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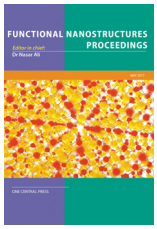

Impact of Crystal Orientation and Conduction Band Nonparabolicity on Diffusion Constant of Nano-scale Si Rectangular Wires - theoretical estimation

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ABSTRACT

In this paper, we address the significant impact of crystal orientation in the estimation of the diffusion constant of Si nanowires confined by (111) surfaces. This calculation applies quantum-mechanical averaging to physical parameters because we must take account of the distinct electronic states of the one-dimensional (1-D) system. For the case of confinement along the <111> direction, it is shown that the diffusion constant is insensitive to width in the approximate equation. This characteristic is slightly impacted by the assumption of the non-parabolic conduction band. On the other hand, Si nanowires confined by (001) and (011) surfaces don't show such interesting behavior.

I. INTRODUCTION

The electrochemical property of one-dimensional materials, which includes Si wire, is attracting intense attention because such materials can realize energy-conversion devices through the Seebeck effect [1, 2] and the photochemical effect. The low thermal conductivity of Si nanowire is also attracting attention. Even though extensive simulation studies of such structures have been performed [3], several physical parameters must be reconsidered because the bulk properties of Si material are expected to alter with scale reduction [3].

In this paper, we calculate, theoretically, the diffusion coefficient of electrons in silicon based on a feasible semi-microscopic theoretical model at around room temperature. We constrain the consideration of the carrier diffusion process to room temperature or thereabout because it allows us to assume the thermal smearing effect of quantum-mechanical transport; *i.e.*, a couple of semiclassical approaches will be shown to be covered by the theoretical calculation of the diffusion process of carriers [4, 5]. We discuss the impacts of crystalline orientation and non-parabolic band effect of conduction band on the diffusion constant.

II. DIFFUSION CONSTANT MODEL

Theoretical Base. The diffusion process is theoretically described by the master equation based on the probability density [6]. For the 1D transport system, the semiclassical diffusion coefficient $D(\omega)$ is expressed as [6]

$$D(\omega) = \sum_{x,x'} \left(-\frac{1}{2}\omega^2 \right) (x - x')^2 \tilde{P}(x, i\omega \,|\, x') \,, \tag{1}$$

where $\tilde{P}(x, i\omega|x')$ is the Fourier transformation of the probability density of finding a particle at site x. For the present topic, we take the limit of $\omega \to 0+$; the static limit of the diffusion coefficient, $D(0+)$, is given. The stochastic motion of particles at the low-field limit yields Einstein's relation, which suggests that the group velocity given by the averaged energy of particles rules the transport of particles. At the low-frequency limit ($\omega \to 0+$), the average trace of particle loci over a certain period should be ruled primarily by a low frequency component because high-

frequency parts would automatically cancel each other out owing to the random-phase behaviors of particles. This yields

$$D(0+) = \lim_{T_v \to \infty} \sum_{x,x'} -\frac{1}{2}\left(\frac{x-x'}{T_v}\right)^2 \tilde{P}(x, i\omega \mid x') \cong \sum_{x,x'} -\frac{1}{2} v(0+)^2_{x-x'} \tilde{P}(x, 0+ \mid x') \tag{2}$$

where T_v is the time constant that characterizes particle behavior and $v(0+)_{x\text{-}x'}^2$ means the square of the mean velocity at the low-frequency limit.

Assuming the diffusion process is *ergodic*, we introduce the following approximate expression for $D(0+)$.

$$D(0+) \cong \sum_{x,x'} -\frac{1}{2} v(0+)^2_{x-x'} \tilde{P}(x, 0+ \mid x') \approx \frac{1}{2}\int_0^\infty < v(0+)^2_{x,x'} > \exp\left(-\frac{t}{T_v}\right) dt \tag{3}$$

This deduction is, in theory, valid provided the temperature is sufficiently high.

