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Transient intervalley scattering and impact ionization in GaAs and InSb in high THz field

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Abstract: The ensemble Monte Carlo method was used to calculate the time-variation of scattering mechanisms and the carrier nonlinear dynamics evolution of n-doped GaAs and InSb in the high terahertz (THz) field. The time information of the electrons scattering into the side valleys and that of the electrons relaxation back into the original energy valley was directly obtained. The carriers transient increase process was also traced. Meanwhile, it showed that the intervalley scattering is the main mechanism of GaAs, while the impact ionization is a key point for InSb in high THz field. Furthermore, the work discussed the influences of the two mechanisms on related physical quantities: average kinetic energy, average velocity, and material conductivity. It indicates that the two mechanisms lead to nonlinear effects and play inverse roles in the two materials. The response time of impact ionization in InSb is longer than that of intervalley scattering in GaAs. The results have some guiding values in THz modulation field.

Key words: THz wave, carrier dynamics, ensemble Monte Carlo, intervalley scattering, impact ionization
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强 THz 场下 GaAs 和 InSb 中瞬态谷间散射和碰撞电离

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摘要:运用系宗蒙特卡罗法计算了强 THz 场作用下,n 型掺杂的 GaAs 和 InSb 中随时间变化的散射机制以及载流子非线性动力学演变,获取了电子散射至卫星谷并弛豫回原能谷的时间信息,并追踪描绘了载流子瞬态增加的过程,结果同时显示了强场作用下谷间散射是 GaAs 中的主要散射机制,而碰撞电离则是 InSb 中的关键因素.此外进一步讨论了这两种机制对于相关物理量:平均动能、平均速度、材料的电导率的影响,结果说明这两种机制导致了非线性效应并在两种材料中起到相反的作用,InSb 中碰撞电离的响应时间比 GaAs 中谷间散射的响应时间更长.该研究结果在 THz 调制领域有一定的指导意义.

关 键 词:THz 波;载流子动力学;系宗蒙特卡罗;谷间散射;碰撞电离

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Introduction

High speed semiconductor device is the important hardware basis of modern information environment, and the effect of the carrier in the picosecond has a direct impact on the device development and application. Especially in the optical field, a wide variety of optoelectronic

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technologies provides effective methods to study carrier transport and scattering effects. Based on its intense field and ultrafast properties, THz pulse has already been a reasonable tool on nonlinear modulating carrier motion characteristics in picosecond and subpicosecond scales[1-5].

Compared with the traditional photoconductive materials such as GaAs, InP and ZnTe, the narrow bandgap material InSb has better performance in high-speed, low-noise, and low-power applications[6-7] with the low-electron effective mass, high-carrier concentration and high mobility. There are lots of researches on carrier transportation and nonlinear effects of GaAs and InSb in THz field. For example, Hoffmann *et al.* studied nonlinear ultrafast optical absorption of intense terahertz pulses in n-doped GaAs and InSb, and the scattering processes have been resolved by THz-pump/THz-probe (TPTP) measurements[8-10]. The sources have allowed the observation of nonlinear THz absorption bleaching due to intervalley scattering in photoexcited GaAs[11-12].

There are many studies on the nonlinear effects of these two materials, however, it is not common for the ensemble Monte Carlo simulation of nonlinear transient response of high THz-field-driven electrons, and the most are based on the classical Drude model. As we know, the carriers gain high-energy in the high field, forming nonparabolic band structure, and the carriers will no longer follow the classic oscillation formula. In addition, without full consideration of the side valleys in the band structure and the effects of spatial carriers distribution, it is difficult for Drude model to solve the complex transient process. Therefore, ensemble Monte Carlo method[13-18] based on semi-classical theory can undoubtedly provide us an effective solution to the problem.

In this paper, we studied the carriers nonlinear transport properties of the n-doped bulk GaAs and InSb crystals in high THz field, discussing the transient change of the average kinetic energy, average electron velocity and the conductivity. The results showed that the time-variation of intervalley scattering and impact ionization lead to different dynamics characteristics for each materials.

