Proceedings of the 16th International Conference on Nanotechnology
Sendai, Japan, August 22-25, 2016

Numerical Simulation of Physical and Electrical Characteristics of Ge/Si Quantum Dots Based Intermediate Band Solar Cell

Ming-Yi Lee*, Yi-Chia Tsai*, Yiming Li* and Seiji Samukawa†
*Institute of Communications Engineering, Department of Electrical and Computer Engineering
National Chiao Tung University, Hsinchu 300, Taiwan (e-mail: ymli@faculty.nctu.edu.tw)
†Institute of Fluid Science and WPI-AIMR, Tohoku University, Sendai 980-8577, Japan

***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 and constrain on QDs superlattice structure. The interaction of electronic structure among Ge/Si QDs with various density of QDs therough QDs dimension and superlattice structure is investigated to provide a design guideline for QDs solar cell.**

I. Introduction

A prospective candidate among the next-generation high efficiency photovoltaic technologies is the use of semiconductor quantum dots (QDs) [1], [2]. The well-aligned QDs plays a crucial role in determining the electronic band structure. For close-packed and well-ordered QDs superlattice, QDs interacts with neighboring QDs that this interactions broaden the discrete quantum levels confined in single QD to form finite-width minibands. The minibands works as the intermediate band (IB) that the sub-bandgap photons can be absorbed and contribute to the photoncurrent for QDs solar cell application [3], [4]. With the advanced 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) [5].

In this work, the dependence of electron structure on the superlattice structure of Ge/Si QDs is studied in further to instruct fabrication and design of more realistic QDs for photovoltaic technologies.

II. Top-Down Process and Computational Model

With the great help of the self-assemble bio-template and damage-free neutral beam etching (NBE) [8], a top-down process is developed to fabricate sub-10-nm uniform and well-aligned QDs superlattice, illustrated in Fig. 1(a). The SEM image in Fig. 1(b) exhibits top-view of well-uniform and aligned germanium QDs after NBE etching. This nanofabrication technique independently controls the QD's height by the deposition thickness of germanium and its diameter by the bio-template dimension that brings the higher flexibility and possibility on engineering the confined quantum levels in QDs.

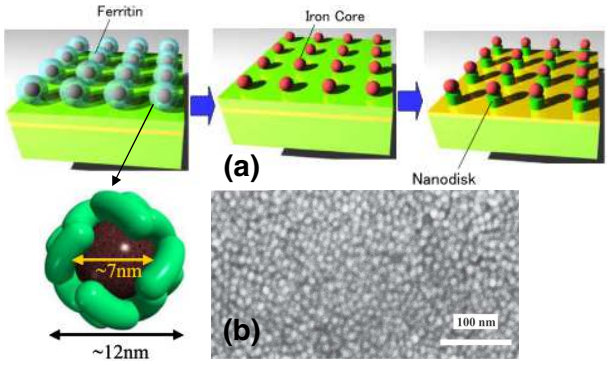

Fig. 1. (a) Neutral beam etching process using the biological supermolecule (protein) ferritin, whose self-organizing properties result in two-dimensional crystallization. The etching mask is made from iron cores encapsulated within the ferritin molecules. By using iron cores with a diameter of 7 nm as etching masks, we can form defect-free nanoscale structures 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.

As shown in Fig. 2, the electronic structure is numerically solved under the Bloch theorem with one-band effective mass approximation [5]. First, a unit cell is defined by the primitive vectors that describe the periodicity of superlattice. Then, according to the symmetry of superlattice, the k-points space in the irreducible Brillouin zone (IBZ) is defined to reduce the sampling size of k-points for simulation. Finally, to get miniband structure $E_{n,k}$ and Bloch function $u_k(r)$ in k-points space, the Schrödinger equation with Bloch wave form,

$$\nabla\left[-\frac{\hbar}{2m^*}\nabla u_k(\boldsymbol{r})\right] - \frac{i\hbar}{m^*}\boldsymbol{k}\cdot\nabla u_k(\boldsymbol{r}) + \left[V(\boldsymbol{r}) + \frac{\hbar k^2}{2m^*}\right] u_k(\boldsymbol{r}) = E_{n,k}u_k(\boldsymbol{r}), \quad (1)$$

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 (n indicates the quantum number). According to the energy distribution in IBZ from Eq. (1), the DoS is calculated by

$$g(E) = \frac{2}{(2\pi)^2}\int_{\mathrm{BZ}}\frac{dl_E}{|\nabla_k E_{n,k}|} = \sum_{n,l} g_{n,l}(E), \quad (2)$$

where the integral is carried out numerically using an im-