Two-Dimensional Diamond Chemical Vapor Deposition Simulation

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A complex mathematical model for Chemical Vapor Deposition of diamond has been formulated. The computational domain consists of an axisymmetrical CVD reactor and the substrate surface. Both gas-phase and surface chemical kinetics are incorporated. Results include flow field, energy field and species distributions in the reactor, and the heat flux and growth characteristics at the substrate. Flow is assumed to be laminar in this stage. The conservation equations for mass, momentum and energy are solved by a modified version of the finite difference code SIMPLER for compressible flow, while composition and chemical and transport properties are supplied and processed by the codes CHEMKIN and SURFACE CHEMKIN.

The model has been applied to a low pressure thermal plasma diamond CVD process in which the argon - hydrogen gas mixture is heated by a d.c. arc and subsequently expanded in a nozzle. For that case, the influence of power input, hydrocarbon introduction method (premixed jet versus peripheral methane injection) and jet characteristics (supersonic versus subsonic jet) are discussed.

It is pointed out that the model predicts that higher velocity of the jet is not always beneficial to the diamond production as it can diminish the jet spread and thus the usable deposition area. Under these conditions, the heat flux to the substrate and the premixed jet diamond deposition rate experience strong peaks at the center of the substrate and strong radial gradients.

The method of the hydrocarbon species introduction is shown to be crucial to the overall diamond production. In case of high velocity jets, the mixing of the reactor gas with the jet gas can be insufficient, and a peripheral injection of the hydrocarbon species might lead to a diamond deposition rate an order of magnitude lower compared to an otherwise identical premixed jet case. A combination of premixing and peripheral injection may lead to the most uniform diamond deposition.