Effect of Relaxation Time on Electron Transport Properties in Double-Barrier Structures *

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Abstract: Using a time-dependent quantum-kinetic simulation for the non-equilibrium electron transport properties of double-barrier devices, we have investigated and analyzed the effects of the relaxation time on electron transport properties in this kind of low dimensional structure. The results show that the relaxation time, which comes from the electron-phonon and electron-defect interactions, greatly affects the current-voltage curves, including the plateau-like gradient and hysteresis width of the current.

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1 Introduction

Recently, the study of electron properties has provided a great deal of information about the nature of electronic devices that operate at the nanostructure level[1~4]. Among these devices, double-barrier resonant tunneling nanodevices have been extensively studied due to their potential applications in various fields[5~7]. Modeling electron transport at the nanoscale poses a great theoretical challenge, because in this region the semiclassical Boltzmann kinetic equation commonly used to describe electron transport is not applicable. Furthermore, the transport processes become non-Markovian due to the memory effects induced by all kinds of scatterings, such as phonon, defect, and impurity scatterings. Hence the device current is strongly dependent on the bias history of the device[8].

The experimental studies by several research groups of double-barrier nanodevices focus on their current-voltage (I-V) relationship[9~11]. There are three main characteristics in I-V curve among these structures: first, a negative differential resistance; second, the current plateau-like structure shown in some experiments[12,13]; and third, the presence of single or double current hysteresis regions[14,15]. All these phenomena strongly depend on the structure of the devices and the experiment parameters. In order to explain the experimental results, researchers have used quantum transport theories[16,17]. Now, some researchers also use numerical simulation methods, such as generalized tunneling theory[18] and the Wigner transport equation[19~21], but they do not consider the effects from the variation of the relaxation time.

2 Theoretical model and method

In this paper, we study the effects of the relaxation time on electron transport properties of an AlGaAs/GaAs/AlGaAs double-barrier device using a time-dependent numerical simulation technique. The potential structure of the device model is shown in Fig. 1. Our results show the effect on the I-V curves from the electron-phonon, electron-defect, and electron-impurity interactions. We use the Wigner function formulation of quantum mechanics because it can handle dissipated and open-boundary systems naturally[22,23]. With the lowest-order approximation to the scattering term, the time-dependent dynamic equation for quantum transport is

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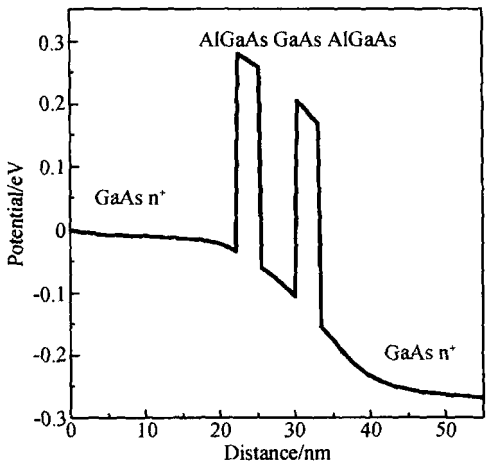

Fig. 1 Potential structure of the simulated device under a certain bias

$$\frac{\partial f(x,k)}{\partial t} = -\frac{\hbar k}{m^*}\times\frac{\partial f(x,k)}{\partial x} - \frac{1}{\hbar}\int_{-\infty}^{\infty}\frac{dk'}{2\pi}f(x,k')V(x,k-k') + \left.\frac{\partial f(x,k)}{\partial t}\right|_{coll} \tag{1}$$

where the kernel of the potential operator is given by

$$V(x,k-k') = \int_{-L/2}^{L/2} dr \sin[(k-k')r]\times[U(x+r/2)-U(x-r/2)] \tag{2}$$

where m^* is the electron effective mass, x and r are the Wigner-Weyl transformation coordinates, U is the conduction-band edge, L is the length of the simulation device, and $f(x,k)$ is the Wigner function. Appropriately treating scattering in semiconductors is very important for obtaining reasonable simulation results. We employ the relaxation-time approximation to deal with the scattering. In the relaxation time approximation, the collision term in the above equation is written as