We assume a sufficiently long wire. If, for simplicity, we assume that the thermalization process is dominated by the primary spectrum of the diffusion process, Eq. (3) can be approximated as [5, 7]

$$D_{T,1D} = \frac{1}{2}\tilde{T} < v^2 >= \frac{1}{2}\tilde{T}\int_0^\infty v^2 f(v) dv \ , \tag{4}$$

where we deduce that $\tilde{T}$ is the characteristic time restricting the primary spectrum of carrier diffusion, v is the one-dimensional carrier velocity, and $f(v)$ is the distribution function of the velocity of the one-dimensional carriers. In this calculation, we apply quantum-mechanical averaging to $<v^2>$ because we must take account of the distinct electronic states of the one-dimensional system; *i.e.,* the quantum states of subbands are not entirely smeared by the thermal energy in narrow semiconductor wires.

Crystalline Orientations. The crystalline orientation of Si nanowires assumed here is shown in Fig. 1; the confinement surface is (010), (011), or (111).

Non-parabolicity of Conduction Band. In this paper, we introduce the following model for the conduction band non-parabolicity.

$$E(1+\alpha E) = \frac{\hbar^2 k^2}{2m^*} \ , \tag{5}$$

where α is the non-parabolicity parameter (units of eV^{-1}), m^* is the effective mass of electrons.

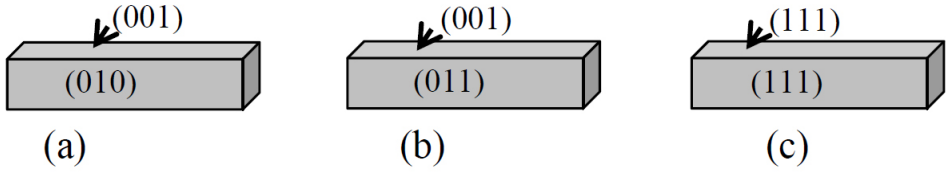

Figure 1 Crystalline orientation of Si-wire surfaces.

III. SIMULATION RESULTS AND DISCUSSION

Calculation results of diffusion constant of Si nanowires are shown in Fig. 2; Figure 2(a) shows those with the assumption of parabolic band structure of the conduction band, and Figure 2(b) shows those with the assumption of non-parabolicity of the conduction band. The diffusion constant slightly depends on the confinement geometry even for large dimensions. When we assume the parabolic band, the diffusion constant for the <111> confinement is almost insensitive to nanowire size in the present model, while the diffusion constant for the <111> confinement falls with wire size when we assume the non-parabolic band structure. On the other hand, for <001> confinement and <011> confinement, the diffusion constant rapidly falls regardless of the band structure as wire size is reduced. For <001> and <011> confinement, the effective density of states is decreased as wire width is reduced, which suppresses the carrier diffusion. In contrast, for <111> confinement, the effective density of states is not significantly decreased as the wire width is reduced. This results in the different behavior of the diffusion constant.

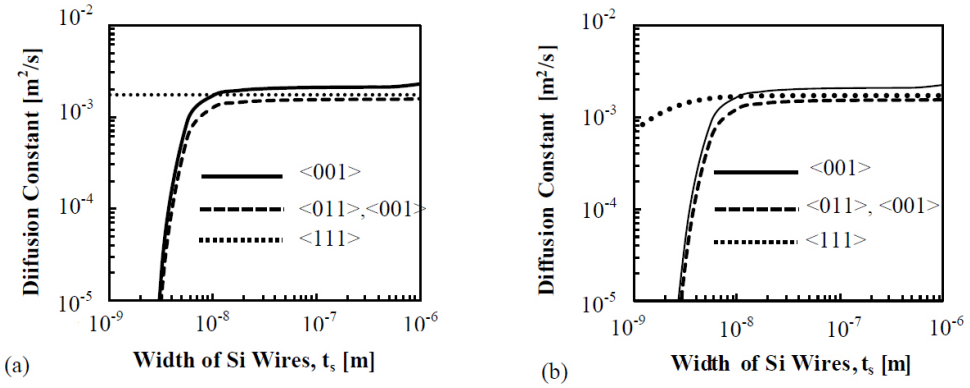

Figure 2 Diffusion constant as a function of Si wire width. (a) Parabolic band model, (b) Non-parabolic band model.

IV. ACKNOWLEDGEMENT

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