

## Impact of Atomic Disorder on Intermediate-Band Structures in Vertically Stacked InAs Quantum Dots

Hiroki Takahashi<sup>1</sup> and Nobuya Mori<sup>1,2</sup>

<sup>1</sup>Graduate School of Engineering, Osaka University,  
2-1 Yamada-oka, Suita, Osaka 565-0871, Japan

Phone: +81-6-6879-7698, E-mail: hiroki@si.eei.eng.osaka-u.ac.jp

<sup>2</sup>CREST, JST, 5 Sanbancho, Chiyoda-ku, Tokyo 102-0075, Japan

The intermediate-band solar cell (IBSC) [1] is a promising device structure for increasing efficiency of solar cells. The IBSCs can be realized with vertically stacked InAs/(Al,Ga)As quantum dots (QDs) [2], which act as an effective one-dimensional superlattice (SL) and produce the intermediate-band (IB) between the conduction and valence bands of the (Al,Ga)As matrix. The electronic properties of vertically stacked QDs can be tuned by adjusting the QD size and the periodicity [3]. Although the uniformity of the QDs is important for improving the efficiency of IBSCs, there should exist fluctuation and disorder in actual QDs. Here we present theoretical study of effects of atomic disorder on the electronic states in vertically stacked InAs/GaAs QD SLs.

We consider vertically stacked InAs/GaAs QDs whose schematic diagram is given in Fig. 1. Each InAs QD has a truncated pyramid-shape with the dot height being  $h_z$ , the side of the square base  $b$ , the side at the dot height  $t$ , and the periodicity  $L_z$ . In the present study, we are interested in effects of the atomic disorder and exclude a wetting layer to simplify the discussion. Since electrons are strongly confined in a QD, the electronic states should be calculated by taking into account the full-band structures. We use an empirical  $sp^3d^5s^*$  tight-binding (TB) method [4] to obtain the energy levels in a vertically stacked InAs/GaAs QD SL, whose atomic structure is relaxed by minimizing the elastic energy with the valence-force-field (VFF) method [5,6]. The relaxed structure contains strain distribution, whose effects on the electronic states are included by scaling the TB matrix elements with respect to the strain tensor and bond-length changes.

Figure 2 shows calculated energy levels as a function of the wavevector,  $k_z$ , along the growth direction in a vertically stacked QD InAs/GaAs SL of  $h_z = 1.1$  nm,  $b = 3.4$  nm,  $t = 2.3$  nm, and  $L_z = 6.2$  nm. We used the following parameters: The bottom of the GaAs conduction band is 0 eV, and the InAs conduction band

offset  $\Delta E_c = 0.6$  eV. We see that the intermediate-band is formed in the GaAs bandgap region. The IB width is found to be  $\sim 17$  meV for this device size.

We introduce atomic disorder by randomly replacing some In atoms on the top surface of a QD with Ga atoms. Typical patterns of the atomic disorder are shown in Fig. 3. Number of replaced In atoms,  $N_{\text{rep}}$  is varied from  $N_{\text{rep}} = 0$  to  $N_{\text{rep}} = 40$ .  $N_{\text{rep}} = 0$  corresponds to an ideal-shaped QD without disorder and  $N_{\text{rep}} = 40$  to that with a smaller height by one monolayer. Figure 4 shows an example of the calculated energy levels of  $N_{\text{rep}} = 20$ . We see that the energy levels shift higher by introducing the atomic disorder. This can be understood by considering the fact that an effective volume,  $V_{\text{eff}}$ , of a QD is reduced by the disorder.

Figure 5 shows the energy shift,  $\Delta E$ , at  $k_z = 0$  as a function of  $N_{\text{rep}}$ . We simulated 10 different patterns for each  $N_{\text{rep}}$ . We find that  $\Delta E$  is mainly determined by  $N_{\text{rep}}$  and is fairly independent of the roughness pattern. This is consistent with the interpretation that  $V_{\text{eff}}$  essentially determines the energy level of a QD. Figure 6 shows the IB width,  $W$ , as a function of  $N_{\text{rep}}$ .  $W$  is also found to be mainly determined by  $N_{\text{rep}}$ .

In summary, we have numerically investigated atomic disorder effects on electronic states in InAs/GaAs intermediate-band solar cells by randomly replacing some In atoms with Ga atoms. We find that the energy levels shift higher by introducing the atomic disorder. We also find that the energy shift and the intermediate-band width are mainly determined by the number of replaced In atoms and are fairly independent of the roughness pattern.

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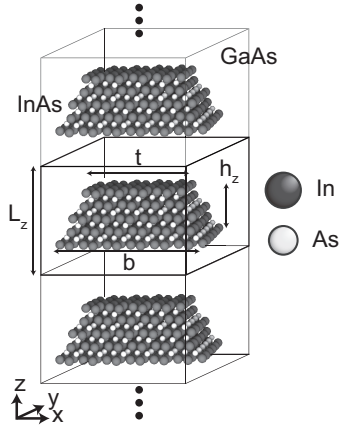


Figure 1: Schematic of a vertically stacked InAs/GaAs QD SL.

