Full Band Monte Carlo Simulation of Electron Transport in Ge with Anisotropic Scattering Process *

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Abstract: The electron transport properties in Ge are calculated by full band Monte Carlo technique with anisotropic scattering consideration. The calculation procedures are as follows: the full band structure is calculated by nonlocal empirical pseudopotential approach; the relative value of density of state (DOS) is computed by counting the number of states located in a certain region of the energy; the phonon dispersion curve is obtained from an adiabatic bond-charge model; the electron-phonon scattering rates are approximated by the nonparabolic model derived from Fermi's golden rule at low energy region and scaled by DOS at higher energy region; the energy and momentum conservations are employed for choosing the final state after scattering. The validity of this Monte Carlo simulator and the physical models that are used is fully confirmed by comparing the program output to experimental results listed in references. As this Monte Carlo model can accurately reproduce the velocity and energy characteristics of electrons in Ge and the DOS scaled scattering rate can significantly reduce the computational cost for scattering rates, this approach is suitable for device simulation.

Key words: Monte Carlo simulation; Fermi's golden rule; transport properties; Ge
PACC: 7210; 7320A; 6300
CLC number: TN304.1 **Document code:** A **Article ID:** 0253-4177(2005)03-0465-07

1 Introduction

As the advancement of modern integrated circuits, the device dimension is scaled down to sub-100nm, and in this small dimensional region, Si MOSFET will reach its limit. Nowadays, Ge is known as a promising candidate for future advanced MOSFET substrate for its high mobility and good interface properties with high *k* dielectric[1,2]. However, in this small dimensional region, some basic physical phenomena such as tunnelling current, blast transport, velocity overshoot, and hot carrier effects will dominate the device characteristics. As a result, it is necessary to account for quantum effects, electron-phonon scattering, impact ionization, and other solid state characteristics to simulate the transport characteristics of semiconductor materials and nano-scaled devices. Among the device simulation techniques, Monte Carlo (MC) approach is the most promising candidate including these foundational physical concepts[3]. In early days, MC model used the analytical parabolic or nonparabolic band structure, thus deduced the isotripic scattering rates and easily choosing of after scattering states in the Brillouin zone from the

* Project supported by the Visiting Research Program of UESTC.

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Received 11 July 2004, revised manuscript received 18 October 2004

valley definition[4]. However, as the electrons get higher energy in small dimensional devices, the band structure can't be expressed analytically and the parabolic or nonparabolic scattering rates model is improper. Furthermore, the post-scattering state can't be selected from the valley model, because the valley is ill defined in the high energy region. The band structure of germanium is complicated and the energy difference between valley L and X is only 0.18eV so that the intervalley scattering is very important, which shows more anisotropic than Si at high energy. Therefore, a wave-vector dependent scattering model is proposed for the high energy transport calculation[5], for which the main defect rests with its much more CPU intensive. Although there is the progress for final state choosing by the analytical fitting band structure[6], the scattering rates calculation is still CPU intensive. In this paper, a Monte Carlo simulator for germanium with anisotropic scattering consideration is developed, the scattering rates at high energy are obtained by the non-parabolic model and scaled by density of states and the final states are chose anisotropically from energy and momentum conservations. Good agreement with experimental results, wave-vector dependent scattering model is achieved. As it is accurate and the scattering rates calculation is efficient, this anisotropic calculation approach not only can be used in device simulation but also can be applied to other complicated band structure materials.

2 Band structure, phonon dispersion, and density of states

For anisotropic MC simulation of electron transport in solid, the band structure, phonon dispersion relation, and the density of states should be obtained as necessary input files.

