

A kinetic model of diamond nucleation and silicon carbide interlayer formation during chemical vapor deposition

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Abstract

The presence of thin silicon carbide intermediate layers on silicon substrates during nucleation and the early stages of diamond deposition have been frequently reported. It is generally accepted that the intermediate layer is formed by the bulk diffusion of carbon atoms into the silicon carbide layer, and the morphology and orientation of the diamond film subsequently grown on the intermediate layer are strongly affected by that layer. While there have been considerable attempts to explain the mechanism for intermediate layer formation, limited quantitative data are available for the layer formation under the operating conditions conducive to diamond nucleation.

This study employs a kinetic model to predict the time evolution of a β -SiC intermediate layer under the operating conditions typical of diamond nucleation in hot filament chemical vapor deposition reactors. The evolution of the layer is calculated by accounting for gas-phase and surface reactions, surface and bulk diffusions, the mechanism for intermediate layer formation, and heterogeneous diamond nucleation kinetics and of its dependence on the operating conditions such as substrate temperature and inlet gas composition. A comparison between the time scales for intermediate layer growth and diamond nuclei growth is also performed. Discrepancies in published adsorption energies of gaseous hydrocarbon precursors on the intermediate layer—ranging from 1.43 to 4.61 eV—are examined to determine the most reasonable value of the adsorption energy consistent with observed saturated thicknesses, 1 to 10 nm, of the intermediate layer reported in the literature. The operating conditions that lead to intermediate layer growth followed by diamond deposition versus those that yield heteroepitaxial diamond nucleation without intermediate layer formation are discerned quantitatively. The calculations show that higher adsorption energies, 3.45 and 4.61 eV, lead to larger surface number densities of carbon atoms, lower saturated nucleation densities, and larger intermediate layer thicknesses. The observed saturated thicknesses of the intermediate layer may be reproduced if the true adsorption energy is in the range of 3.7 to 4.5 eV. The intermediate layer thickness increases by increasing substrate temperature and inlet hydrocarbon concentration, and the dependence of the thickness on substrate temperature is especially significant. Heteroepitaxial diamond nucleation without intermediate layer formation reported in experimental results can be readily explained by the significant decrease of the intermediate layer thickness at lower substrate temperatures and at higher diamond nucleation densities. Further, the present model results indicate that the intermediate layer thickness becomes saturated when growing diamond nuclei cover a very small surface area of that layer.

Keywords: Diamond; Silicon carbide; Chemical vapor deposition; Nucleation; Intermediate layer; Adsorption energy

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