Quantum-chemical simulation of interaction of hydrogen atoms with diamond nanoclasters

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Hydrogen is one of the most important adsorbate which interacts with a diamond surface. Unique physical properties of the hydrogenated C(100) surface makes this material perspective for creation of nano- and microelectronic devices [1, 2]. Vacancies are the important surface defects influencing electric and optical properties. At formation of defect the process of the surface reconstruction, local regibridization of the electronic states, formation or break of bonds between superficial atoms may essentially influence energy characteristics and strongly complicate available models of hydrogen adsorption and desorption [3].

In this work using MNDO semiempirical method (Modified Neglect of Differential Overlap) and MOPAC program package calculations were carried out. Investigations of vacancy defect configurations on C(100)-2×1 surface at different hydrogen coverage are presented. Diamond nanoclasters $C_{63}H_{59}$ and $C_{126}H_{91}$ were used for C(100)-2×1 surface simulation. The potential primary adsorption centres of vacancy defect area and energy characteristics of adsorption - activation energy of chemisorption and C-H bond energy in mono- and dyhidride states have been defined. The analysis of molecular orbital compositions were carried out. Possible mechanisms of hydrogen desorption from mono- and dyhidride states in the defect are offered. The possibility of existence of two states of vacancy defect on a clean C(100)-2×1 surface with different geometry, electronic properties and energy of formation is discussed. It was found, that the activation barriers for hydrogen desorption from C(100) diamond surface containing the vacancy defect make values E_D =1,2÷4,3 eV, depending on the defect state and degree of surface hydrogenation.

However, full saturation by hydrogen of any of defect state leads to a uniform state in which carbon atoms occupy positions close to C(100)-1×1 surface.

[1] Ristein J., *Surface Science* **600**, 3677 (2006).
[2] Tachiki M., Kaibara Yu, Sumikawa Yu, Shigeno M., Kanazawa H., Banno T., Song K.S., Umesawa H., Kawarada H. *Surface Science* **581**, 207 (2005).
[3] Liu F.B., Wang J.D.,, Chen D.R., Liu B., *Solid State Phenomena* **121**, 1119 (2007).