1 Physical mechanism and model

Both transient and steady state transport variables can be obtained from an ensemble Monte Carlo simulation. It is particularly important to observe transient evolution under non-uniform electric field, especially in high field. Therefore, we use the ensemble Monte Carlo method to study the dynamical evolution of the carriers in the high THz field, which is described by the Boltzmann equations[15-18]:

$$\frac{\partial f_k}{\partial t} = \left.\frac{\partial f_k}{\partial t}\right|_{c-ph} + \left.\frac{\partial f_k}{\partial t}\right|_{c-im} + \left.\frac{\partial f_k}{\partial t}\right|_{c-l} + \frac{eE_t(t)}{\hbar}\nabla_k f_k \quad , \tag{1}$$

where f_k is the electron distribution function; $\partial f_k/\partial t|_{c-ph}$ is the carrier-phonon interaction rates; $\partial f_k/\partial t|_{c-im}$ the carrier-impurity interaction rates; $\partial f_k/\partial t|_{c-l}$ the carrier-lattice interaction rates. $eE_t(t)\nabla_k f_k/\hbar$ is the THz-filed-driven process, with $\hbar$ the Planck constant divided by 2π; e the unit charge for electron. The first air-sample interface of the THz field transmission is described by $E_t = 2Y_0E_{THz}/(Y_0+Y_s)$[12], where E_{THz} is the incident THz field; Y_0 the free-space admittances; Y_s the sample admittances.

The scattering mechanism describes the macroscopic properties of electrons transport, which enable the electrons to have a certain movement. We can use Fermi's Golden rule, the effective mass, Born approximations, etc. to calculate the scattering rates. Several important scattering rates were taken into account in this paper, such as ionized impurity scattering, acoustic phonon scattering, intervalley scattering, intravalley scattering, and polar optical phonon scattering. It is worth mentioning that another kind of mechanism should be considered for the narrow band gap semiconductors. Since the band gap energy is lower than the energy needed for the intervalley transition, the free electrons with high energy also have the chance to proceed in impact ionization with the occurrence of intervalley scattering. That is to say, an electron transfers energy to an electron on the valence band through collision. Meanwhile, the electron on the valence band is directly excited to the conduction band, producing two free electrons. This impact ionization process can be used as a scattering mechanism in Monte Carlo simulation, which is described by the Keldysh statistical form[19]: $P(E) = S[(E-E_{TH})/E_{TH}]^2$ when $E > E_{TH}$, and $P(E)=0$ when $E \leqslant E_{TH}$, wherein E is the electron energy, and E_{th} a threshold energy ($E_{th} = 1.08E_g$). According to the present experimental results, the impact ionization probability factor S is generally taken as 10^{12} s^{-1}.

In the simulation, the samples are n-doped, and their carrier concentrations are about 10^{16}/cm^3 at 300 K. Both x and y directions are 1 mm thick, and they can be considered as uniform systems with the large width. Three valley model (Γ-L-X) is used to describe the conduction band structure. The sampling time interval is 1fs, and the electric field and number of electrons are updated after each time period. The holes are not taken into consideration with its slow motion. Moreover, the particles go through the mirror reflection process when they reach the boundary. The parameters used in the simulation are shown in Table 1[14,19-21].

Table 1 Parameters used in the simulation
表1 模拟中使用的参数

Parameters	GaAs	InSb	Unit
Band gap	1.42	0.18	eV
Intervalley Energy $E_{\Gamma\text{-}L}$	0.29	0.76	eV
$E_{\Gamma\text{-}X}$	0.52	0.45	eV
Effective mass m_Γ	0.067	0.014	m_0
$m_L(m_X)$	0.22(0.58)	0.22(0.13)	m_0
LO phonon energy	35	24.4	meV
Intervalley phonon energy	27.8	19.9	eV
Density	5.360	5.790	g/cm^3
Sound velocity	5 240	4 060	m/s
Static dielectric function ε_0	12.9	17.65	
High-frequencydielectric function ε_∞	10.92	15.68	

