Adhesion of electrodes on diamond (111) surface: A DFT study.

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ABSTRACT

We explore possible candidates for metallic electrodes of diamond semiconductor from twenty kinds of metallic sheets on oxygen- or hydrogen-terminated diamond (111) surface as well as pristine one. Their adhesion strengths and electric characteristics of contacts (i.e. either Ohmic, Schottky or neither) are both considered as figures of merit. The former is measured as work of separation, Wsep, obtained from density functional theory (DFT) simulations. The latter is inferred from DOS (density of states) analysis based on DFT, by checking whether or not the in-gap peak disappears and if there is a large DOS around the Fermi level. We found that (1) Ti on pristine surface has both the best Ohmic contact and fairly strong adhesion and (2) Ti and Cr on oxygenated surfaces have the strongest adhesion with good Schottky contact.

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