2.1 Band structure

The pseudopotential Harmiltonian matrix element was given by Potz and Vogl[7]:

$$H_{KK'} = \frac{\hbar^2}{2m} K^2 \delta_{KK'} + [V^S(|K - K'|) + V_{NL}^S(K, K')]\cos[(K - K')\tau] \quad (1)$$

where m^* is an effective mass, k is the wave vector in the first brillouin zone and $K = k + G$, $K' = k + G'$, G and G′ are reciprocal lattice vector, and the nonlocal part $V_{NL}^S(K, K')$ is expressed as

$$V_{NL}^S(K, K') = \frac{4\pi}{\Omega_a} \sum_{l=0,2} A_l^i (2l + 1) P_l(\cos\theta_{KK'}) F_l^i(K, K') \quad (2)$$

where $P_l(x)$ is Legendre polynomials, $\theta_{KK'}$ denotes the angle between K and K′, A_l^i is a parameter and only $l = 2$ should be computed for Ge, Ω_a is the atomic volume, a is the lattice constant and

$$F_l^i(K, K') = \int_0^\infty r^2 j_l(Kr) f_l^i(r) j_l(Kr) \mathrm{d}r \quad (3)$$

where $j_l(x)$ is the sphere Bessel function and $f_l^i(r) = \exp(-r^2/R_l^{i2})$.

Then, the energy eigenvalues and eigenvectors are found by solving the secular equation

$$\det | H_{KK'}(k) - E(k)\delta_{KK'} | = 0 \quad (4)$$

Figure 1 shows the conductance band structure for germanium calculated by the above nonlocal pseudopotential using the parameters listed in Table 1. By detailed comparisons of critical point energies calculated by this pseudopotential method and measured by photoemission experiments[8], we conform the validity of the calculation.

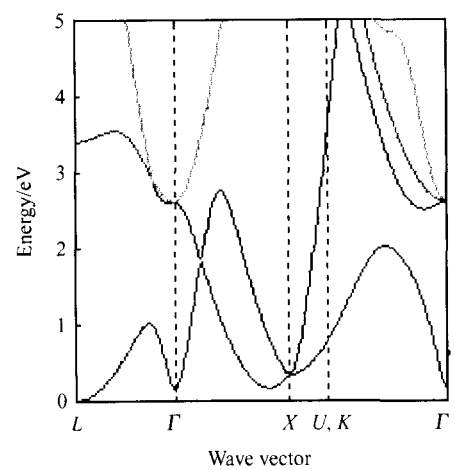

Fig. 1 Conductance band structure for Ge calculated by nonlocal pseudopotential approach

Table 1　Local and nonlocal pseudopotential parameters for Ge

Material	Lattice constant/ nm	Form factors(Ry)				Nonlocal parameters				
		$V^s(3)$	$V^s(4)$	$V^s(8)$	$V^s(11)$	α_0(Ry)	β_0	A_2(Ry)	R_0	R_2
Ge	0.565	-0.2378	-0.1600	0.0053	0.0678	0	0	0.275	0	1.22

2.2　Phonon dispersion relation

The phonon energy is very important to determine the scattering rate or the post-scattering state. There are several approaches to calculate the phonon dispersion curves. In this MC calculation, the adiabatic bond charge model for the dynamics of diamond-type crystals is adopted to calculate the phonon dispersion relation for Ge in the irreducible wedge of the first brillouin zone[9] ;four types of interactions are used: (1) central ion-ion forces; (2) Coulomb interactions of the ions and bond charges (BC 's) ; (3) central ion-BC forces; (4) bond-bending forces. The results are shown in Fig. 2. Note that the result is satisfactory by comparing with Ref. [9] or even a text book.

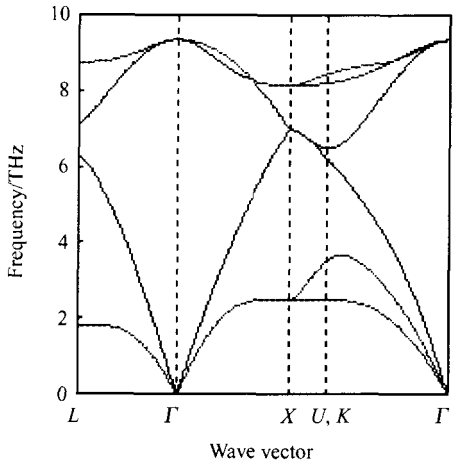

Fig. 2　Phonon dispersion relation for Ge calculated by adiabatic bond-charge model

2.3　Density of states

According to the definition, DOS can be obtained from the full band structure in the Brillouin zone as follows:

$$D(E) = \sum \delta(E(k) - E) \tag{6}$$

where E is the energy.