2　Results and discussion

Figure 1 shows the time-domain spectra (a) and frequency spectra (b) of the incident THz pulse. The pulse center frequency is 1 THz with the width of 0.5 THz. The intense THz field can directly accelerate free carriers in n-doped semiconductors with high mobility[22]. In this process, the carriers energy is increased rapidly and the nonlinear dynamic response occurs. The two kinds of materials GaAs and InSb, which have high mobilities of ~8 500 $cm^2/V/s$ and ~76 000 $cm^2/V/s$, are easy to achieve this process[8-12].

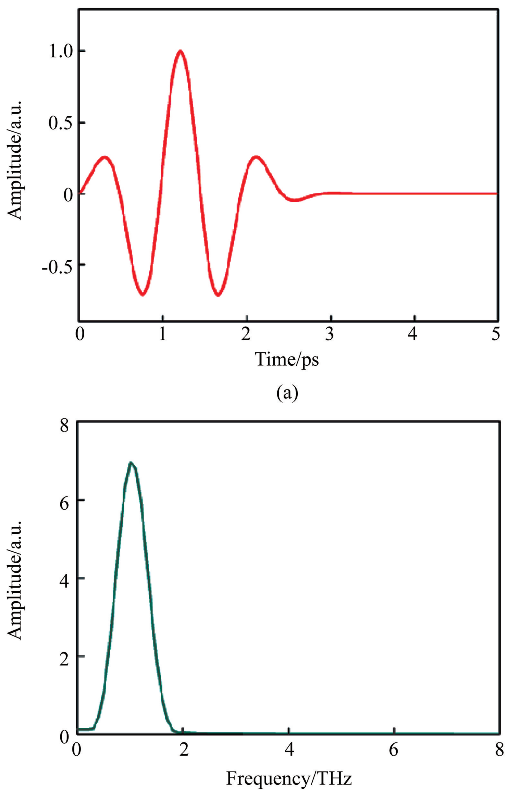


Fig. 1　(a) The spectra of time-domain and (b) frequency domain of the incident THz pulse
图 1　入射 THz 脉冲的时域谱(a)和频谱(b)

Figure 2 shows several important scattering probabilities in GaAs and InSb in the Γ valley at 300 K. It can be seen that when the electron energy is small, the ionized impurity scattering dominates in GaAs, and the polar optical phonon scattering also account for a large proportion. While in InSb, the polar optical phonon scattering plays a major role. However, when the electron energy increases, these two kinds of scatterings change slowly, and their variation degrees are far below the intervalley scattering and impact ionization. In the high field, the electron energy increases rapidly, and the effect of the ionized impurity scattering and the polar optical phonon scattering gradually becomes unimportant. Meanwhile, the intervalley scattering of GaAs intensifies in the high energy, becoming the main scattering mechanisms.

