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Tight-binding Approach to Electron Transport in Nanostructured Semiconductors

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We report an analysis on electron transport in nanostructured semiconductors within the tight-binding framework. We employ the Chebyshev expansion to calculate the time-evolution of single-electron wave function. The mean-square displacement and diffusivity of electron in Si chains are obtained for atomic orbitals taken as initial states. The results show ballistic behavior of electron in the pure Si chain. Substitution of impurity atom (Ge) reduces the ballistic regime due to impurity scattering.
Key words: semiconductor, nanowire, electron transport, tight-binding model

1. INTRODUCTION

Recent progress in nanotechnology has made electron dynamics in nanostructures extremely important. For example, FET that consists of one semiconducting single-wall carbon nanotube has been fabricated [1]. Electron transport in such nanoscale devices has shown essential differences in its mechanisms from those described by conventional approaches for bulk semiconductors. Most of the theoretical approaches to electron dynamics in bulk semiconductors have been based on the effective mass method, which has been quite successful for their macroscopic properties. However, the standard effective mass method cannot be applied to nanostructures, because the method describes only the envelope of electron wave functions and neglects interband electron transitions. In the present study, we use the Heisenberg operator for electronic positions to calculate electron dynamics following the idea D. Mayou *et al.*[2,3,4] have developed. In Ref. 2, the authors calculated DC conductivity of quasicrystals using Kubo-Greenwood formula. They adopted the Chebyshev expansion for calculating efficiently the Heisenberg operator. The same technique has been applied to an analysis on the electron diffusivity in a grain boundary of SiC [5]. Here, we use similar technique for calculating electron diffusivity in silicon chain, as a model system of nanostructured semiconductor.

2. BASIC FORMALISM

Time evolution of an electronic state can be described as

$$|\Psi_{i\alpha}(t)\rangle = \exp(-i\hat{H}t/\hbar)|i\alpha\rangle \,, \quad (1)$$

where $|i\alpha\rangle \equiv |\Psi_{i\alpha}(t=0)\rangle$ is the initial state. In this study we take atomic-like orbitals as initial states. These i and α denote indices of atom and its associated orbital, respectively.

The electron diffusivity is defined as

$$D_{i\alpha}(t) \equiv \frac{1}{t}\langle \Psi_{i\alpha}(t)|\hat{X}^2|\Psi_{i\alpha}(t)\rangle \ . \quad (2)$$

Assuming that those atomic-like functions form a complete orthogonal set, equation (2) can be rewritten as

$$D_{i\alpha}(t) = \frac{1}{t}\Big[\sum_{j_1\beta_1}\sum_{j_2\beta_2}\sum_{j_3\beta_3} \langle i\alpha|e^{i\hat{H}t/\hbar}|j_1\beta_1\rangle\langle j_1\beta_1|\hat{X}|j_2\beta_2\rangle \times \langle j_2\beta_2|\hat{X}|j_3\beta_3\rangle\langle j_3\beta_3|e^{-i\hat{H}t/\hbar}|i\alpha\rangle \Big] . \quad (3)$$

Here, j's and β's also denote indices of atomic position and atomic orbital, respectively.

The time-evolution operator $\exp(-i\hat{H}\,t/\hbar)$ in Eq.(3) is calculated approximately by the Chebyshev expansion of the first kind. For scalar argument x, the Chebyshev expansion of a function f is defined as follows:

$$f(x) \cong \sum_{k=0}^{n-1} d_k T_k(x) \,, \quad (4)$$

where

$$d_0 = \frac{1}{n}\sum_{j=1}^{n} f(x_j) \,, \ d_k = \frac{2}{n}\sum_{j=1}^{n} T_k(x_j) f(x_j), \quad (5)$$

and

$$x_j = \cos\frac{(2j-1)\pi}{2n} . \quad (6)$$

The Chebyshev polynomial of degree n denoted by $T_n(x)$ is given by the explicit formula,

$$T_n(x) = \cos\{n \arccos(x)\} \ . \quad (7)$$

For T_n holds a recurrence relation;

$$T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x) \,, \quad n \geq 2$$
$$T_0(x) = 1, \quad T_1(x) = x \ . \quad (8)$$

The time-evolution operator can be expanded by the Chebyshev polynomials as

$$\langle j_1\beta_1|e^{-i\hat{H}t/\hbar}|j_2\beta_2\rangle = \sum_{k=0}^{n-1} d_k(t)\langle j_1\beta_1|T_k(\hat{H})|j_2\beta_2\rangle . \quad (9)$$

The Chebyshev polynomials of the Hamiltonian operator are calculated using the recurrence formula Eq.(8), replacing x with the Hamiltonian matrix. Here we use

tight-binding model for the Hamiltonian matrix, which includes only the effects of the nearest neighbor atoms. Thus, the mean displacement of electron is approximated by

$$\sum_{j_1\beta_1}\sum_{j_2\beta_2}\langle j_1\beta_1|\hat{X}|j_2\beta_2\rangle = \sum_{j_1\beta_1}[\ \langle j_1\beta_1|\hat{X}|j_1-1,\beta_1\rangle + \langle j_1\beta_1|\hat{X}|j_1\beta_1\rangle + \langle j_1\beta_1|\hat{X}|j_1+1,\beta_1\rangle\ ]. \quad (10)$$

We then assume that the integrals have nonzero values only when the two orbitals are of the same kind. The integrals with orbitals on the same atom are approximated as positions of the atom accompanying the orbitals. Similarly, the integrals with the nearest-neighbor orbitals are approximated as the positions of their bond center.

