Ab initio-based approach to adsorption of In atom with strain relaxation on InAs wetting layer surface grown on GaAs(001)

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InAs/GaAs(001) lattice mismatched system has been paid much attentions to fabricate low dimensional nanostructures such as self-assembled quantum dots (QDs) by molecular beam epitaxy (MBE) [1]. Despite the importance of the InAs/GaAs(001) system, there has been few theoretical studies for the QD formation mechanisms because of the difficulty of understanding the behavior of InAs wetting layer (WL) grown on GaAs substrate by *ab initio* calculations. We previously revealed that the growth of InAs and resultant surface structural change cannot proceed without eliminating lattice strain in the InAs WL at 0.96 monolayer (ML) [2]. Furthermore, we recently clarified that misfit dislocation (MD) formation as one of promising candidates for strain relaxation mechanisms starts at the InAs/GaAs(001) interface from 0.5ML during the growth [3]. These findings suggest that the InAs growth and its surface structural change are closely related to the lattice relaxation mechanisms on the InAs WL. In order to clarify the relationship between the growth process and the strain relaxation, lattice relaxation mechanisms on the InAs WL, we investigate the adsorption behavior of In atom on InAs WL surfaces including various lattice strain conditions on the basis of *ab initio* calculations.

Figure 1 shows the calculated adsorption energy of In atom on the (4×3) reconstructed surface consisting of In-As dimers as a function of hypothetical lattice constant of the InAs WL, which corresponds to the strain relaxation of the InAs WL. The calculated adsorption energy on the (4×3) surface with lattice constant a=5.76 Å, which corresponds to InAs WL without strain relaxation, is larger than that for adsorption of In atom under the MBE condition at 730 K (-2.63 eV). This indicates the adsorption does not occur without strain relaxation [3]. In contrast, the adsorption energy of In atom drastically decreases when lattice constant is larger than 6.08 Å, and becomes close to the value for fully relaxed InAs WL of -2.63 eV. The reduction of adsorption energy around a=6.08 Å thus manifests that the adsorption of In atom and resultant surface structural change toward the (2×4) reconstruction [4] can be realized by eliminating lattice strain of the InAs WL such as MD formation.

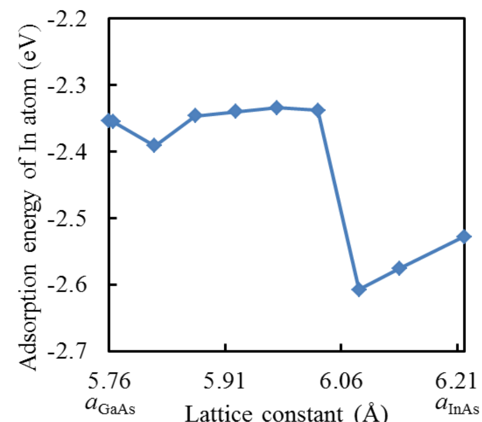

Fig. 1. Calculated adsorption energy of In atom on the (4×3) reconstructed surface including In-As dimers as a function of hypothetical lattice constant of the InAs WL. a_{GaAs}=5.76 and a_{InAs}=6.21 Å are calculated lattice constant of bulk-GaAs and InAs, respectively.

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