Adhesion of the electrodes on diamond device surfaces

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ABSTRACT

Appropriate candidates of the metallic sheet used for the electrodes of diamond semiconductor are investigated using computational ap-proaches based on density functional theory (DFT). For twenty kinds of metallic elements x, we modeled a diamond-metal interface andevaluated its work of separation, Wsep(x), as a possible measure of anti-peeling strength. The appropriateness of the Ohmic contact wasinferred from DOS (density of states) analysis of diamond-metal interface by looking at whether an in-gap (isolated/localized) peak disap-pears as well as a sufficient amount of DOS value exists around the Fermi level. Our DFT simulation confirmed that a typical electrode, Au,is not adhesive enough for power devices [Wsep(Au) = 0.80 J/m2], though showing the Ohmic contact. In contrast, some transition metalswere found to possess Ohmic features with much stronger adhesion than Au [e.g.,Wsep(Cr/Ti) = 6.02/4.03 J/m2]