Nanostructured surfaces

The adsorption properties of the diamond surface (111)-2×1 with the divacancy V–C=C–V defect: quantum-chemical simulation

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Experimental and theoretical works [1] are mainly devoted to the study of stability and influence of vacancy and divacancy defects on the bulk properties of diamonds. However, the structure and properties of defects on a clean diamond surface remain insufficiently studied. This paper presents the results of calculations of the geometric, electronic, and adsorption properties of divacancy defects on the C(100) and C(111) diamond surfaces. As adsorbate particles, were selected the molecules of hydrogen H_2 and water H_2O.

Defective conditions on a clean, reconstructed surface are considered; stable configurations of divacancy defects differing in geometries, electronic properties, and formation energy are determined. We also evaluate the energy barriers between the V–C–C–V; V–C=C–V, and divacancy V_2 states.

The presence of defects leads to a change in surface adsorption activity and significantly affects the energy of adsorption and desorption of the particles. The potential primary adsorption centres of vacancy defect area and energy characteristics of adsorption - activation energy of chemisorption and heat of adsorption have been defined. The analysis of molecular orbital compositions was carried out. Possible mechanisms of molecules adsorption in the defect area are offered.

1. *Khmelnitsky R.A., Dravin V.A., Tal A.A., Latushko M.I., Khomich A.A., Khomich A.V., Trushin A.S., Alekseev A.A., Terentiev S.A* Mechanical stresses and amorphization of ion-implanted diamond. // Nuclear Instruments and Methods in Physics Research B. – 2013. - **304,** - P. 5-10.