

Chemisorption of hydrocarbon species on transition metals during diamond chemical vapor deposition

Pushpa Mahalingam, Huimin Liu and David S. Dandy
Department of Chemical Engineering
Colorado State University
Fort Collins, CO 80523-1370

Abstract

This paper presents a brief discussion of the phenomena associated with chemisorption of hydrocarbon species on transition metals during diamond chemical vapor deposition. The concepts relevant to the surface energetics are summarized, and the methods developed for the calculation of surface chemisorption energies are reviewed. Chemisorption energies of methyl radicals on transition metals are estimated on the basis of published results. The estimated chemisorption energies of CH₃ on Ni, Co, Fe, W (Mo), Ta and Ti are 36, 34, 43, 64, 85 and 85 kcal/mole, respectively. The results provide the necessary input parameters for studies of diamond nucleation kinetics.

Submitted to *Chemical Physics Letters* on October 18, 1995