$$\frac{\partial f(x,k)}{\partial t} = \frac{1}{\tau}\left[\frac{f_0(x,k)}{\int f_0(x,k)\,dk}\int f(x,k)\,dk - f(x,k)\right] \tag{3}$$

where τ is the relaxation time, and f_0 is the equilibrium Wigner function. The boundary conditions used are the same as those given by Frenslay[22]:

$$f(-L/2,k)|_{k>0} = \frac{m^* k_B T}{\pi\hbar^2}\times\ln\left\{1+\exp\left[-\frac{1}{k_B T}\left(\frac{\hbar^2 k^2}{2m^*}-\mu_L\right)\right]\right\} \tag{4}$$

$$f(L/2,k)|_{k<0} = \frac{m^* k_B T}{\pi\hbar^2}\times\ln\left\{1+\exp\left[-\frac{1}{k_B T}\left(\frac{\hbar^2 k^2}{2m^*}-\mu_L\right)\right]\right\} \tag{5}$$

Each term in Eq. (1) can be discretized, and for the steady state case the entire equation is written as

$$(T+V+S)\cdot f = B \tag{6}$$

where T, V, and S are the kinetic, potential, and scattering operators, respectively, B is the boundary condition term, and f is the Wigner function. To discretize the problem, we use a picture of a "simulation box" in phase space. The spatial length of the simulation region is L, and momentum space is from $-|K_{max}|$ to $|K_{max}|$. $K_{max} = \frac{\pi(N_x-1)}{2L}$, where N_x is the discrete point in position space.

The time-dependent simulation can be found in Ref. [21]. The corresponding electron and current density may be obtained by the k-space integral of the Wigner function. Another important equation in our model is the Poisson equation (PE):

$$\frac{d}{dx^2}u(x) = \frac{q^2}{\varepsilon}[N_d(x)-n(x)] \tag{7}$$

where ε is the dielectric permittivity, $u(x)$ is the electrostatic potential, q is the electronic charge, $N_d(x)$ is the concentration of ionized dopants, and $n(x)$ is the density of electrons.

3 Results and discussion

We have studied the effects of the relaxation time on the I-V curves in symmetrical double-barrier structures using the transient Wigner-Poisson transport method. We simulate the intensity of electron-phonon interactions by changing the relaxation time. The parameters used in the simulation are as follows. The momentum and position spaces are broken into 72 and 86 points, respectively. The donor density is $N_d = 2.0\times10^{18}\,cm^{-3}$, and the quantum well and barrier regions are undoped. The compensation ratio for scattering calculations is 0.3, and the barrier and quantum well widths are 3 and 5nm, respectively. The simulation box is 55nm, and the barrier potential is 317meV. The device temperature is 77K, and the effective mass of an electron is assumed to be a constant of $0.0667m_0$. The doping extends to 3nm before the emitter barrier and after the collector barrier.

We first study the mean I-V relationship in

the forward bias sweep process for the double-barrier structure. The results are shown in Fig. 2, which give the mean *I-V* curves for relaxation times ranging from 100 to 1000fs. Here different relaxation times mean different electron-phonon interactions.

