DYNAMICAL BASIS OF THE STRUCTURE ZONE MODEL OF THIN SOLID FILMS GROWTH

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Thin solid films grown by various techniques of vapor deposition onto a substrate often exhibit different characteristic morphologies as the temperature of the substrate and the energy of the impinging atoms are varied. These morphologies have been universally classified by means of empirical schemes known as Structure Zone Models (SZM)[1,2,3,4]. In spite of the fact that thin films growth have been extensively simulated by means of ballistic aggregation models, molecular dynamics and partial differential equations with moving boundaries, none of these studies have addressed rigourously the question of to what extent these models are able to reproduce and predict the phase diagrams implied by the SZM.
Our present work represents the first step of a comprehensive program to thoroughly investigate this question. We started off considering the Structure Zone Models produced by ballistic deposition models in 1+1 dimensions. In particular, we have considered a modern implementation of these type of simulations which includes surface thermal diffusion and the two possible coexisting micro-configurations[5]: one with hexagonal and another with square packing symmetries. We show that this model displays at least the three columnar structures of the simplest SZM thus improving the description of previous single lattice models. Interestingly, the model also presents a microstructural phase transition from the coexistence of the square and the hexagonal to the only hexagonal packing configuration that we are able to detect and characterize.

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