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POSTER SESSION 1

June 25, 2019

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Growth mechanism of III-V nanowires depending on the temperature and pressure: ab-initio thermodynamic study

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The nanowires of III-V compound semiconductors have been widely studied for a variety of applications such as complementary metal oxide semiconductor field-effect transistor (CMOS FET), light emitting diode, laser, solar cell, and quantum transport circuit, etc. To improve the device performance, understanding and control of the morphology of the nanowires are crucial. Among various methods to growth the III-V nanowires, the catalyst-free growth methods, such as the selective-area metal-organic vapor-phase epitaxy (SA-MOVPE) and selective-area molecular beam epitaxy (SA-MBE) are based on the thermodynamic control of the formation of facets and preferential adsorption, which play important roles in the preferential one-dimensional growth along a specific crystallographic orientation.

In this study, we theoretically investigate the mechanism of the catalyst-free growth of the III-V nanowires by using GaAs as a model system. To do this, we first calculate surface energy [1] and the equilibrium crystal shape (ECS) [2] as a function of temperature (T) and pressure (P) in the combined framework of density functional theory (DFT) calculations and thermodynamics. To compare the theory and experiment directly, this methodology is more favorable compared with the previous DFT studies, which provide the surface energy and ECS as a function of chemical potential (μ). Note that the T and P are the experimentally controllable thermodynamic variables, while μ cannot be controlled experimentally. Therefore, the theoretical calculations as a function of T and P is a prerequisite to compare directly with experimental conditions. From these calculations, the variation of the surface reconstruction of several low-index facets depending on T and P can be extensively examined. Then, we calculate and compare the adsorption energy of Ga and As on the stable reconstruction of various facets with the chemical potential in their gas phase to determine whether the adsorption occurs or not as a function of T and P. Finally, we make a comparison our theoretical prediction with the previous experiments and explain the preferential growth along the <111>B orientation observed in experiments, validating our methodology. In these calculations, the consideration of the surface vibration is indispensable to predict the stable reconstruction. It is confirmed that the As adsorption on the (111)B surface is exclusively favorable under conditions where the growth of GaAs nanowires has been successful. It explains that the driving force for the 1D growth along the <111>B orientation is the preferential adsorption of As on the (111)B surface under the given specific conditions. In particular, the (111)B Ga vacancy α(2×2) reconstruction, which was calculated to be stable at high T by considering the vibrational effect [2], is identified to offer the preferential adsorption sites for the incoming vapor reactants.

Our work not only provides new and practically applicable findings on the surface reconstructions and the growth of nanowires of GaAs but also does a general calculation methodology, which can be applied to a broad range of materials and surfaces based on the ab-initio thermodynamics.

[1] I. W. Yeu, J. Park, G. Han, C. S. Hwang, and J.-H. Choi, Sci. Rep. 7 (2017) 10691
[2] I. W. Yeu, G. Han, J. Park, C. S. Hwang, and J.-H. Choi, Sci. Rep. in press

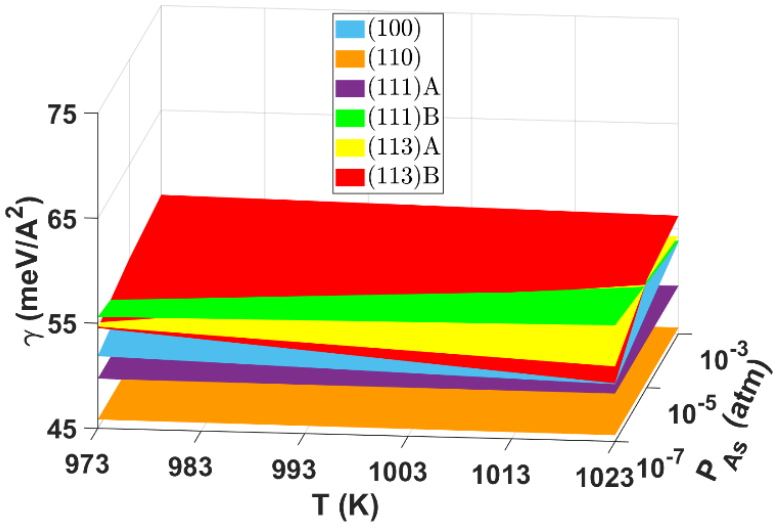

Figure 1. Calculated minimum surface energies composed the electronic and vibrational energy terms ($\gamma = \gamma^{elec} + \Delta\gamma^{vib}$) of each surface orientation for GaAs as a function of T and P_{As} [2].

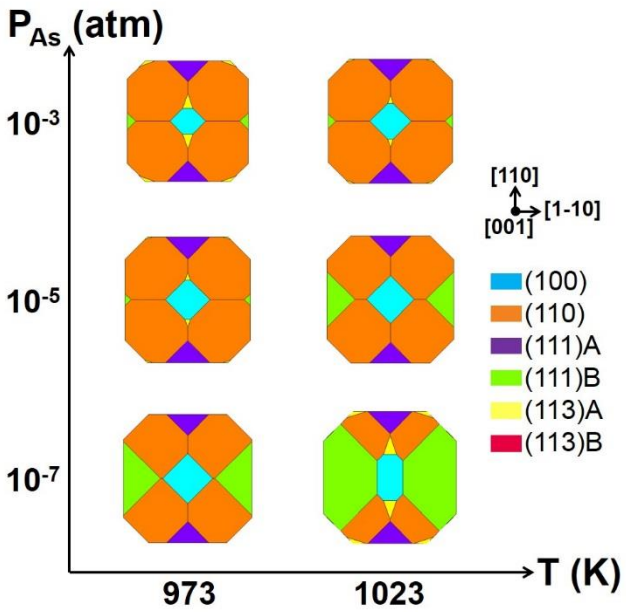

Figure 2. Top view of the ECSs of GaAs along the [001] direction at around the experimental growth conditions after including the surface vibration and the newly suggested (111)B Ⅲ vacancy(2×2) [2].