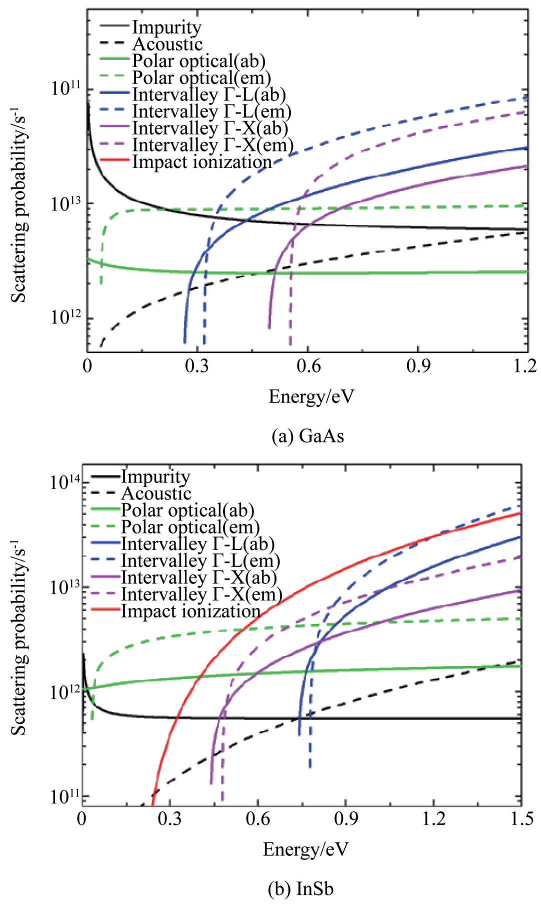
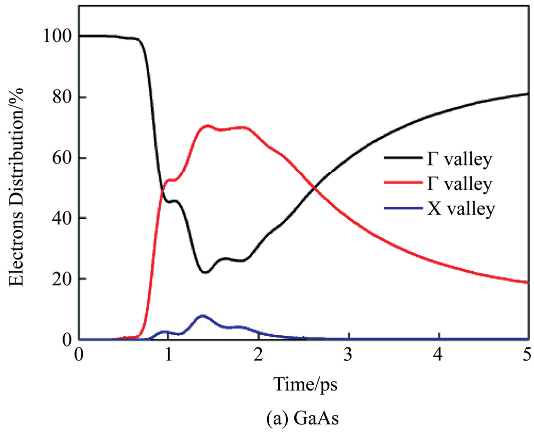


Fig. 2　Various types of scattering probabilities in (a) GaAs and (b) InSb in the Γ valley at 300 K
图 2　300 K 时 GaAs(a)和 InSb(b)的 Γ 能谷中各种类型的散射几率

The impact ionization probability is very small in this material due to the wider band gap, and the red curve in Fig. 2(a) is invisible. In InSb, the impact ionization is easy to occur with the small effective electron mass and narrow band gap energy. In addition, acoustic phonon scattering probability increases with the electron energy, but it has little influence because of the small overall probability. Thus, in the high THz field, we focused on the intervalley scattering and the impact ionization mechanisms.

2.1　Transient processes of intervalley scattering and impact ionization

Scattering between different energy valleys will make electron absorb or emit energy additionally, thus satisfying the energy conservation condition of transition. Under the high outfield, the intervalley scattering will generally cause a dramatic change in the momentum and kinetic energy of electrons. In order to analyze the specific process of carriers intervalley scattering in semiconductor materials, we calculated the transient electron distribution percentages of three valleys under the high THz field of 100 kV/cm (the peak amplitude). It was found that the electron ratios of different valleys change rapidly. The two kinds of materials have undergone different degrees of intervalley scattering, and both of them reach the peak value in the vicinity of 1.4 ps.



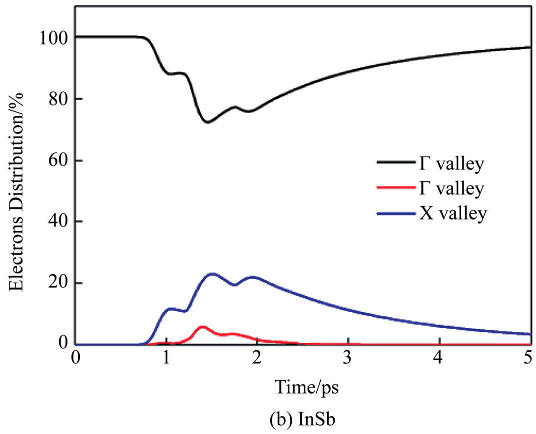


Fig. 3 Transient electron distribution of each energy valley in (a) GaAs and (b) InSb at high THz field of 100 kV/cm