Once the diffusivity is calculated, DC conductivity of the system at T=0K can be obtained from Kubo-Greenwood formula

$$\sigma_{DC}(E) = \frac{2\hbar e^2\pi}{\Omega}\lim_{t\to\infty}\sum_{i\alpha} D_{i\alpha}(t)\frac{\langle\Psi_{i\alpha}(t)|\hat{X}\delta(\hat{E}-\hat{H})\hat{X}|\Psi_{i\alpha}(t)\rangle}{\langle\Psi_{i\alpha}(t)|\hat{X}^2|\Psi_{i\alpha}(t)\rangle}. \quad (11)$$

The calculation of σ_{DC} usually requires very large system in order to achieve the convergence for $t\to\infty$. In the present study, on the other hand, we only need short-time regimes since the system of our interest is of nanoscale. Therefore, we only focus on the analyses of the diffusivity of electrons.

3. MODEL FOR ANALYSIS

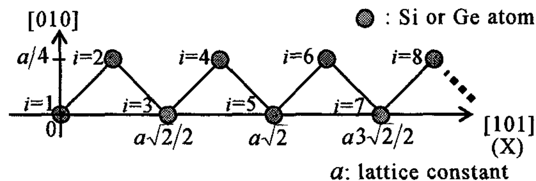

Fig.1 Semiconductor chain model

The model system we adopted is Si chains shown in Fig.1, where a is chosen to be the bulk value of lattice constant for diamond structure. The principal axis of the chain is equivalent to that along the [101] direction in diamond structure. We consider four Si chains, the composed of N=4, 8, 12, and 16 Si atoms with lengths 0.5760, 1.3441, 2.1122 and 2.8802nm, respectively. We also consider Ge impurity substituted in the Si chain N=16.

For calculating the time-evolution operator, we adopt sp^3s^* model for the tight-binding Hamiltonian of Si and Ge given by P.Vogl et al. [6].

4. RESULTS

Figure 2 shows calculated diffusivity for Si chain with N=4, 8, 12 and 16. Diffusivity depends on the initial position i and the initial orbital α. In Fig.2, we show the orbital dependence of the diffusivity for the electron initially at i=1. Figure 2(a) indicates that the diffusivities are small and there are no significant differences among orbitals. In Figs.2(b), (c) and (d), the diffusivity for s orbital is larger than other orbitals and increases linearly up to around 1.2fs, 1.8fs, and 2.4fs, respectively. Thus, the time scale, in which the diffusivity increases linearly, becomes longer as the length of Si chain increases.

