Nanostructured surfaces

Quantum-chemical modeling of the diamond surface reactive ion etching in gas mixtures containing fluorine atoms

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Plasma with different composition and content of components was used for reactive ion etching of diamond surfaces. A mixture of carbon tetrafluoride and oxygen was used in a number of works [1]. In this paper, we used the quantum chemistry methods to investigate the chemical interaction of F atoms with the clean orderly surface and point defects on the reconstructed diamond surface C(100)-(2×1): single vacancies and divacancies. Simulation of a clean reconstructed diamond surface C(100)-(2×1) was carried out on a $C_{195}H_{112}$ cluster using a semi-empirical technique involving a MOPAC software package. Modeling the fluorine atoms adsorption on a diamond surface was carried out using reaction coordinate calculations.

Analyzing the quantum-chemical calculations results for the energy characteristics of the fluorine atoms interaction with the C(100)-(2×1) diamond surface, we can conclude on the following:

1. Formation of difluoride states of carbon atoms on an ordered diamond surface in the atomic fluorine atmosphere requires a 2.9 eV activation energy and leads to the destruction of surface dimers. As a result, there appear two types of potential centers of CF_x fragments desorption on the surface involving gas phase fluorine atoms: a difluoride and a monofluoride one.

2. A vacancy on the surface leads to a decrease in the activation energy (E_{act}=1.85 eV) of difluoride states formation on the atoms of the neighboring dimers in the same dimer row where the vacancy is located. This suggests that vacancies on the C(100)-(2×1) surface trigger further formation of linear defects in the form of "empty" dimer rows.

1. *Kunuku S., Sankaran K.J., Tsai C.-Y. et al.* Investigations on diamond nanostructuring of different morphologies by the reactive-ion etching process and their potential applications // ACS Appl. Mater. Interfaces. – 2013. – **5**, - P. 7439-7449.