The absolute value of DOS is given by the surface integral over the equal energy E,

$$D(E) = \oint \frac{\mathrm{d}s}{\nabla_k E(k)} \tag{7}$$

where ds denotes the area of iso-energy surface in the Brillouin zone grid. This integral can be evaluated by numerical method.

As the DOS is used to scale the scattering rates obtained from the valley model, the relative value of DOS at different energy is adequate. Therefore, a relatively simple method can be used which accounts the number of the states in the k space between the range from $E-\Delta E$ to $E+\Delta E$. It can give the relative value of DOS, that is, the DOS calculated by this method has the arbitrary units. This result shown in Fig. 3 is used to scale the scattering rate of the valley model at higher energy.

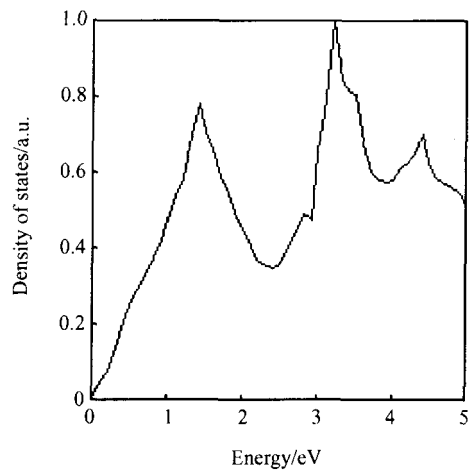

Fig. 3　Density of states obtained from band structure of Ge

3　Efficient anisotropic scattering rates calculation

Actually, the electron state transition rate from k to k $\pm$q 'is given by Fermi 's golden rule[4] ,

$$p(k, k\pm q) = \frac{2\pi}{\hbar}|\langle v', k\pm q, N_q \mp 1| H' |v, k, N_q\rangle|^2 \times \delta(\varepsilon(k\pm q) - \varepsilon(k) \mp \hbar\omega_q) \tag{8}$$

Subtration and plus signs correspond to emission and absorption of a phonon, respectively.

While anisotropic scattering rates are wave-vector and energy band dependent, its calculation may be very time-consuming when using first principle from the full band discrete results. In a simplified approach, the rates may be obtained with the standard non-parabolic band approach. A scaling based on the knowledge of the full band density of states is applied to get the proper behavior. This may be accepted since at high energy the DOS is expected to play a more important role than the details of band structure[6] are. Also, this procedure is acceptable for most device simulation applications and it adds negligible cost with respect to the standard Monte Carlo approach. It is then possible to update scattering table on-the-fly if one wants to change temperature, material composition, etc.

At low energy level, the classical non-parabolic model is valid and the scattering rates[4] can be used. At high energy the scattering rates should be numerically calculated using the full band structure. However, as a first approximation, we decide to account for the band-structure effect only through the DOS term.

$$p(\varepsilon) = \begin{cases} p(\text{nonparabolic}), & \varepsilon \leq \varepsilon_0 \\ p(\text{nonparabolic}) \dfrac{\text{DOS}(\varepsilon)}{\text{DOS}(\varepsilon_0)}, & \varepsilon > \varepsilon_0 \end{cases} \quad (9)$$

where p(nonparabolic) is the scattering rates obtained with the standard non-parabolic band approach, DOS(ε) and DOS(ε_0) are the density of states at energy ε and ε_0, respectively, ε_0 is the threshold energy below which the nonparabolic model is valid, which equals to 0.4eV in this simulator. The energy dependent scattering rate is calculated and shown in Fig. 4.

We take into account the following scattering mechanisms: acoustic phonon absorption, acoustic phonon emission, optical phonon absorption, optical phonon emission, ionized impurity, impact-ionization, and self-scattering. The energy dependent Ridley and Keldysh formulation are used for ionized impurity scattering and impact ionization rate, respectively.