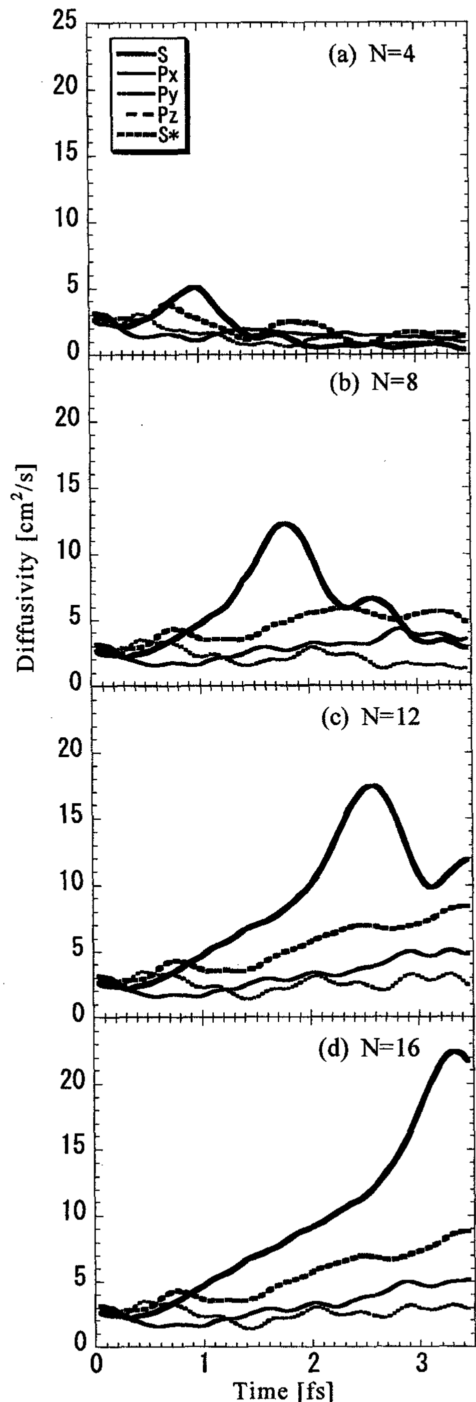

Fig.2 Diffusivity vs. time for different lengths N. (a), (b), (c) and (d) are the cases of N=4, 8, 12 and 16, respectively. The time scale, in which the diffusivity increases linearly, is getting longer with increase of N.

Figure 3 shows calculated electron diffusivity in Si chain (N=16) with a Ge impurity. The positions of Ge atom are set to be i=4, 7, 10 and 13 in the chain. In Fig.3(a), diffusivities are small and there are no significant differences among all orbitals. In Fig.3(b), (c)

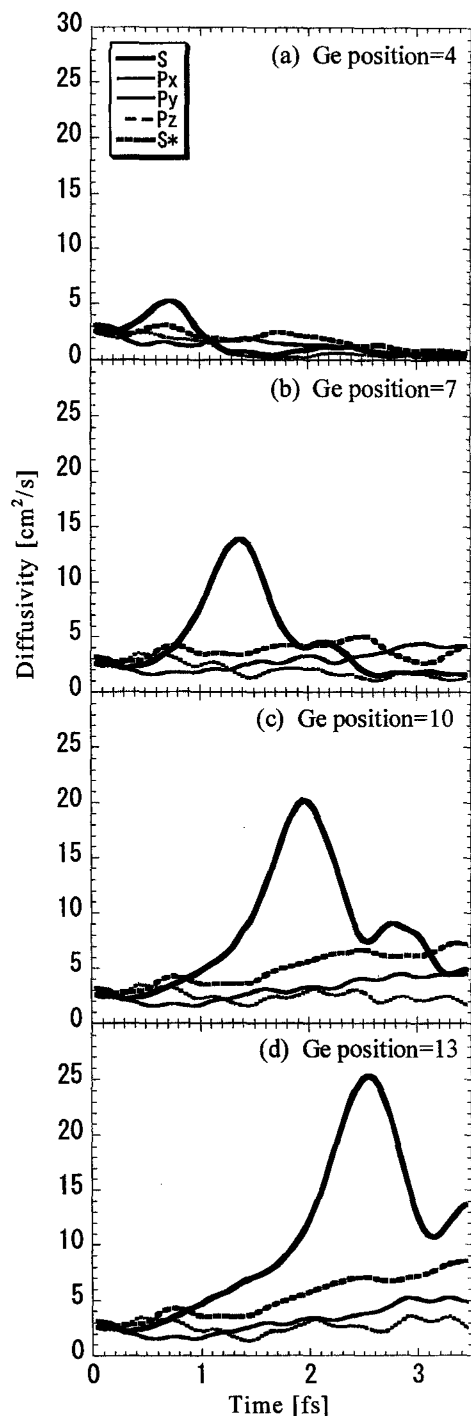

Fig.3 Diffusivity vs. time for different Ge positions. (a), (b), (c) and (d) are the cases of Ge position at 4, 7, 10 and 13, respectively. The time scale, in which the diffusivity increases linearly, is getting longer with increase of the distance between the initial position of electron and the Ge atom.

and (d), the diffusivity of *s* orbital is larger than other orbitals and increases linearly up to around 0.6fs, 1.1fs and 1.6fs, respectively. Thus, the time scale in which diffusivity increases linearly becomes longer as the distance between the initial position of electron and the Ge atom increases, similarly to the results shown in Fig.2.

5. CONCLUSION

The time scale in which the diffusivity increases linearly corresponds to a ballistic regime of electron motion and the length of ballistic motion is equal to the mean free path of an electron in the system. Consequently, our model shows a ballistic behavior of *s* electrons in Si chains. It is also shown that the diffusivity depends on the position of Ge atom in Si chain. This can be interpreted as the effect of impurity scattering in the conventional Boltzmann theory. The decrease of diffusivity after the peak may be due to the interference with the electron reflected at the end of Si chain.

The remaining issues are the following. First, the expectation values of position X in Eq.(10) has to be calculated exactly, starting from each orbital type. Here we have assumed that the integral with same orbitals is finite and the integral with different orbitals is zero: We have to confirm the validity of this assumption. Second, we should be able to study much larger system using the present scheme. We may also need to consider better tight-binding parameters for the system studied here. Accuracy in describing π bonding of conduction state and dangling-bond state can be essential for electron dynamics in such nanostructures.

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