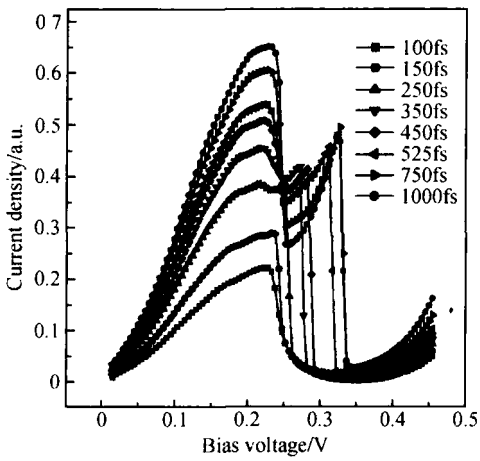

Fig. 2 *I-V* curves under different relaxation times in the forward bias sweep

From the figure, we can see that for different relaxation times, the peak value of current and the width of the current hysteresis plateau-like structure are different. Here small relaxation times correspond to strong scattering systems, i.e., larger electron-phonon and electron-defect interactions. With the increase of relaxation time, the electron scattering is weakened, and the current curve shows the following main characteristics: (1) The change trend of the main current peak value is shown in Fig. 3 (a), which shows a nonlinear change; (2) The main peak-valley ratio increases with the relaxation time and shows a linear-like change, as shown in Fig. 3(b); (3) The hysteresis-peak value of the current increases with the relaxation time, and the change mainly happens in 525fs, which is the relaxation time of the body material, as shown in Fig. 3(c); (4) The width of the hysteresis of the current only changes around the relaxation time of the body material, as shown in Fig. 3 (d), and shows stable saturation for low and high relaxation times; and (5) The gradient of the plateau-like structure increases gradually with the relaxation time.

In our former studies[24], we pointed out that there are two factors determining the plateau-like

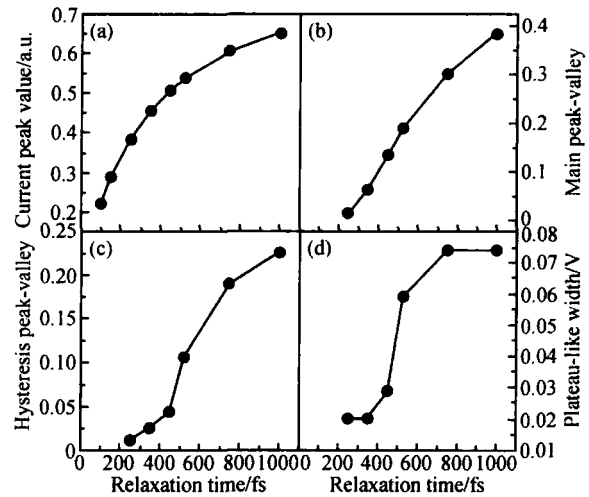

Fig. 3 Effect of relaxation time on the current peak value (a), the main peak-valley ratio (b), the hysteresis current peak (c), and the width of the plateau-like structure of the current (d)

structure of the current: one is the coupling of the energy level between the main quantum well and the emitter quantum well, which leads to the increase of the current density; the other is the electronexciton interactions, such as the electron-phonon and electron-defect interactions, which weaken the current density. Our theoretical calculation also verifies this viewpoint, i.e., the strong interactions lead to a decrease in the width and gradient degree of the plateau-like structure of the current, even making the plateau-like structure of the current disappear.

For the backward bias sweep process, Figure 4 shows that the relaxation time does not affect the position of the current and the negative differential conductance, while only affecting the height of the current peak. The above results show that for the devices with the same material, various fabrication techniques sometimes lead to the disappearance of the hysteresis of the current and the current bistability after the resonant bias. In order to find the hysteresis and bistability of the current, apart from decreasing the bias step on the device, we must improve the fabrication techniques to obtain good samples.

In order to explain the effect of the relaxation time on the mean current, we give the time-dependent current curves and local electron density distribution for the different relaxation times in the forward bias sweep process. Figure 5 shows the time-