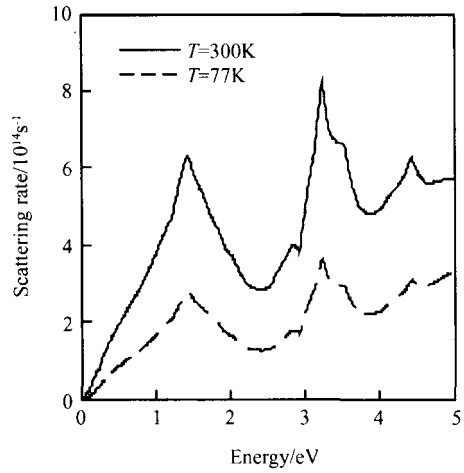

Fig. 4 Total phonon scattering rate for Ge calculated by valley model and scaled by density of states

4 Calculation procedure

In this MC simulator, the 1/48 irreducible wedge of the first brillouin zone is discretized with the mesh spacing of 0.025 in units of $2\pi/a$, where a is the lattice constant, the wedge is discretized by 7544 grids. In each grid, the band structure and phonon dispersion curves are calculated. The discrete band and phonon information, along with DOS, are created as input files in the main program.

At free flight, the semiclassical equations describing the motion of an electron in the reciprocal and real space, are written, respectively, as

$$\frac{\mathrm{d}\mathbf{k}}{\mathrm{d}t} = -\frac{e\mathbf{F}}{\hbar} \quad (10)$$

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = \frac{1}{\hbar}\nabla_{\mathbf{k}} E(\mathbf{k}) \quad (11)$$

Under the electric field, some electrons suffer free flight but others will scat according to their scattering rates, and the types of scattering will be chosen stochastically.

After scattering the electron state is changed according to the nature of the scattering. The selection of post-scattering is another CPU intensive procedure of MC simulation state because of the discrete band structure and phonon disperasion re-

lation. In this simulator ,it is assumed that energy and momentum conservation is held in the selection. The selection of the post scattering state in k space consists of three parts. Firstly ,simulator selects the cubes whose energy are within the range of energies plus/ minus phonon maximum energy 40meV in the wedge of first Brillouin zone[11] ,significantly reducing the computation costs. Secondly ,these cubes are mapped to the whole Brillouin zone according to the symmetry property. Finally , the final states are chosen stochastically in the isoenergy surface of the selected cubes defined by Fermi 's golden rule[12] .

5 Results and discussion

The new Monte Carlo simulator has been applied to the transport properties in bulk germanium. Figure 5 shows the average velocity of electrons in Ge versus electrical field at 77 K and 300 K respectively. The experimental results are also shown in this figure for comparison[13] . Since the electrons with higher energy will experience larger scattering rates ,as shown in Fig. 4 ,the drift velocity deviates from linearity at high electric field region. On the other hand ,the drift velocity decreases at higher temperature because of the larger scattering rates also shown in Fig. 4. It is also found from Fig. 5 that the electron velocities show strong anisotropicity at lower temperature ,and a negative differential mobility (NDM) occurs at 77 K along the (100) direction ,which is attributed to transfer electron mechanism and the non-parabolicity of the lower valleys[4,13] .

The average electron energy simulated versus electrical field at different temperatures ,along with the previous MC work ,is shown in Fig. 6[3,4] . Almost no anisotropicity was found in the simulation , so the results in the figure represent along both (100) and (111) directions. It can be seen that when electric field is higher than 10^4 V/ cm ,the average energy is larger than the energy gap between valley L and X ,thus will induce the inter-

