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Metal-Semiconductor Ohmic Contacts: An ab initio Density Functional Theory Study of the Structural and Electronic Properties of Metal-Diamond (111)-(1x1) Interfaces.

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<p>Metal contacts on clean, hydrogenated and oxygenated diamond surfaces have been studied using ab initio Density Functional Theory. Five metals, i.e., gold, titanium, tantalum, vanadium and palladium on the three surfaces were considered. Gold and palladium were found to form weak bonds on clean, hydrogenated or oxygenated diamond (111) surfaces compared to the other three metals. Bulk properties were also studied following the formation of the respective ohmic contacts on the three surfaces. The clean diamond surface was found to have surface states which were modified by oxygen but removed by hydrogen. Density of states studies revealed that all the investigated metals had an effect on the electrical properties of the diamond surface. A peak that is characteristic of diamond was observed at ≈ -11.8 eV. For the clean diamond surface terminated with gold and palladium, states due to Au-2p orbitals were observed at ≈ -2.5 eV and ≈ -1.5 eV, while Pd-5s orbitals were located at ≈ -1.7 eV and ≈ -0.5 eV on the same surface. Titanium, tantalum and vanadium showed unique states at high binding energies of ≈ -38 eV for vanadium, ≈ -34 eV for tantalum and ≈ -32.5 eV for titanium, which were thought to be responsible for their strong bonding. Key words: Metal-diamond interface, Adsorption, ohmic contacts

Level (Hons, MSc,
   PhD, other)?

PhD Student

Consider for a student
   award (Yes / No)?

Yes

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

Yes

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