

Nucleation and growth of cubic monolayers at a truncated solid-liquid interface in III-V nanowires

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Although cubic zinc blende (ZB) / hexagonal wurtzite (WZ) polytypism was observed in III-V nanowires (NWs) grown in the vapor-liquid-solid (VLS) mode nearly 30 years ago [1], it is still far from being fully understood. The first explanations, based on the calculation of total energies for fully formed NWs, predicted the occurrence of WZ only below critical diameters of the order of few nm, which is contradicted by the experiment. In 2007, we proposed the first nucleation-based model that explained the formation of WZ via a nucleation of the NW monolayers (MLs) at the triple phase line (TPL) at intermediate droplet contact angles, provided the chemical potential $\Delta\mu$ of a III-V pair in the liquid (with respect to the solid) is high enough [2]. The LS interface was then assumed to be planar and the chemical potential constant during steady state growth.

Later experiments showed that the LS interface may actually be truncated [3] and revealed strong morpho-structural correlations, namely planar-WZ and truncated-ZB [4,5]. The planar case fits rather well our initial model [2]: *in situ* experiments confirm TPL nucleation [6], although we now know that, even in stationary growth, $\Delta\mu$ varies considerably during the formation cycle of each ML [7]. Calculations show that the LS interface morphology is determined by the droplet contact angle and $\Delta\mu$ [4], but the impact on crystal structure is unclear. In particular, the current morphology-related models of polytypism return to total energy calculations and ignore nucleation [5].

Here, we discuss the more complex case of the truncated interface. We argue that a proper explanation of the formation of ZB in this case has to treat nucleation explicitly. We consider that, both at the nucleation stage and during the subsequent extension of the ML, material may be provided by the liquid but also, as is generally accepted now, by the solid via a cyclic enlargement of the truncation. We show that the respective contributions of these two pathways depend on the extent of the truncation and on the chemical potential before nucleation and that they vary with time during each ML cycle. We discuss the implications of these findings for the formation of the ZB phase in this situation.

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