Simulation of morphological instabilities during diamond chemical vapor deposition

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Abstract

The diamond chemical vapor deposition (CVD) process has been investigated theoretically and the morphological instabilities associated with the growth of diamond films have been examined with a model based on the continuum species conservation equation coupled to surface reaction kinetics. A linear stability analysis and numerical calculations have been carried out to determine critical parameters affecting the diamond deposition layer morphology. A two-dimensional model describes the evolution of the gas-solid interface. The dynamic behavior of the interface depends on the reactants' diffusivity and surface kinetics. These factors depend upon the reactant material properties and film growth conditions such as the reactor temperature and pressure. From the analyses, it has been found that the ratio ($\mathcal{D}/k$) of gas phase diffusivity ($\mathcal{D}$) to the surface reaction rate constant (k) plays the critical role in promoting diamond morphological instabilities because the film morphology stabilizing processes of surface diffusion and re-evaporation are absent or negligible during diamond CVD. It is found that the film non-uniformity increases as the ratio ($\mathcal{D}/k$) decreases. Increasing growth rates also result in increasing morphological instability, leading to rough surfaces. It is shown that increasing reactor pressure and decreasing gas-phase temperature and/or substrate temperature promote deposition layer non-uniformity. An approach to avoiding these instabilities is proposed.