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A quasi-equilibrium model for the prediction of interlayer chemistry during diamond chemical vapor deposition

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Abstract

The chemistry of the intermediate layer that develops at the interface between diamond and a non-diamond substrate during diamond chemical vapor deposition is analyzed using a thermodynamic quasi-equilibrium model. Substrates of Si, Mo, W, Ti, Ta, Fe and Ni are examined, and the physical parameters such as substrate temperature, reactor pressure, and CH_4/H_2 ratio in the gas phase required for the growth of respective metal carbides/solid carbon as intermediate layers between the substrate and diamond is predicted. The intermediate layers that are considered to be formed on Si, Mo, W, Ti, Ta, Fe, and Ni are SiC, Mo_2C, WC, TiC, TaC, Fe_3C, and Ni_3C, respectively, in addition to diamond and graphite. A quasi-equilibrium treatment of heterogeneous reactions at the gas–substrate interface is used to compute the desorption rates of volatile species formed in the reaction of gaseous H_2/H with the substrate. A phase diagram is obtained for the hydrogen and metal carbides/solid carbon (graphite, diamond). Good qualitative agreement is obtained between the model predictions and existing experimental data for the chemistry of the intermediate layer formed on the substrate at various temperatures and pressures commonly employed during diamond chemical vapor deposition.

Keywords: Diamond films; Chemical vapor deposition; Quasi-equilibrium model