KN0200

Growth kinetics of plasma deposited microcrystalline silicon thin films

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Hydrogenated microcrystalline silicon (μc-Si:H) has attracted particular attention due to its successful application in tandem 'micromorph' solar cells. There are several experimental and theoretical investigations in literature, aiming to propose adequate mechanisms leading to the formation of nanocrystals in relatively low substrate temperature conditions (< 250 °C). However, most of these efforts suffer from the lack of in-situ and non intrusive experimental feedback and are either based on indirect observations or on ex-situ measurements. On the other hand, simulations of μc-Si:H deposition are either limited to the gas phase, treating indirectly the film growth, or to small-scale atomistic modeling of specific material phase transformations. Both can give valuable information on the mechanisms of nanocrystallization but cannot describe the nucleation kinetics or the nucleus size distribution and growth. In this work, we present a model of μc-Si:H growth kinetics based on the solution of time-dependent mass balance equations for the species reaching the surface. The mass balances are expressed in terms of the surface fractional coverage θ_i by different species and include possible surface reactions (abstraction, physisorption, chemisorption, etching, sputtering, Eley Rideal and Langmuir Hinshelwood mechanisms) for production and annihilation of the surface sites and diffusion of the species in the sub-surface. The fluxes of species (radicals, ions and hydrogen atoms), are taken from gas phase simulations in industrially relevant conditions corresponding to deposition rates > 5 Å/sec. The surface model results include growth rate, species sticking coefficients, nucleation rates, critical nucleus size, hydrogen content and finally small scale (1x1 μm) topography. These results are compared against experimental film topographies (AFM, TEM), FTIR hydrogen content and bonding. The main parameters affecting nucleation kinetics are presented and discussed.

Keywords
microcrystalline silicon
nanostructure
solar cells
PECVD
modeling