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Enhancement of Electrical Conductivity by Miniband Formation In Silicon Quantum Dot Superlattice Structure

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1. Introduction

Quantum dot (QD) superlattice excites great interest of both physical scientist and device researchers. With quantum dots approaching and forming quasi-crystal structure, electron wavefunctions diffuse and overlap, which merges discrete quantum levels into minibands. This band rearrangement has significant applications for many novel opto-/electronic devices. For example, the quantum dot solar cell, the most exciting photovoltaic device with more than 63% conversion efficiency, has to utilize minibands for carrier transport and additional optical transition.

Ideal superlattice means a great challenge to present nanotechnologies. Several technologies, chemical solution method, molecular beam epitaxy (MBE) and so on, convincingly fabricate relative-uniform quantum dots; however, very few technologies can finitely arrange QDs to form quasi-crystal structure. The well-developed MBE technology can only achieve very limited control along growth direction, more seriously which induces mixture state from the wet-layer. The direct idea is developing the top-down nanotechnology. However, nanometer order size exceeds most light/electron beam limitation, and also seems impossible to get a proper mask. Very recently, our developed Neutral Beam Etching and ferritin bio-template bring a great breakthrough: we successfully fabricated the 2-dimensional array Si nanodisks (Si-NDs) with sub-10 nm, high density (>10^{11} cm^{-2}), and quasi-hexagonal crystallization [1-4].

The photovoltaic conversion efficiency is determined by the light absorbance and carrier collection efficiency. Our previous works have proved that the wavefunction coupling relaxes the selection ruler to induce additional optical transitions. In this paper, we firstly observed an enhanced conductivity in 2D array Si-NDs with SiC matrix. And within the envelop function theory and Anderson Hamiltonian method, we calculated electronic structures and the current transport, which theoretically proved that minibands enhanced the conductivity. These enhanced optical/electrical properties indicates a potential application for the ultra-high efficiency quantum dot solar cell.

2. Results and discussion

The conductive atomic force microscopy (c-AFM) has been used to investigate the conductivity, as shown in Fig. 1. Different from that in SiO_2 matrix, the 2D array Si-NDs in SiC matrix has a uniform current distribution except edge area, which indicates a strong in-plane electrical connection due to enhanced lateral coupling of wave functions. In addition, changing the matrix from SiO_2 to SiC greatly increases the current and decreases the threshold voltage. One cause is that minibands enhance the conductivity, which is revealed in the later theoretical simulation. More significantly, we first found that the 2D array Si-NDs in SiC matrix has better conductivity than the SiC thin film. This means it has great potential in carrier transport.

Our developed top-down nanotechnology achieves great flexibility in designing parts of the quantum structure, such as the independently controllable diameter and thickness, high-aspect ratio, different matrix materials, and so on. The finite element method is very suitable to describe complex quantum structures. Within the envelope function theory, the electronic structure and wavefunction are presented as

$$-\nabla \cdot \left(\frac{h^2}{2m} \nabla \phi \right) + V\phi = E\phi \quad (1)$$

Here, we mainly consider the matrix material and realistic geometry structure. A distinct feature is that due to the higher band-offset of Si/SiO_2 interface, electron wavefunctions are more strongly confined in the Si-NDs in SiO_2 matrix, as shown in Fig.2.(a). Thus, they result in the higher quantum levels. In addition, in the same geometry alignment, the stronger confinement means the weaker coupling of wavefunction and narrower miniband. In Fig.2.(b), when the matrix changes from SiC to SiO_2, the miniband width decreases from 1.04 meV to 0.37 meV.
With the Anderson Hamiltonian model, Chang et al. considered interdot coupling to deduce the below tunneling current density as

$$J = \frac{2eN}{h} \int_0^\infty d\varepsilon_z \int dk_{xy} \left\{ f_t[\varepsilon(k) - Ef_t] - f_d[\varepsilon(k) - Ef_d] \right\} \cdot \frac{\Gamma_t \Gamma_d}{\Gamma_t + \Gamma_d} \operatorname{Im} G_\sigma^r[\varepsilon(k), E(k_{xy})] \quad (2)$$

Here, *$E(k_{xy})$* is related to the energy discrepancy, ***t***, due to in-plane ND coupling E(kxy) = 2*t* [cos(k_xR) + cos(k_yR)].