图 3 在 100 kV/cm 的强 THz 场作用下(a)GaAs 和(b)InSb 中各能谷瞬态电子分布

When electron energy reaches the threshold of the intervalley transition, electrons are scattered from Γ Valley to L Valley or X Valley. In GaAs, the Γ Valley scattering begins from 0.25 ps, and the maximum proportion reaches 80%. While in InSb, the Γ Valley scattering begins from 0.6 ps, and the maximum proportion only reaches about 25%. It shows that the intervalley scattering of GaAs is much stronger than that of InSb. After 1.4 ps, with the weakening of the external electric field, most of the out-scattered carriers gradually relax back into the original valley. We can see that the fastest electron transfer time back to the Γ valley of GaAs is about 1.15 ps, and the slow electrons need 3.5 ps or more. These values can be compared with the results of 1.9 ps in the THz-pump/THz-probe experiment[8] and 3 ps in the optical-pump/THz-probe experiment[12]. For the weak intervalley scattering material InSb, the relaxation time is relative short. In addition, it is shown the scattering proportion from Γ Valley to the L Valley in GaAs is higher than that from Γ Valley to the X valley. It acts exactly the opposite way in InSb because of valley energy difference $\Delta E_{\Gamma X} > \Delta E_{\Gamma L}$ in GaAs and $\Delta E_{\Gamma X} < \Delta E_{\Gamma L}$ in InSb (See Table 1).

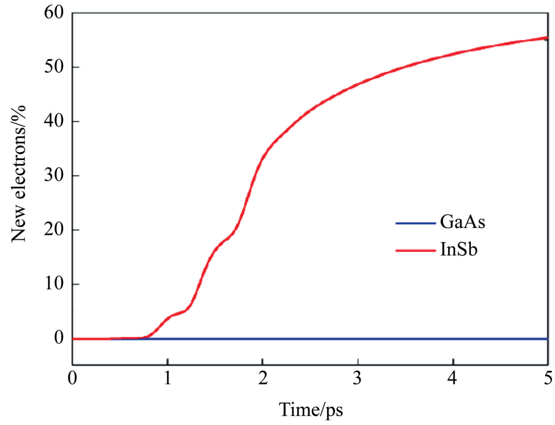


Fig. 4 Percentage of new electrons in GaAs (blue line) and InSb (red line) excited by impact ionization dependence of time at high THz field of 100 kV/cm

图 4 在 100 kV/cm 的强 THz 场作用下,GaAs(蓝线)和 InSb(红线)中由碰撞电离激发的新增电子比例随时间的变化

We further analyzed the impact ionization effect of different materials in the high field. Figure 4 shows the percentage of total number of electrons excited by impact ionization in the two materials in the 100 kV/cm driving strength. Since the impact ionization generates new electron-hole pairs, the total number of carriers is updated on each time step. For GaAs, the total number of electrons is almost the same, indicating that the impact ionization hardly occurs. It is because that this material has large effective mass ($m_\Gamma = 0.067 m_0$, $m_L = 0.22 m_0$, *and* $m_X = 0.58 m_0$) and wide band gap ($E_g = 1.42$ eV), the electron acceleration kinetic energy cannot reach impact ionization threshold. For InSb, the adding electrons proportion increases from 0.38ps and reaches 55% at the end of 5ps, changing gently in the late stage. Compared with the Fig. 3(b), the impact ionization occurs much earlier and the response time is longer than intervalley scattering. For this material, the effective electron mass ($m_\Gamma = 0.014 m_0$, $m_L = 0.22 m_0$, *and* $m_X = 0.13 m_0$) and band gap energy ($E_g = 0.18$ eV) are very small. It is easy to produce impact ionization, which leads to dramatical increase of the number of carriers and inhibits the increase of intervalley scattering.

As is shown above, we obtained the detail of response time of the intervalley scattering and impact ionization. It also shows that the intervalley scattering is the main scattering mechanisms of GaAs, while the impact ionization is a key point for InSb in the high THz field.

