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Atomistic understanding on the growth and stacking-fault of GaAs nanowires grown by noncatalytic method

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The growth of III-V nanowire on Si substrate has been developed to integrate the novel functionalities on the low-cost commercial substrate. Dislocation and crack caused by the mismatch in lattice constant and thermal expansion coefficient have been effectively reduced by the small contact area between the nanowire and Si substrate. The remaining difficulty is the precise control in the growth and stacking-fault (SF), which is shown to be abundant and randomly distributed to date. In this study, the growth and SF mechanism in GaAs nanowire grown by noncatalytic facet-driven method is theoretically explained using the ab-initio thermodynamic and nucleation models. The changes in the chemical potential and interface energy are calculated as a function of temperature (T) and pressure (P). By considering the growth condition dependence of Gibbs energy of the related subsystems, the element transport from vapor source to crystal through adsorption and nucleation could be compared among different faceted surfaces. As a result, the reason why the GaAs crystal grows preferentially in one direction is confirmed to be the excessive concentration of sources on the growing surface induced by preferential adsorption under narrow (T, P) conditions [1]. In addition, the effects of growth conditions and directions on SF density are predicted, which agrees with previous experimental observations [2].

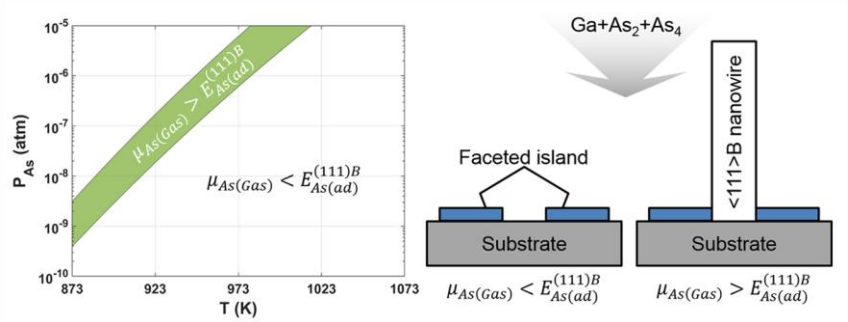

Fig 1. Schematic of GaAs nanowire growth by preferential adsorption on the growing surface [1].

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References [1] In Won Yeu et al., Appl. Surf. Sci. 497, 143740 (2019). [2] In Won Yeu et al., in preparation.