in GaAs p-i-n diodes under high electric fields by means of self-consistent ensemble Monte Carlo method [4] It is concluded that the time variation of velocity overshoot plays an important role to determine the features of THz radiation from coherent LO phonon oscillations.

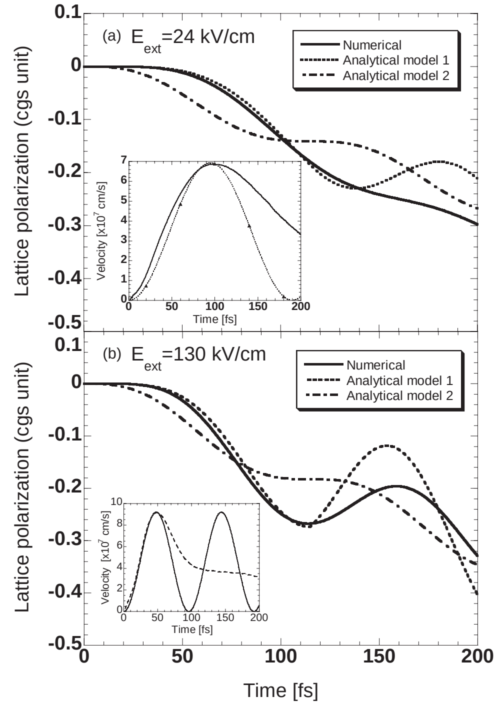

Fig. 4. (a) $P_L(t)$ versus time at E_{ext} = 24 kV/cm; (b) $P_L(t)$ versus time at E_{ext} = 130 kV/cm, the inset shows the curve fitting of the numerical results (dashed line) in figure 2 (a) with $v_{e-h}(t) = A(1-\cos(\omega_0 t))$ (solid line).

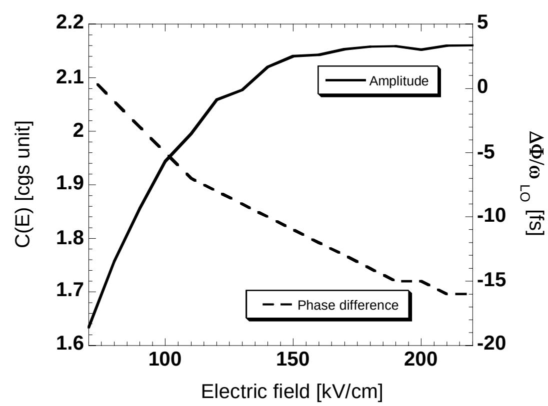

Figure 5: Amplitude $C(E)$ and phase difference $\Delta\Phi(E)$ of THz signal due to coherent LO phonon versus electric field.

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Contents

List of publications

Papers presented in Journals

(1) D. N. Thao, S. Katayama, T. D. Khoa and M. Iida, "Calculation of THz radiation due to coherent polar-phonon oscillations in p-i-n diode structure at high electric field", Semicond. Sci. Technol. ***19*** (2004), S304-S307.
(2) D. N. Thao, S. Katayama, and K. Tomizawa "Numerical simulation of THz radiation by coherent LO phonons in GaAs p-i-n diodes under high electric fields", Journal of the Physical Society of Japan, Vol. ***73,*** No. 11, 2004, in press.

Papers presented in International Conferences:

(1) D. N. Thao, S. Katayama, T. D. Khoa and M. Iida, "Calculation of THz radiation due to coherent polar-phonon oscillations in p-i-n diode structure at high electric field", in "The 13th Int. Conf. on Nonequilibrium Carrier Dynamics in Semiconductors (HCIS13)", Modena, Italy, July 28 - August 1, 2003, Conf. Abst. p. Th6-15.
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(3) D. N. Thao, S. Katayama, K. Tomizawa, "Numerical analysis of THz radiation by coherent LO phonon oscillations in GaAs p-i-n diodes under high electric fields", in "The 31st International Symposium on Compound Semiconductors (ISCS-2004)", Seoul National University, Seoul, Korea, Sept. 12 - 16, 2004.

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(1) D. N. Thao, S. Katayama and K. Tomizawa, "Ultrafast carrier dynamics and generation of coherent oscillations in GaAs p-i-n diodes", Kyushu university, Fukuoka, March 27-30, 2004, Meeting Abst. Vol. ***59***, No. 1-4, p. 763 (30aPS-36).