2.2 Influences of intervalley scattering and impact ionization on related physical quantities

In high-field transport calculations, carriers can have very high kinetic energy E. A more appropriate description of E-k relationship can express practical energy band structure[14] as $E(1+\alpha E) = \gamma(k) = \frac{\hbar^2 k^2}{2m^*}$, where k is wave vector; α is the nonparabolicity coefficient: $\alpha = (1 - \frac{m^*}{m_0})^2 / E_g$, where E_g is the energy gap; m^* is the effective electron mass at the band edge and m_0 is the free electron mass.

By Monte Carlo method, the energy-wave vector relationship (energy band structure) of carriers determines their dynamical properties under the influence of an external force. Once the band structure is known, the velocity v associated with a state k can be calculated from the expression: $v(k) = \frac{1}{\hbar}\nabla_k E(k)$. In the case of a nonparabolic band, the velocity is given by $v = \frac{\hbar k}{m^*(1+2\alpha E)}$. With the excitation of the external field, the intervalley scattering and the impact ionization effects will lead to a series of changes such as the carrier effective mass and the number of carriers as well as the average kinetic energy and the average velocity.

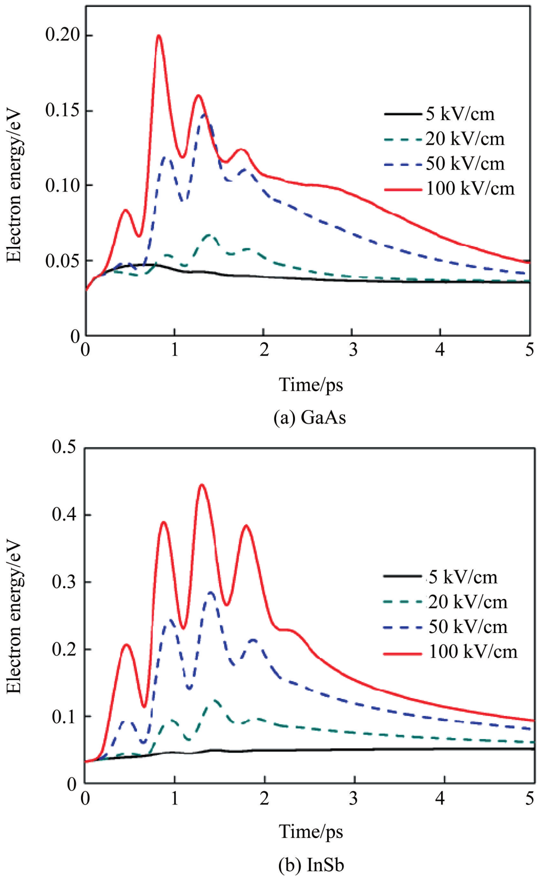


Fig. 5 Average electron kinetic energy in (a) GaAs and (b) InSb at various THz field strength
图 5 不同 THz 强度下(a)GaAs 和(b)InSb 中电子的平均动能

Figure 5 shows changing process of average electron kinetic energy over time. As can be seen, the kinetic energy change trend of two materials are similar when the electric field is lower than 50 kV/cm. In such field strength, it is not obvious for intervalley scattering and impact ionization. When the field is increased to 100 kV/cm, the kinetic energy peak can be quickly formed in the early stage. The stronger field leads to the higher peak value. The reason for the formation of peak value is that the electron energy is very low in the initial stage, which is not high enough to produce the intervalley scattering and the impact ionization. A quasi-ballistic transport can form in a high energy electric field in a short time, and the electron energy increases rapidly during transport period without changing other scatterings. With the increase of energy, the intervalley scattering and the impact ionization rates will rise rapidly as a response, and finally reaches the steady state of the electrons average kinetic energy. The average kinetic energy of GaAs quickly reduces after the initial peak, because of the intervalley scattering appearance in the intense field. Electrons transfer from the low energy valley to high energy valleys with the increased effective mass and the substantially-reduced electron kinetic energy. While for InSb, impact ionization is the main mechanism that inhibits the aggravation of the intervalley scattering and excites the cascaded carriers. Large numbers of electrons are accelerated in the outfield, making the duration time of the increasing average kinetic energy become longer.