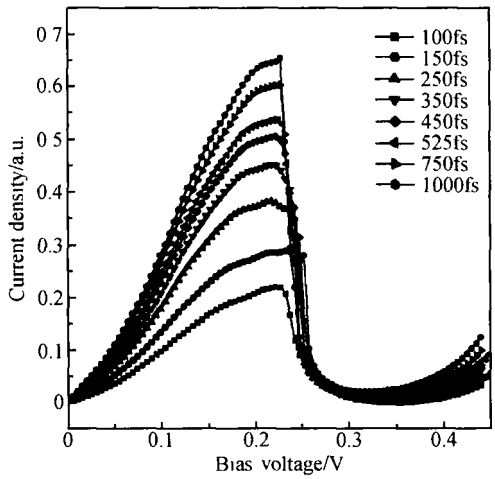

Fig. 4 *I-V* curves under different relaxation times under backward bias sweep The inset gives the relaxation time in the unit of fs

dependent current curves in a bias vol-tage lying in the window of the hysteresis region. From the figure ,we can see that the amplitude of the time-dependent current oscillation increases gradually with the relaxation time. This further verifies that the electron-phonon interactions weaken the oscillation

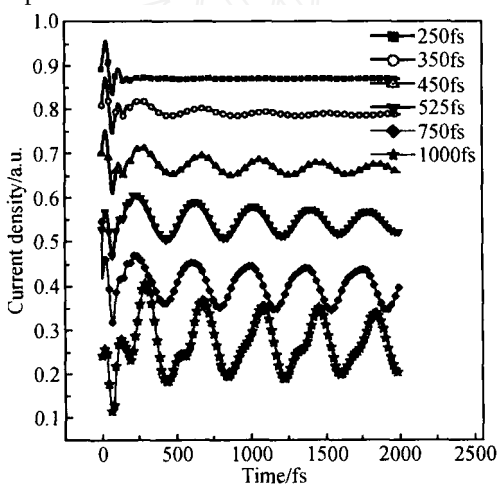

Fig. 5 Time-dependent current curves under different relaxation times under a bias lying in the window of the current hysteresis region

of the current ,destroying the coupling model of the energy level. According to our coupling theory ,the coupling is due to the formation of the emitter quantum well , so the relaxation time must affect the distribution of the electron density. Figure 6 shows that the exhaust layer of electron density before the emitter barrier increases with the relaxation time , affecting the formation of the emitter quantum well.

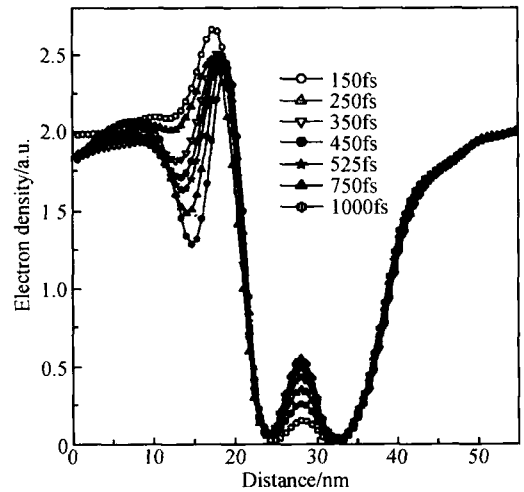

Fig. 6 Local electron density distributions under different relaxation times under a bias lying in the window of the current hysteresis region

4 Conclusion

From the above analysis ,we know that the relaxation time (the mean collision scattering time of an electron) has an important effect on the *I-V* behavior in double-barrier structures. An increase of electron scattering time leads to an increase in the width and gradient degree of the current hysteresis plateau-like structure. In a strong electron scattering situation ,there is only negative differential conductance ,and the hysteresis of the current and the plateau-like structure of the current disappear completely. At the same time ,the scattering also affects the current peak-valley ratio. In order to obtain a large current peak-valley ratio and an obvious current bistability after the resonant bias , we must fabricate a high-quality double-barrier sample.

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弛豫时间对双势垒结构电子输运性质的影响*

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摘要: 利用对双势垒器件非平衡态电子输运性质的含时动力学模拟计算,分析了弛豫时间对这类低维器件电子输运特性的影响. 结果表明,由于电子-声子、电子-杂质和电子-缺陷等相互作用导致的弛豫时间对器件 *I-V* 曲线产生很大的影响,即电流滞后类平台结构的倾斜度以及电流滞后区的宽度.

关键词: 非平衡; Wigner 函数; 电子输运
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