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Kinetic-control of morphology and composition during the 3D growth of semiconductor nanostructures

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Growing three-dimensional epitaxial nanostructures opens a new world of opportunities, unique properties and novel designs for next-generation semiconductor devices. However, the increased complexity and wide variability of parameters to be controlled in order to achieve the desired structures demand for an in-depth understanding of the growth mechanism. In particular, the morphology of the growing crystal stems from the interplay of either thermodynamic and kinetic driving forces, whose relative strenght depends on the actual growth conditions and is strongly influenced, if not directly templated, by the substrate geometry and patterning. Moreover, in the case of alloys, the local composition tightly binds to such a dynamics, frequently resulting in different faceting and/or segregation effects. The development of reliable growth models and simulations comprising all of these physical contributions is then of great value for the characterization of growth experiments and to restrict the parameter space for targeting a desired outcome. Here we present a growth model based on a phase-field approach [1], including both deposition and surface diffusion dynamics, and allowing for the modeling of morphological and compositional evolution in single-component and alloyed materials on different substrate geometries. First, the faceted growth of ring-like structures [1], as obtained experimentally by selected-area epitaxy, will be analysed. The different role of anisotropic surface energy density, orientation-dependent incorporation rates and nonuniform deposition fluxes in determining the crystal shape will be investigated. In particular, it will be discussed how the behavior of convex and concave regions reveals the dominance of thermodynamic or kinetic contributions. Then, the case of alloyed core-shell nanowires will be inspected as a peculiar example of kinetically-coupled morphology-composition dynamics. In particular, the occurence of segregation in Ge-GeSn [2] and GaP-Si-SiGe(hex.) [3] core-shell nanowires will be discussed and related to the deposition-vs-diffusion ratio.

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[3] R. Bergamaschini, R.C. Plantenga, M. Albani, E. Scalise, Y. Ren, H.I.T. Hauge, S. Kölling, F. Montalenti, E.P.A.M. Bakkers, M.A. Verheijen, L. Miglio Nanoscale 2021, 13, 9436

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