With it, we simulated the I-V properties of our structures. Results are shown in Fig. 3. Calculated results also reveal that the wider miniband in SiC matrix brings a better transport property than that in SiO_2 matrix. A simplified, but not too distorted, explanation is that miniband formation broadens the resonance levels to increase the joint-state-density. The carrier transport in this two-barrier structure mainly depends on the resonant tunneling. Moreover, if the Coulomb blockade effect is neglected, the tunneling joint-sate-density in Eq. 2 can be simplified as a parabola function with a resonant peak at $\sim E_0 - E(k_{xy})$. Miniband formation broadens resonant peak to allow more states to approach the maximum, which results in the enhanced current. Thus, the wider miniband means a higher current density and lower threshold voltage, as shown in the Si-NDs in the SiC matrix. In addition, the 2D array of Si-NDs in the SiC matrix has a lower miniband level, E_0, which also shifts the I-V curves to a lower threshold voltage. This tendency closely matches our experimental results, and due to the larger tunneling resistance in the SiO_2 interlayer (C_t), the threshold voltage (V) is further increased in realistic I-V curves.

The enhanced conductivity is very significant for electronic/optoelectronic devices, which indicates high charge-injection efficiency in lasers and carriers collection efficiency in solar cells. In Fig. 4, by stacking our NDs from one layer to 10 layers, the miniband gradually broadens; and around four to six layers, the broadening velocity seems to saturate. The probability of wavefunction diffusing into barrier exponentially decays with distance, which indicates that wavefunction coupling exponentially saturates as the number of layers increases. Perhaps, four or six layers NDs are enough to maximize the advantage of minibands.

3. Conclusions

We developed an advanced top-down technology to fabricate the stacked Si NDs with high-aspect ratio, clear interface, and uniform size. Moreover, our theoretical calculation proved that miniband form enhanced the tunneling current, which well supports our previous experimental results. This enhanced transport indicated a high carrier's collection efficiency in solar cells. Further analysis revealed four or more Si NDs basically maximize the advantage of minibands in our structure.

References

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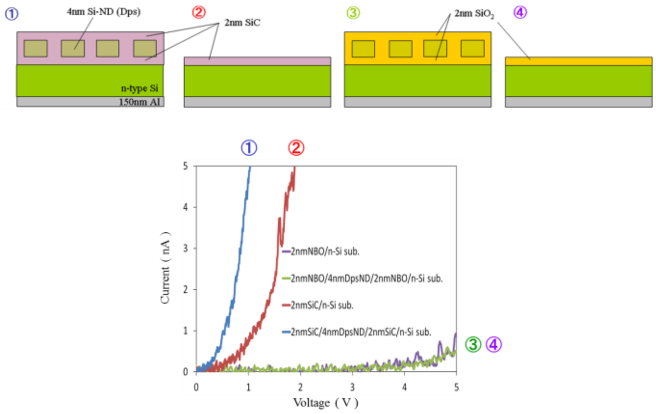

Figure 1 C-AFM measurements of the 2D array Si-NDs in SiC or SiO_2 matrix. The same thick SiC or SiO_2 films are measured as references.

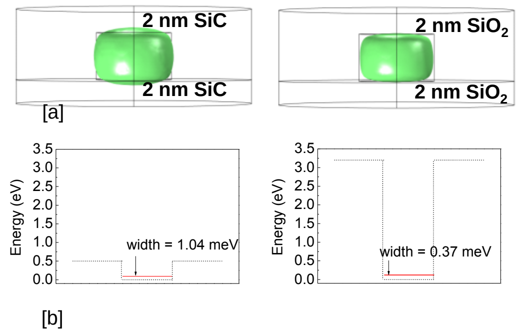

Figure 2 (a) Wavefunctions and (b) minibands in the 2D array Si-NDs in SiC or SiO_2 matrix. SiC/Si structure has the lower band-offset, 0.5 eV, which results in the weaker wavefunction confinement and the wider miniband.

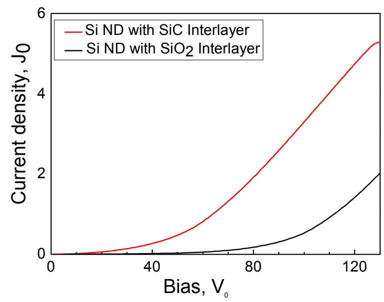

Figure 3 Calculated I-V plot of the 2D array Si-NDs in SiC or SiO_2 matrix. The wider miniband greatly increases the joint-state-density and finally increases the current.

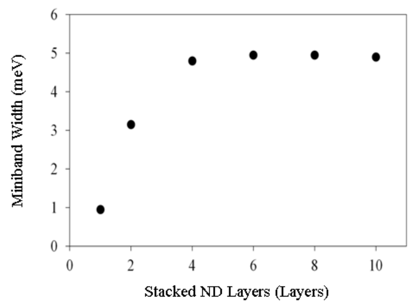

Figure 4 Miniband Broadening in staked Si ND array. It nearly saturates in 4~6 layers structure.