A Phase-Field Model for Solvent Evaporation in Thin-Film Solar Cell Fabrication

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ABSTRACT

With renewable energy becoming a high priority in recent times, the ability to harness solar power efficiently and cheaply is proving to be an essential task. Thin film organic-inorganic solar cells have the potential to make great leaps in this area due to their low-energy production and high efficiency [1].

Fabrication of thin film solar cells consists of depositing a solution of the absorbing material mixed with a solvent onto a substrate followed by an annealing period during which the solvent evaporates and the morphology of the absorbing layer evolves. The changing morphology within the thin film is driven by energy minimisation and can be described by 3D phase field models [2]. Lack of surface coverage of the thin film is a major issue for cell efficiency [3], and it is known that solvent evaporation causes pinholes to grow, thereby decreasing surface coverage [4].

We propose a simple, geometrically reduced, phase field model for pinhole growth in evaporating thin films based on the Cahn-Hilliard equation with reactive terms which, as usual [5], dissipates a suitable free energy. Linear finite elements are used for the spatial discretisation and a novel third order IMEX Runge-Kutta method is employed for the time stepping.

We use our computational model to simulate surface coverage in an effort to identify which parameters need to be controlled to achieve maximum coverage.

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