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Hierarchical simulation of microcrystalline PECVD silicon film growth and structure

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We have designed and implemented a hierarchical simulation methodology for the study of Plasma Enhanced Chemical Vapor Deposition of silicon films. Our main objective is to elucidate the microscopic mechanisms as well as the interplay between atomic level and macroscopic design parameters associated with the development of nano- or micro-scale crystalline regions in the grown film. The ultimate goal is to use multi-scale modeling as a design tool for tackling the issue of local crystallization depending on the environment, thus also of the growth parameters. Our simulation approach is based on the design of a very efficient, large-scale kinetic Monte Carlo (kMC) algorithm capable of generating samples of representative Si films based on a validated chemistry model. In a second step, the generated film is subjected to an atomistic simulation study restoring the molecular details lost or ignored in the kMC model and tuning the local structure i.e. the important morphological details associated with the presence of crystalline and amorphous regions (and the intervening interfacial domains) in the grown film. The kMC methodallows us to study several seconds of film growth, resulting in thicknesses in the order of tenths of nanometers. The validity of the method was investigated via computational experiments over a wide range of dilution ratios and by comparing the numerical results for the growth rate and roughness with the corresponding experimental data; very good agreement is observed in most cases. The 3-d structures generated with kMC are used as input in large-scale MD simulations for times up to several microseconds to allow the system further relax towards the preferred morphological state at the conditions of interest. This will allow us to obtain predictions for other industrially relevant quantities and observables (e.g. hydrogen content and crystallinity which are experimentally accessible by FTIR and Raman spectroscopy), thus opening the way to fully understanding the underlying molecular mechanisms responsible for the growth of micro- or nanocrystalline films.

Keywords
silicon growth
plasma CVD
thin films