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Numerical Simulation of Hole Transport in Silicon Nanostructures

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INTRODUCTION

In ultra-small MOSFETs, quantum-mechanical effects, such as quantum confinement and source-drain direct tunneling, significantly affect device characteristics. To simulate electron transport in such devices, quantum-transport modeling is necessary. For CMOS application, quantum simulation of hole transport is also required. For hole transport modeling, it is desirable to include the valence-band structure using an accurate method, such as an empirical tight-binding method, since the valence-band structure is complex and makes the hole effective mass dependent on the axis orientation. Quantum simulation with the complex valence-band structure, however, requires expensive computational costs, which may restrict the device size that can be simulated. The tradeoff between accuracy and computational costs is one of important issues associated with the quantum simulation of hole transport. In order to address this issue, we have performed numerical simulation of hole transport in nanoscale Si structures within a nonequilibrium Green's function formalism combining with three different types of methods for band structure calculation; an empirical $sp^3d^5s^*$ tight-binding method (TBM) [1], $\boldsymbol{k}\cdot\boldsymbol{p}$ multiband approximation (MBA) [2], and effective-mass approximation (EMA).

METHOD

We consider a (100)-oriented p^+pp^+ Si nanostructure whose schematic diagram is given in Fig. 1. The device structure is the same as that considered in Ref. [3] except for the type of doping. For the longitudinal direction (x direction), we use a discrete lattice in real space. For the transverse directions (y-z directions), we assume periodic boundary conditions and use the eigenstate basis labeled by two-dimensional wavevectors $\boldsymbol{k} = (k_y, k_z)$. We descritize the two-dimensional $\boldsymbol{k}$-space into triangular meshes and evaluate spectral functions, $A(\boldsymbol{k}, E)$, and transmission functions, $T(\boldsymbol{k}, E)$, at each mesh point. Hole density and the total transmission are then calculated by summing those functions over $\boldsymbol{k}$- and energy-spaces.

RESULTS AND DISCUSSION

We used the parameters of Ref. [4] for TBM and those of Ref. [2] for MBA. For EMA, we adjust the heavy hole mass so as that the density of states agrees with that of TBM (see Fig. 2). Fig. 3 shows a density plot of $A(\boldsymbol{k}, E)$ at Γ-point calculated with EMA for $V_\mathrm{d} = 50\,\mathrm{meV}$. The self-consistent potential profile is also plotted by solid line. Figs. 4 and 5 represent $A(\boldsymbol{k}, E)$ at Γ-point calculated with MBA and TBM, respectively, for the same potential profile given in Fig. 3. Performing similar calculations for other $\boldsymbol{k}$ mesh points, we obtain the hole density profile and current density. In Fig. 6, the calculated hole density profile is plotted for $V_\mathrm{d} = 50\,\mathrm{meV}$. We see that EMA is insufficient for an accurate modeling of hole transport in Si nanostructures.

ACKNOWLEDGMENT

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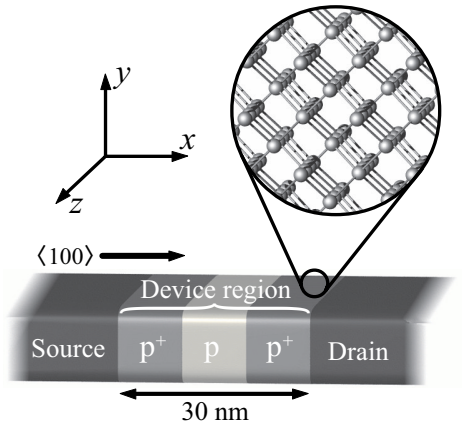

Fig. 1. Schematic diagram of the device structure together with the coordinate axis.

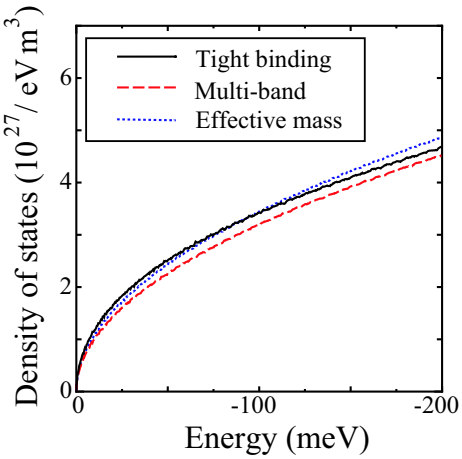

Fig. 2. Density of states calculated with the tight-binding method (solid line), $\boldsymbol{k}\cdot\boldsymbol{p}$ perturbation (dashed line), and effective-mass approximation (dotted line).

