The role of Ga-Ga and Ga-SiO_x interactions in Ga-assisted GaAs nanowire growth on Si(111)

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Integrating III-V materials on Si is highly desirable. In this context, the Ga-assisted growth of GaAs nanowires (NWs) on Si is a popular approach, and a number of interesting growth phenomena have been identified. Each crucial insight into NW growth was obtained within a discrete NW growth regime. It is, however, often unclear what determines the exact growth regime and how regimes are related. In molecular beam epitaxy (MBE) the growth parameters form a 3D variable set consisting of growth temperature (T_{grow}), As flux and Ga flux. We have determined the inter-dependency of these growth parameters by the systematic variation of each variable across the entire NW growth window. The window spans 110 K of T_{grow} and two orders of magnitude in V:III ratio, whereas the conditions to obtain NW samples of "good" morphology are restricted to a 10 K variation in T_{grow} and a V:III ratio of ~1.2±10%. We observed a range of GaAs structures, progressing from pure Ga droplets under negligible As flux through horizontal NWs, tilted NWs, vertical NWs, NWs without droplets to 3D crystallites as the As flux is increased. Similarly, the parasitic growth evolves with T_{grow} from polycrystalline mounds at low T_{grow} to crystalline mounds, and is finally suppressed to a minimum at the optimum T_{grow}. We performed a quantitative analysis of the resulting NW morphology in terms of NW number density, diameter, elongation rate, vertical yield, polytypism and the type and areal coverage of parasitic growth. The results obtained were highly repeatable on substrates from the same batch and also readily facilitated the transfer of a desired NW growth regime to other substrates. Whilst the desired NW morphology was consistently obtained the results indicate that the optimum As:Ga ratio for NW *nucleation* is approximately double that required for later *elongation* and hence the two processes must be optimised independently.

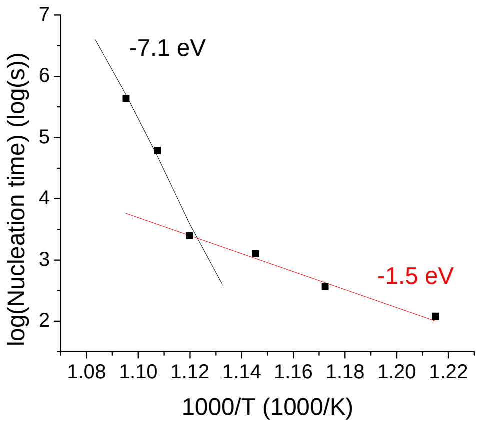

Figure 1: Graph of log(nucleation time) vs 1000/T_{grow} (1000/K). Black squares indicate onset of NW growth as determined by RHEED diffraction spots. Lines of fitting indicate the Arrhenius behaviour at a fixed V:III ratio is distinct above and below optimum T_{grow}.

In order to obtain a deeper understanding, we investigated the nucleation kinetics. To this end, we monitored the onset of NW nucleation *in situ,* defined by the emergence of characteristic NW spots on the reflection high-energy electron (RHEED) pattern. The Arrhenius plot for the NW nucleation time measured under concurrent As and Ga fluxes is shown in Figure 1. Two distinct nucleation energies are found under constant global V:III ratio. We interpret them to correspond to the Ga droplet nucleation energy (-1.5 eV) and the interaction of Ga with SiO_x (-7.1 eV). The two different nucleation processes dominate the NW morphology on either side of the optimum T_{grow} corresponding to the inflection point. In addition these processes underpin all temperature dependent NW morphologies obtained under constant V:III ratio outlined in the previous paragraph.

Our systematic study has led to a comprehensive understanding of the mechanics of NW growth and enables a grower to optimise NW growth conditions regardless of the initial starting point.