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Ab-Initio Molecular Dynamics Study of the Structural Stability of fcc-Carbon on Diamond[1] CHARLES CHIN-CANCHE, CESAR CAB, JORGE-ALEJANDRO TAPIA, Facultad de Ingenieria, Universidad Autonoma de Yucatan, GABRIEL MURRIETA, Facultad de Matematicas, Universidad Autonoma de Yucatan, ROMEO DE COSS, Departamento de Fisica Aplicada, Cinvestav-Merida — The observation of a new carbon phase in thin films on diamond has been reported. High Resolution Electron Microscopy studies of the carbon thin films revealed a face-centered-cubic (fcc) crystal structure with a lattice constant of 3.563 Å. It is interesting to note that this value is very close to that of carbon in the cubic diamond phase (3.567 Å), suggesting that the substrate is contributing to the stabilization of fcc-carbon. Thus, in the present work we have studied the structural stability of fcc-C on the surface (001) of diamond. We have used the Density Functional Theory and the Molecular Dynamics approach in the slab configuration. The calculations where performed with the pseudopotentials LCAO method (SIESTA code) and the Generalized Gradient Approximation (GGA) for the exchange-correlation potential. We have analyzed the changes in the atomic structure, density of states (LDOS), and the local orbital population. We found that the carbon layers in the fcc structure on diamond are unstable.

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