

# Theoretical aspects of nanowire formation: growth kinetics, morphology and crystallographic structure

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This talk presents an overview of recently obtained results in the field of nanowire growth theory. Presentation splits into the introduction and three major parts. The first part of the talk is devoted to modeling of growth kinetics. We discuss different kinetic processes contributing to nanowire formation in the vapor-liquid-solid mechanism [1]: adatom diffusion, direct impingement, crystallization of supersaturated liquid alloy on the wire top, re-evaporation and 2D surface growth. It is demonstrated that in the most cases the growth process is controlled by the adatom diffusion [2-5]. The model for calculation of wire growth rate in the diffusion induced mode is presented and analyzed [6]. In the second part of the talk we discuss different models of morphological transformations during nanowire formation: tapering effect in high vacuum deposition [7] and sidewall nucleation resulting in lateral growth and conical shape of crystals [8,9]. In particular, it is shown that lateral growth is pronounced at lower substrate temperatures and almost absent at higher  $T$ . In the third part we consider the model for the growth thermodynamics and polytypism of zinc blende III-V nanowires [10,11]. Formation energy of a nanowire ensemble is calculated and different polytypes between cubic and hexagonal structure are analyzed. One of the conclusions is that polytypism of III-V nanowires requires high supersaturation of gaseous phase and small wire radius, because the surface energy of polytypes is smaller than that of pure zinc blende phase [12]. The second important result shows that 4H polytype has the lowest formation energy and should be considered as the one controlling the wire structure from thermodynamic point of view.

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