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Interfacial properties and electron structure of Al/B4C interface: A first-principle study

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This research aims at investigating the structural, mechanical and electronic properties of the Al (111)/B4C (0001) interface by first-principles calculations. This model geometry Al (111)/B4C (0001) is chosen because the close-packed planes of Al and B4C have the (111) and (0001) orientation, respectively, and the lattice mismatch is only ~2.1%. Among four B4C (0001) surfaces with different terminations, our calculation of surface free energies predicted that C-terminated B4C (0001) surface is the most stable one. Relaxed atomic geometries, the work of adhesion and interfacial free energies were calculated for three C-terminated B4C (0001)/Al (111) interfaces with different stacking sequences (top-site, hollow-site and bridge-site). Results reveal that the relaxed top-site (hollow-site-like) Al/B4C interface has the best adhesion force and also be the most stable. The interfacial electron structure including charge density difference, Bader charge and density of states (DOS) is analyzed to determine the nature of metal/carbide bonding and we find the formation of AleC bond and possibly the formation of Al4C3 in the interface.

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Modeling and simulation of radiation effects on charge coupled devices induced by proton and neutron beams

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Charge coupled devices (CCDs) have extensive applications in particle detection, space mission, medical imaging, and nuclear industry. However, the CCDs used in these particular applications are susceptible to radiation damage. The radiation-induced damages can be separated into two phenomena: ionization damage effects and displacement damage effects. Ionizing damage induces an increase in trapped oxide charges and bulk-oxide interface traps which cause an increase in surface dark signals and dark signal non-uniformity (DSNU) of the CCDs. Displacement damage caused by energetic particles such as protons or neutrons induces stable bulk traps with energy levels within the band-gap which can lead to the degradations on the CCDs. Fewer studies have focused on the details of simulation results and with generally only limited information about modeling and simulation process. A method is presented for modeling and simulation of radiation effects on CCDs irradiated by proton and neutron beams. The device model, clock pulse driver circuit models, radiation effect models, and solution methods are described in detail. The mechanism of dark signal and charge transfer inefficiency (CTI) increase, induced by proton radiation is analyzed. The proton radiation modeling is established to simulate the degradation of dark signal and CTI in a CCD by the device simulator. The simulation results show that the CTI increase induced by protons is mainly due to the trap with energy level of Ec-0.42eV (E centers) and the total dark signal increase is dominated by the surface dark signal increase. The mechanism of CTI increase induced by neutron radiation is analyzed. The neutron radiation modeling is established to simulate the CTI degradation in a CCD. The tendencies of the simulation results are in agreement with the experimental results of the correlative literatures.

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