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Resonance-enhanced Tunneling Current through Doped Si-p/n Junction; Theoretical Study

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Abstract

Tunneling current in Si-based TFETs is markedly enhanced when the isoelectronic co-doping of Al and N atoms is realized at the p/n junction. In this work, we studied why such doping enhances the current and what types of dopants are desirable, by the numerical simulation using a simple atomistic model. It is shown that the tunneling current is enhanced when discrete electronic states of dopants resonate and mix with continuous conduction/valence-band states of host Si at the p/n junction. Moreover, we show that the further increase of tunneling ratio is expected by controlling the dopant characteristics such as the spatial position of dopants in the junction and the energy position of dopant electronic state.

1. Introduction

Tunnel field-effect transistor (TFET) is one of promising candidates for energy-saving devices due to a much steeper switching, compared to conventional metal-oxide-semiconductor FETs (MOSFETs). However, the ON current is still low in the case of Si-based TFETs because of the indirect band-to-band transitions in Si [1]. Recently, Mori and his coworkers succeeded in remarkably enhancing a tunneling current in Si-based TFETs utilizing an isoelectronic co-doping of Al and N atoms around the p/n junction [2]. Correspondingly, we showed by first-principles calculations that the Al+N co-doping produces weakly-localized electronic states in Si band gap [3]. However, it is still unclear why the tunneling current is enhanced by such electronic states.

Tunneling current is traditionally calculated by the Kane's type formula assuming the plane p/n junction and the electric-field-induced band-to-band transitions. However, these methods are not applicable to the present doped Si-p/n junction. In this work, we perform the numerical simulation adopting a simple model of doped p/n junction, and clarify why the tunneling current is enhanced by the doping and what characters of dopants are important to increase the tunneling current.

2. Calculation Model and Method

To simulate the Si-p/n junction, we adopt a simple one-dimensional two-band tight-binding model shown in Fig.1, where the left and right regions correspond to p- and n-type Si, respectively. We use Wannier-orbital bases and assign a Si primitive unit cell to a single tight-binding site, thus the electrons in valence and conduction bands being transferred between nearest-neighboring sites. On-site energies are aligned in the junction region responding to the original alignment of p/n junction and the applied electric field. The electric-field-induced inter-band transitions occur from valence to conduction bands in this p/n junction and produce the tunneling current. The dopants having different on-site energies E_d are incorporated in the p/n junction region.

Tunneling is realized by tracing the time evolution of electron wave packets. Wave packets of valence electrons

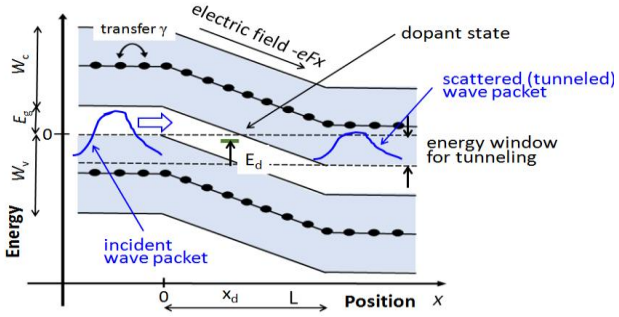

Fig.1. Schematic picture of atomistic tight-binding model of Si-p/n junction adopted in this work. Lower and upper connecting dots denote tight-binding sites of valence and conduction bands, respectively. Dopants are embedded in the junction region. Electron wave packets are incident from left p-type region, while the tunneling electrons are obtained as scattered wave packets in right n-type region. Typical parameters for Si are E_g=1eV (band gap), W_c=W_v=8eV (band width), L=5nm (junction length), F=4MV/cm (electric field). x_d and E_d are spatial and energy positions of dopants, respectively.

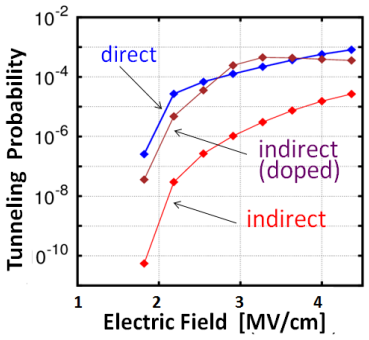

Fig.2. Calculated tunneling probability through the p/n junction of indirect band-gap semiconductor, as a function of electric field strength, for the cases with and without dopants. The probability for the direct-gap system is also shown for reference.

