Modeling of the growth of ZnO nanorods in batch and flow reactors

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Chemical bath deposition is an attractive method for the preparation of semiconductor nanostructures. This method is cost-efficient, scalable, can be easily implemented, and takes place at temperatures below water boiling point, which allows for the deposition on a large variety of substrates. Various shapes and properties of the nanostructures can be achieved by controlling the interface supersaturation during the growth process. The interface supersaturation is, however, a complex function of many parameters, such as the chemical reactive environment, the transport of growth units to the growth front of nanostructures, and the structure and morphology of the substrate on which the nanostructures grow. As the growth proceeds, these parameters vary, which results in temporal and spatial variation of the interface supersaturation. Determination of the temporal and spatial variation of the interface supersaturation is essential to understand the growth mechanism of semiconductor nanostructures.

In most cases, the growth is carried out in batch reactors without a continual addition of reactants, where the concentration of chemical precursors, and thus also the supersaturation, decreases with time, which can affect the growth mechanism of the grown nanostructures. On the other hand, continuous flow reactors with constant inflow of reactants establish a time-independent supersaturation in a particular position on the sample. To understand the role of substrate, we prepared nanostructures on ZnO seed layers with a non-regular distribution of ZnO seeds and on patterned substrates with precise control over the position of ZnO seeds. To analyse the interface supersaturation, we prepared samples in both types of reactors on both patterned and non-patterned substrates. The growth velocities and the surface area of the growth front were then determined from SEM images. A model of transport phenomena using the measured reaction kinetics was implemented in COMSOL Multiphysics. The solution of the model was used to estimate the interface supersaturation and to compare it with experimentally collected data.

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[1] Černohorský, O., J. Grym, H. Faitová, N. Bašinová, Š. Kučerová, R. Yatskiv and J. Veselý, Modeling of Solution Growth of ZnO Hexagonal Nanorod Arrays in Batch Reactors. Crystal Growth & Design, 2020