A model for the nucleation of diamond clusters on Si(111) substrates

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

Abstract

A theoretical study of the nucleation, size and structure of diamond phase carbon clusters on Si(111) substrates is presented. Molecular mechanics analysis has been utilized to predict energetically and entropically feasible pathways for nucleation of the carbon clusters. Several mechanistic pathways for nucleation of carbon clusters are examined with C_2H_2 and/or CH_3 as the nucleation precursors. A possible model for the nucleation mechanism of diamond-phase carbon clusters on the β-SiC(111) surface, which forms epitaxially on Si(111) substrates, is presented. The critical size of the carbon clusters is computed based on the atomistic theory of nucleation and the proposed nucleation mechanisms.

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