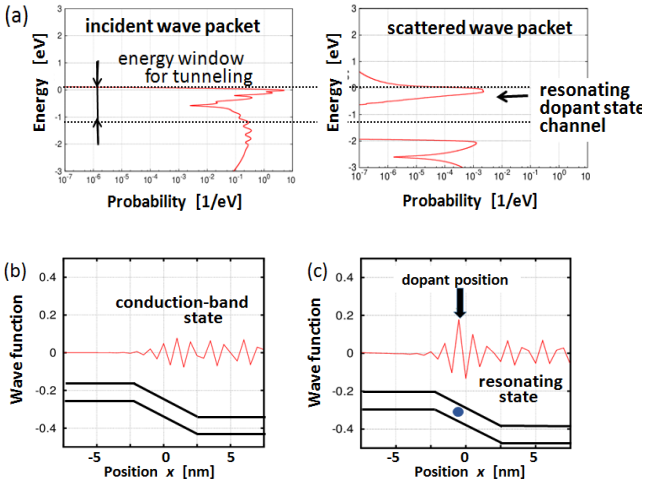

Fig. 3. (a) Energy distributions of incident and scattered (tunneled) wave packets. Scattered conduction-band final states after the tunneling (b) without and (c) with dopants in the p/n region.

are first prepared in the left p-type region, and then incident to the junction. The tunneling probability is obtained as a probability of scattered wave packets located in the conduction-band states in the right n-type region.

3. Results and Discussions

Origin of tunneling-current enhancement by dopants

First, we consider why the dopants in the Si p/n junction region increase the tunneling current. Figure 2 shows the tunneling probability of electrons from valence bands of left p-Si layers to conduction bands of right n-Si layers, as a function of applied electric field F, for the cases with and without dopants. For reference, the probability of direct band-gap system is also shown. Compared to the direct-gap system, the tunneling probability is small for the indirect-gap Si system due to the mismatch of Bloch wave numbers between valence and conduction bands. However, we can clearly see the remarkable increase of probability in the case with dopants.

To clarify the origin of tunneling-current enhancement by the dopants, we show the energy distributions of incident and scattered (tunneled) wave packets in Fig. 3(a), around the energy window of tunneling. Incident packet is mainly made of valence-band states of left p-Si, while tunneled packet is made of conduction-band states of right n-Si. The most notable feature is that the scattered (tunneled) packet has large components at the specific energy. By analyzing electronic states, we found that such energy corresponds to the electronic states of dopants.

Figures 3(b) and 3(c) show the final conduction-band states after the tunneling in the cases without and with dopants, respectively. In the former case, the conduction-band state is simply located in the n-Si side. In the latter case, however, the conduction-band state has large amplitude at the dopant position. This indicates that the electronic states of dopants resonate and mix with conduction-band states in the right n-Si layers. Since the dopants are located in the

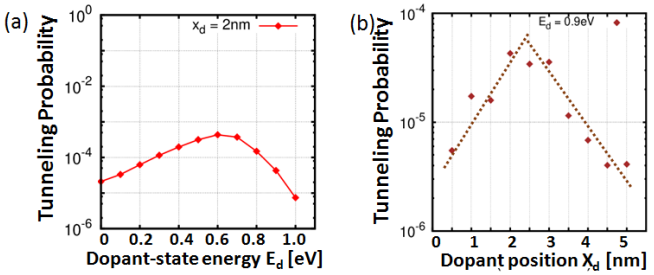

Fig. 4. Calculated tunneling probabilities as a function of (a) energy position of dopant electronic state in Si band gap and (b) spatial position of dopant in the p/n-junction region.

p/n-junction region and work as step stones for tunneling, the tunneling probability from left p-Si to right n-Si layers markedly increases in the case of doped Si-p/n junction.

Dependence of tunneling current on dopant characteristics

Then, we consider how the tunneling current changes with varying the dopant characteristics such as the energy and spatial positions. Figure 4(a) shows the tunneling probability as a function of the energy position E_d of dopant state in the Si band gap. The probability has the largest value around E_d=0.65eV. This is because the scattered conduction-band final state has large amplitude at the dopant site for this energy. When the energy of dopant state approaches the edges of conduction and valence bands of bulk Si, this state is embedded in the continuous spectra of bulk bands and thus the enhancement does not occur.

Figure 4(b) shows the tunneling probability as a function of the spatial position x_d of dopant in the p/n-junction region. The probability is large when the dopant is located around the center of junction. This is because the resonating dopant state is located around the center of the energy window of tunneling. When the dopant approaches to left and right edges of junction, the energy of dopant state becomes outside the window and thus the probability sharply decreases. In this way, the increase of tunneling current strongly depends on the dopant characteristics.

4. Conclusions

Tunneling probability of electrons through doped Si-p/n junction was studied by the time evolution of wave packets based on the simple tight-binding model. It was shown that the probability enhancement occurs when the dopant states resonate and mix with the conduction/valence-band states of host Si in the junction. In addition, we showed that the probability strongly depends on the spatial and energy positions of dopant electronic states.

Acknowledgements

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