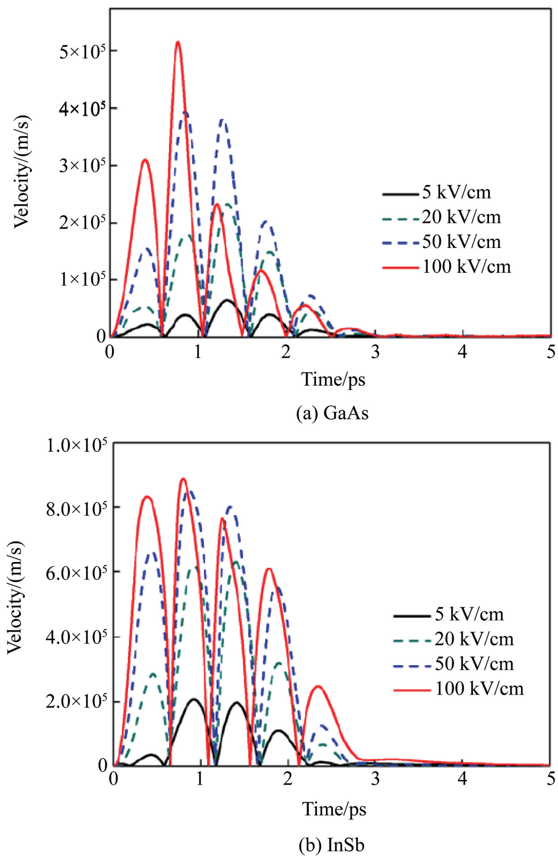


Fig. 6 velocity overshoot effect in (a) GaAs and (b) InSb at various THz field strength
图 6 不同 THz 强度下(a)GaAs 和(b)InSb 中的速度过冲效应

Velocity overshoot effect is a kind of transient transport phenomena under the high electric field. The effect is that the carrier drift velocity exceeds the normal steady state drift velocity. It has relatively large impact on the performance of small size devices and compound semiconductor devices, improving the operating frequency and speed of the device. Figure 6 shows the time-variation of average velocity curves of two materials in different THz fields. Compared with Fig. 5, we can see that the momentum relaxation time is much less than the energy relaxation time.

In the weak outfield (peak amplitude 5 kV/cm), the velocities change little, while in the high field (100 kV/cm), the electron velocity peak can be quickly formed in the early stage. That is to say, the obvious velocity overshoot phenomenon can be observed. The reason of its peak form is similar to that of the average kinetic energy. The peak velocity of GaAs can reach 5.2×10^5 m/s (See Fig. 6 (a)). This value can be compared with the data of Su *et al.* [12]. In their study, the electron peak velocity of GaAs was ~ 8×10^5 m/s under the high THz field of 173 kV/cm. As we know, the intervalley scattering reduces a great deal of initial kinetic energy, making the electron group velocity drastically decreased. Figure 6(a) shows the velocity decreases rapidly after 1ps, and reaches a steady state after 3 ps. For InSb, peak velocity can reach 8.9×10^5 m/s (See Fig. 6(b)). Impact ionization is the main scatter mechanism of this material, exciting large number of new carriers. It not only increases the peak velocity, but also prolongs the velocity overshoot response time, longer than 3 ps.

Conductivity reflects the conductive properties of materials. As we know, the conductivity is proportional to the electron concentration n, and inversely proportional to the electron effective mass m^*. It is expressed as $\sigma \propto \frac{n\tau}{m^*}$, where τ is the time interval between two scatterings. In the electron scattering mechanisms, the intervalley scattering and impact ionization are the main factors in high electron energy. The previous analysis shows that electrons are transferred to the satellite valley and the effective mass becomes larger by intervalley scattering mechanism, resulting in the reduction of conductivity. Furthermore, new electron-hole pairs are generated by impact ionization, which increases the carrier concentration and the conductivity. Therefore, impact ionization can contribute to high conductivity while intervalley scattering plays an inverse role.

