136d Kinetic Monte-Carlo Simulations of Nanowire Growth

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We have modeled nanowire growth using a kinetic Monte-Carlo scheme to understand the following: faceting, growth direction, and the growth kinetics. The main feature of these simulations is the use of a dynamic size constraint, i.e., the diameter of the growth surface is kept constant, compared to previous approaches which use periodic boundary conditions on a fixed surface. This allows our simulations to predict the growth direction depending upon the growth parameters used. The simulations start with a certain area defined by a circle of a pre-chosen diameter on a two-dimensional surface (say a (100) surface). The growth is modeled using adatom adsorption and desorption with a set of rate constants depending upon the neighborhood of the chosen site while incrementing in time. The programs are written in C++ for implementations on UNIX and Windows platforms and are initially intended for diamond cubic materials systems such as Si, Ge and diamond.

The simulation results show a linear relationship for length as time increases ($V \sim t$), which is expected for 1-D growth under kinetic control. Simulations with a set of rate constants allowing ‘faster' growth led to nanowires with <100> growth directions while slower growth led to nanowires with <111> growth directions. Nanowires grown epitaxially on <100> substrates attain <111> growth directions depending upon the process conditions. In addition, the faceting of nanowires with <100> growth directions indicate four-fold faceting while nanowires with <111> directions yield faceting that varies from triangular to 3-dimensional at their tips.