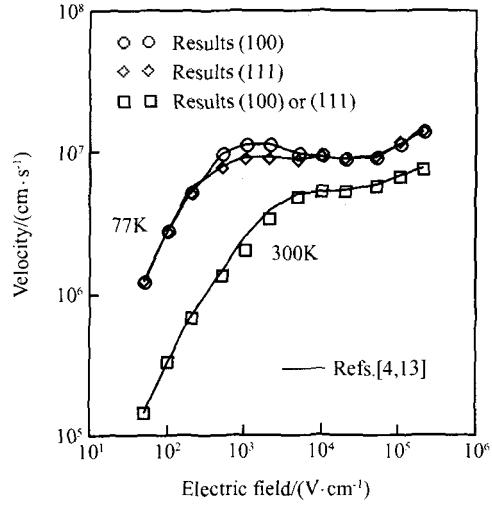

Fig. 5　Dependence of average drift velocity of electrons in Ge on electric field at different temperatures

valley scattering from L to X in Ge ,and this transfer electron effect causes the NDM in v-E curve. For present small dimensional devices ,the electric field exceeds 10^4 V/ cm in considerable part of the channel ,the inter-valley scattering has a significant impact on device behavior. As the parabolic or non-parabolic band structure is out of the range of validity at this energy ,the selection of post-scattering state based on discrete band structure and energy-momentum conservation is necessary.

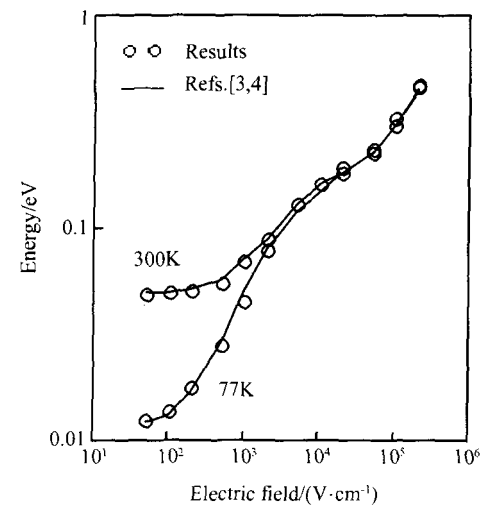

Fig. 6　Average energy of electrons in Ge as a function of electric field at different temperatures

From these figures ,it is found that this MC simulator with anisotropic scattering consideration

can accurately reproduce experimental or previous MC results at a wide range of temperature and electric field. As this DOS scaled scattering rates can be obtained efficiently and the results are satisfactory in the range of normal device operation, it can be used in device simulator.

6 Conclusion

Monte Carlo simulator for the electron transport in germanium is developed. By the full band structure, phonon dispersion relation and density of states as inputs, the energy dependent scattering rates are obtained with nonparabolic approach and scaled by density of states at higher energy range. The after-scattering state is selected based on energy and momentum conservation in the discrete k space anisotropically. The results in the range of normal device operation are satisfactory by comparing with the experiment data or previous MC simulator. As it's DOS scaled scattering rates can minimize the calculation time, this approach is suitable for the device simulator.

Acknowledgments The authors would like to thank the Beckman Institute, University of Illinois at Urbana-Champaign (UIUC) for kindly providing the research facilities and other helps.

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考虑各项异性散射的锗中电子输运的全能带蒙特卡洛模拟 *

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摘要: 在考虑各向异性散射的基础上,对锗中电子输运特性进行了全能带蒙特卡洛模拟. 计算过程如下:锗的全能带由 nonlocal empirical pseudopotential 方法求得;态密度的相对值通过不同能量的状态数得到;声子色散谱由 adiabatic bond-charge 模型求出;电子-声子散射率在低能量时采用费米黄金律得出的非抛物线散射率,高能量则通过态密度对其修正而得到;散射后的状态满足能量守恒和动量守恒. 通过比较计算结果与实验报道,证实了该模型算法的正确性,由于该模型能正确反映锗中电子的速度与能量特性,同时又能大大降低散射率的计算成本,故可运用在器件模拟中.

关键词: 蒙特卡洛模拟; 费米黄金律; 输运特性; 锗

PACC: 7210; 7320A; 6300

中图分类号: TN304. 1　　**文献标识码**: A　　**文章编号**: 0253-4177(2005)03-0465-07

* UESTC 访问研究计划资助项目

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2004-07-11 收到,2004-10-18 定稿