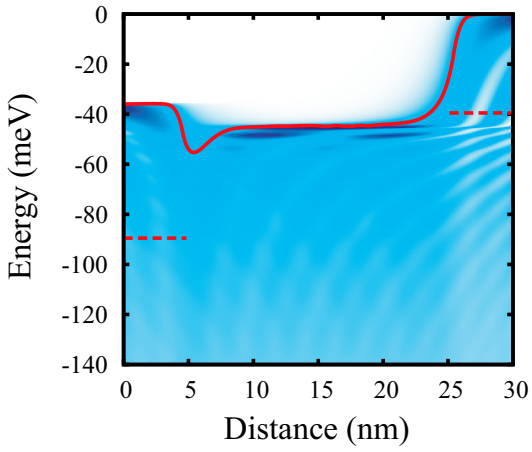

Fig. 3. Spectral function at Γ-point calculated with the effective-mass approximation. Solid line represents the self-consistent potential profile and dashed lines the Fermi levels.

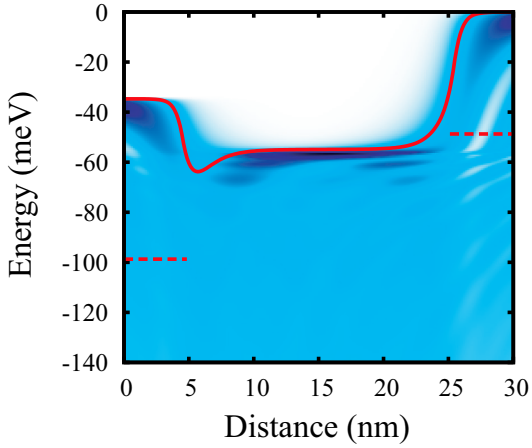

Fig. 4. The same as Fig. 3 but for the $\boldsymbol{k}\cdot\boldsymbol{p}$ perturbation.

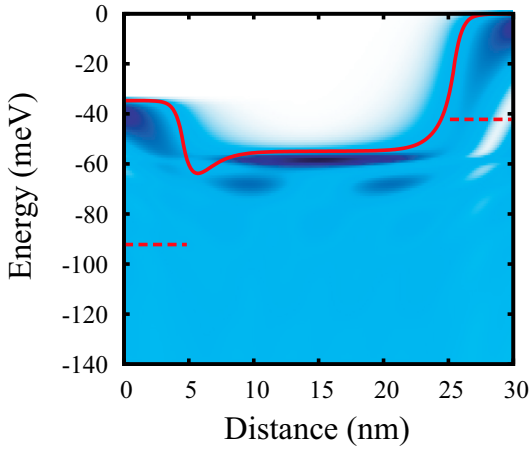

Fig. 5. The same as Fig. 3 but for the tight-binding method.

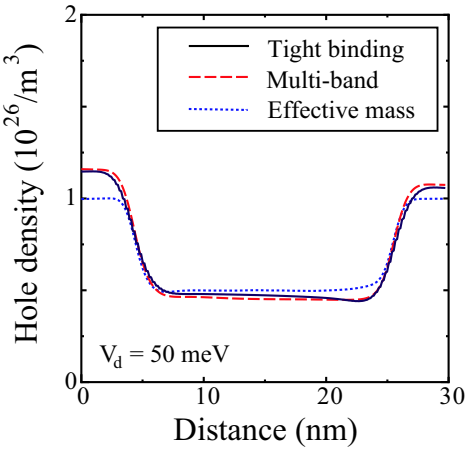

Fig. 6. Hole density profile calculated with the tight-binding method (solid line), $\boldsymbol{k}\cdot\boldsymbol{p}$ perturbation (dashed line), and effective-mass approximation (dotted line).