Figure 7 shows the conductivity changing process of two kinds of materials over time in different THz fields. There are few changes and slight undulation when outfield is lower than 50 kV/cm, but under the 100 kV/cm field, great changes have taken place. For GaAs, the conductivity decreases sharply after 1ps because of the strong intervalley scattering. For InSb, the impact ionization process occurs and the number of carriers dramatic increases, leading to the fact that the conductivity increases rapidly after 1 ps at 100 kV/cm high field. We can also see that the response time of impact ionization in InSb is longer than that of intervalley scattering in GaAs.

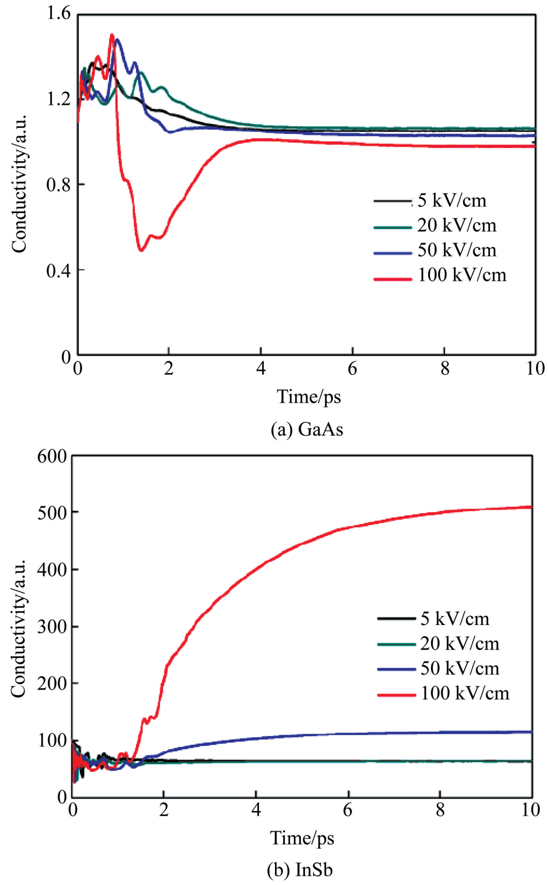


Fig. 7 Conductivity in (a) GaAs and (b) InSb at various THz field strength

图 7 不同 THz 强度下(a)GaAs 和(b)InSb 中的电导率

3 Conclusions

The ensemble Monte Carlo method was used to calculate the transient scattering mechanisms and the carrier nonlinear dynamics evolution of n-doped GaAs and InSb in high THz field. The results were as follows: Firstly, we obtained the detail of response time of the intervalley scattering and the impact ionization. The intervalley scattering is the main mechanism of GaAs, while impact ionization is a key point for InSb. Secondly, the average kinetic energy peak is rapidly formed in the high THz field. The intervalley scattering quickly reduces the average kinetic energy of GaAs after the initial peak, while the impact ionization makes the duration time of the increasing average kinetic energy become longer in InSb. Thirdly, the obvious velocity overshoot phenomenon was observed under the high THz field. The intervalley scattering makes the electron group velocity drastically decrease, while the impact ionization increases the peak velocity sharply and prolonges the velocity overshoot response time. Fourthly, under the high THz field, the intervalley scattering decreases the conductivity deeply, while the impact ionization acts an inverse role. The response time of impact ionization in InSb is longer than that of intervalley scattering in GaAs. Further research can provide more reliable results considering the full band structure, the effects of hole mobility, electron-electron scattering, electron-hole scattering, etc. We will also improve the model to make clear the influence of doping content on average kinetic energy, average velocity and material conductivity in different THz fields. The analysis of bulk semiconductor has important guiding values to study the characteristics of semiconductor optoelectronic

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devices such as III-V MOSFETs, HEMTs, IMOS, and IMPATT diodes in THz field.

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