

Integrated Multi-Scale Modeling of Diamond Chemical Vapor Deposition

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Abstract

The fundamental mechanisms of diamond growth occur on the atomic scale. However, the geometry of the deposition reactor and the other operating parameters directly affect the chemical composition of the gas and the temperature at the growth surface. The properties are in turn controlled by both atomic- and microstructural-scale features. By developing diamond growth models at each length scale and coupling the output of one model into the next, a comprehensive, integrated simulation scheme for diamond deposition is realized. This approach provides the missing link between CVD reactor design / operating conditions and the material structure / properties.