

Influence of the gas phase on doping in diamond chemical vapor deposition

David S. Dandy*

Dept. of Chemical Engineering, Colorado State University, Fort Collins, Colorado 80523-1370

A series of calculations has been carried out to examine the relationship between gas phase composition and film composition in diamond chemical vapor deposition. It is predicted that the ability to carry out *in situ* doping of films with N and S, and the inability to dope with O, can be explained from a simple thermodynamic perspective. Probable precursor dopant species are identified as $\cdot\text{CN}$ and $\cdot\text{SH}$ for the $\text{CH}_4/\text{H}_2/\text{N}_2$ and $\text{CH}_4/\text{H}_2/\text{H}_2\text{S}$ systems, although it is expected that these are the most likely precursors regardless of the initial forms of nitrogen and sulfur.

Keywords: Diamond, deposition process, semiconductors, chemical vapour deposition, chemisorption.

* *Tel:* +1-970-491-7437; *Fax:* +1-970-491-7369; *Email:* david.dandy@colostate.edu.