Theoretical Investigations for Strain Relaxation and Resultant Growth Mode in InAs/GaAs Heteroepitaxial System

Tomonori Ito, Toru Akiyama, Kohji Nakamura
Department of Physics Engineering, Mie University, Tsu 514-8507, Japan

It is well known that InAs grown on GaAs(001) produces three-dimensional (3D) island shaped quantum dots. Despite a constant lattice mismatch, InAs thin films fabricated on the GaAs(111)A and GaAs(110) exhibit two-dimensional (2D) growth contradicting the 3D growth of InAs on GaAs(001) [1]. In this study, the growth mode of InAs/GaAs depending on orientations is systematically investigated using macroscopic free energy, microscopic emprical interatomic potential, and nanoscopic ab initio calculations to clarify the contribution of strain relaxation at their interfaces and surfaces to the resultant growth modes.

Figure 1 shows the calculated free energy differences among various growth modes as a function of layer thickness h for InAs/GaAs with different orientations. The growth mode in (110) (Fig. 1(a)) changes from the 2D-coherent (2D-coh) to the 2D growth with misfit dislocation (2D-MD) at h~1 monolayer (ML), while the 2D-3D growth mode transition appears inserting $In_{0.25}Ga_{0.75}As$ layer between InAs and GaAs that reduces surface energy γ from 51 to 49 meV/Å^2. On the other hand, (111)A (Fig. 1(b)) keeps the 2D growth mode from the 2D-coh to the 2D-MD via stacking-fault tetrahedron (SFT) formation (2D-SFT) at h~3 ML. The SFT formation near surface reduces strain energy more effectively than island and MD formations at the initial growth stage. For (001) (Fig. 1(c)), the strain relaxation occurs at h~0.5-0.6 ML where the macroscopic theory is no longer applicable. At this early stage, the strain is relaxed on the InAs reconstructed surface with missing surface dimer to substitute for In-As dimer going so far as to break the electron counting rule. These suggest that the growth mode in InAs/GaAs is closely related to the strain relaxation at the interface for (110), at both the surface and the interface for (111)A, and on the surface for (001).

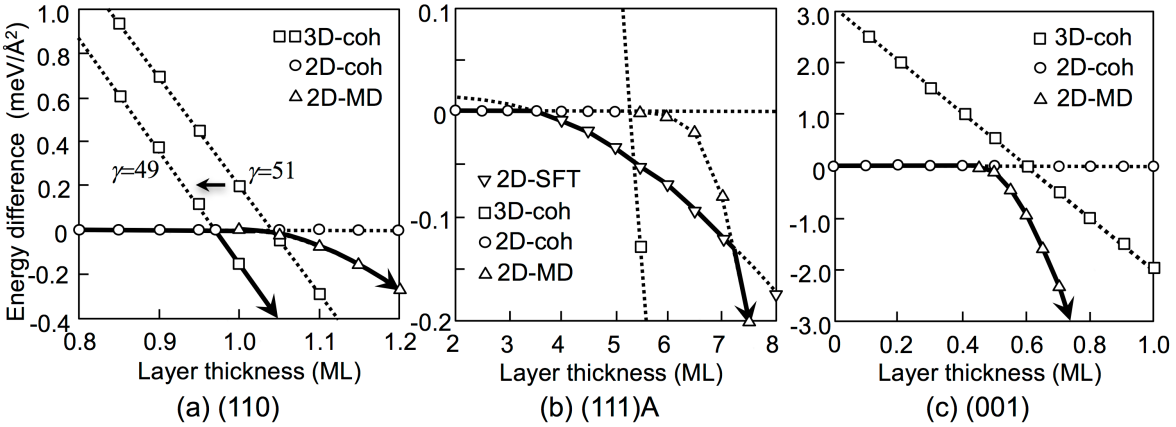

Figure 1 Calculated energy differences for various growth modes in InAs/GaAs systems.

[1] B. A. Joyce et. al., Jpn. J. Appl. Phys. **36**, 4111 (1997).

+ Author for correspondence: tom@phen.mie-u.ac.jp

Suplementary Page (Optional)

For strain relaxation processes found on InAs reconstructed surface grown on GaAs(001), Fig. 2(a) shows the calculated phase diagram of InAs(001)-($n \times 3$) wetting layer surface obtained by our ab initio-based approach. The stable (8×3) surface conforming to the electron counting rule appears under experimental growth conditions (closed diamond) at layer thickness h~0.6 ML corresponding to the initiation of strain relaxation due to MD and 3D-island formation shown in Fig. 1(c). On the (8×3) surface consisting of seven As-dimers and one missing dimer, In adsorption on the missing dimer site induces simultaneous As-dimer desorption to relieve strain on the surface. This surface is equivalent to (4×3) surface shown in Fig. 3, often found experimentally, without conforming to the electron counting rule. On the (4×3) surface, we confirmed that In adsorption and subsequent As-dimer desorption consecutively occurs to replace for In-As dimer as schematically shown in Fig. 3. Therefore, initial strain relaxation during epitaxial growth is not due to the conventional MD and 3D-island formations but is owing to rearrangements of surface atoms on the (001) surface.

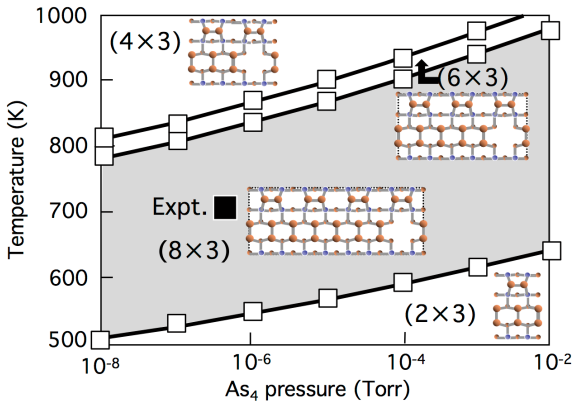

Figure 2 Calculated phase diagram for InAs(001)-($n \times 3$) wetting layer surface at h~0.6 ML.

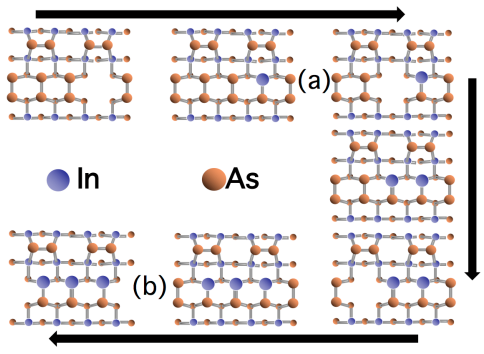

Figure 3 Simulated growth process on InAs(001)-(4×3) wetting layer surface.