Miniband Dependence on the Density of Ge/Si Quantum Dots for Solar Cell Application

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Abstract—According to the Bloch theorem and the symmetry of superlattice configuration, a new 3D finite element method is employed to calculate the miniband structure and density of state for well-aligned Ge/Si QDs array. This method can overcome the approximation of multi-dimensional Kronig-Penny model with constrain of QDs structure. The interaction of electronic structure among Ge/Si QDs with various density of QDs is studied to provide a guideline of QDs solar cell design.

I. INTRODUCTION

A prospective candidate among the next-generation high efficiency photovoltaic technologies is the use of semiconductor quantum dots (QDs) [1]. The well-aligned QDs work plays a crucial role in determining the electronic band structure. For close-packed and well-ordered QDs superlattice, QDs couples with neighboring QDs to broaden the discrete quantum levels to form finite-width miniband. With the great development of nanotechnologies and device processes, a 3D finite element method without constraining on QDs structure is needed and proposed to simulate miniband structure and density of state (DoS) [2]. In this work, the dependence of electron structure on the density of Ge/Si QDs array is studied in further to instruct realistic QDs fabrication and design for photovoltaic technologies.

II. TOP-DOWN PROCESS AND COMPUTATIONAL MODEL

By combining the self-assemble bio-template and damage-free neutral beam etching, a top-down process, illustrated in Fig. 1(a), is used to fabricate sub-10-nm uniform and well-aligned QDs superlattice [3]. The SEM image in Fig. 1(b) exhibits good uniformity and alignment of germanium QDs. This nanofabrication technique, which controls the QDs thickness by the deposition thickness and its diameter by the bio-template, brings the higher flexibility on engineering quantum levels. As in Fig. 2, the electronic structure is numerically solved under the Bloch theorem. First, a unit cell formed by the primitive vectors is defined. Then, based on the symmetry of superlattice, the k-points space is defined in the irreducible Brillouin zone (IBZ). Finally, to get band structure En,k and Bloch function u(k) (r), Eq. (1) is discretized within a unit cell in real space and solved by a 3D finite element method solver for each sampling k-point in IBZ. The DoS is calculated from the energy distribution in IBZ by Eq. (2) illustrated in Fig. 2 [4]. To calculate the conversion efficiency of intermediate-band solar cell (IBSC) formed by QDs superlattice as in Fig. 5(a), Luque theory [5] is modified to consider the density of QDs as Eq. (3) [2].

III. RESULTS AND DISCUSSION

Fig. 3 shows the calculated band dispersion relation and DoS for QDs with the varied interdot space s from 2.3 to 0.3 nm. As the interdot space decreasing, the interaction between QDs and discrete levels increases that minibands become broad with finite bandwidth and meanwhile miniband mixing phenomenon occurs especially for higher excited states. Because the highest excited states are mixed and become continuous energy levels to Si barrier, the effective bandgap of bulk Si decreases. This reduction of effective bandgap impacts the conversion efficiency of QDs solar cell. The effect of superlattice structure, such as square and hexagonal lattice in Fig. 4(a), on miniband is investigated. Fig. 4(b) shows the compatible bandwidth under strong interactions between QDs with s = 0.3 nm but different DoS distribution based on the corresponding symmetry of superlattice.

To investigate the density effect due to QDs dimension and lattice structure on IBSC as shown in Fig. 5(a), Eq. (3) is used to calculate the J-V characteristics. In Fig. 5(b), the short-circuit current increase with density of QDs as interdot space decrease due to increase of volume ratio of QDs to bulk Si. However, the open-circuit voltage decrease with interdot space due to the reduction of effective bandgap from strong band mixing. Thus, the conversion efficiency for QDs IBSC increase with QDs density at low QD density but turn around at high QDs density (> 2.5 × 1012/cm2 for s = 0.3 nm). The conversion efficiency map with dependence of r and h under s = 0.3 nm is illustrated in Fig. 5(d) and Fig. 5(e). Comparing to the square superlattice, the hexagonal superlattice has higher efficiency due to higher density under the same QDs dimension and reach the maximum efficiency 40.6% at r = 4 nm and h = 2 nm. However, the more sensitivity of conversion efficiency on radius (distance between QDs) for hexagonal superlattice is revealed due to the stronger interactions between QDs.

IV. CONCLUSION

The FEM method by a unit cell with consideration of translation symmetry was applied on Ge/Si QDs array fabricated by an advanced top-down process for guiding QDs solar cell design. With the varied dimension and lattice of QDs, the miniband formation and mixing affects sub-bandgap and the effective bandgap of bulk Si, which results in a turn-around phenomenon for conversion efficiency with QDs density for IBSC application.
REFERENCES


Fig. 1. (a) Neutral beam etching process using the biological supermolecule (protein) ferritin, whose self-organizing properties result in two-dimensional crystallization. The etching mask is made from iron cores encapsulated within the ferritin molecules. By using iron cores with a diameter of 7 nm as etching masks, we can form defect-free ultrananostructures with a size of less than 10 nm. (b) SEM image of defect-free nanodisc structures (diameter 10 nm) formed with a uniform density and regular arrangement for germanium.

Fig. 2. The simulation flow chart proposed for an in-plane 3D QDs square superlattice to get band structure by solving Eq. (1) and material parameters used for simulation. The density of state \( g(E) \) is calculated from the energy distribution in IBZ by using an improved triangle method Eq. (2).

Fig. 3. The band structure along symmetry point \( \Gamma - X - M - \Gamma \) and the density of states for Ge/Si QDs square superlattice with QD radius 3 nm, thickness 4 nm, and interdot space 2.3 nm (dash line) and 0.3 nm (solid line).

Fig. 4. (a) QDs square and hexagonal superlattice with the corresponding IBZ and symmetry points. (b) The density of states for square and hexagonal superlattice with QD radius 3 nm, thickness 4 nm, and interdot space 0.3 nm.

Fig. 5. (a) The QDs IBSC consists of quantum dots as IB materials and p-n-junction as emitter at both end of the terminals. Eq.(3) is used for calculation of \( J-V \) characteristics. The example shown in (b) for QDs in dimension of \( r = 3 \text{ nm} \) and \( h = 4 \text{ nm} \) with varied interdot space \( s \). (c) The conversion efficiency for QDs IBSC increases with QDs density at low QD density but turn around at high QDs density (> \( 2.5 \times 10^{12} \text{cm}^{-2} \) for \( s = 0.3 \text{ nm} \)). This turn-around phenomenon could be explained by the increase of short-circuit current due to the increase of QDs density and the reduction of open-circuit voltage due to the band mixing and reduction of effective bandgap as in Fig. 3. The conversion-efficiency map with parameters of \( r \) and \( h \) under \( s = 0 \text{ nm} \) for (d) square and (e) hexagonal superlattice. The hexagonal superlattice has the maximum efficiency 40.6% at \( r = 4 \text{ nm} \) and \( h = 2 \text{ nm} \).