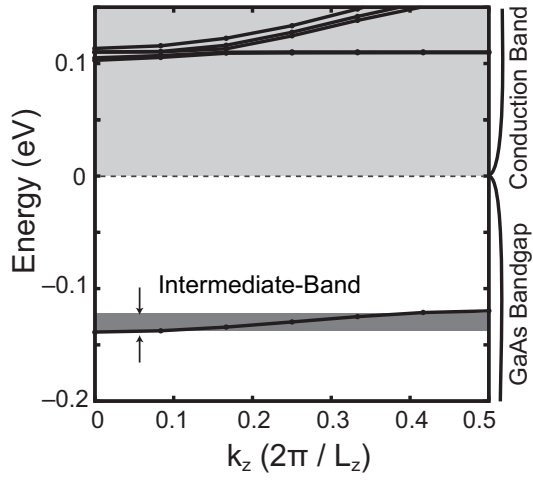


Figure 2: Energy levels as a function of the wavevector along the growth direction.

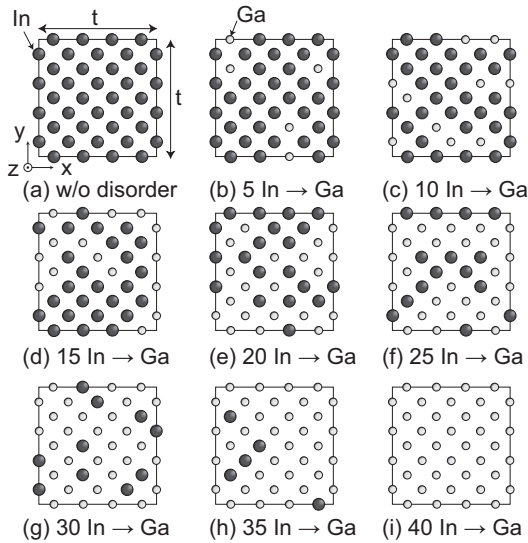


Figure 3: Typical patterns of atomic disorder used in the simulation from (a)  $N_{\text{rep}} = 0$  to (i) 40.

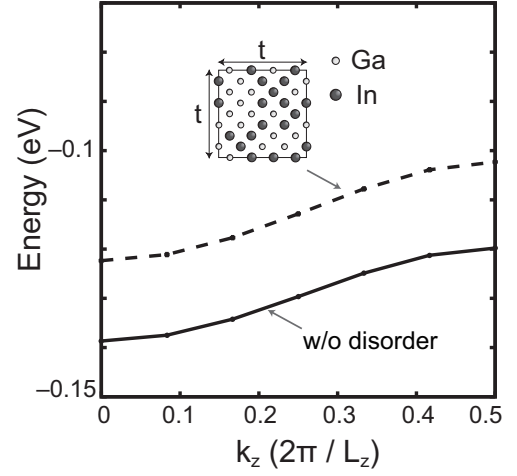


Figure 4: Energy levels of a vertically stacked InAs/GaAs QD SLs without the disorder (solid line) and with the disorder of  $N_{\text{rep}} = 20$  (dashed line).

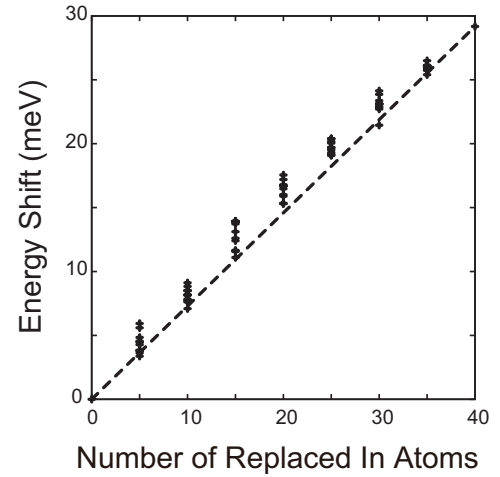


Figure 5: Energy shift,  $\Delta E$ , at  $k_z = 0$  as a function of  $N_{\text{rep}}$ .

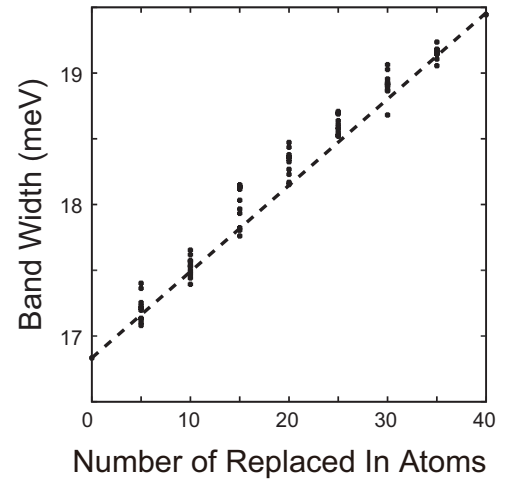


Figure 6: IB width as a function of  $N_{\text{rep}}$ .