On charging effects at SiC/nitride interfaces – *ab initio* studies

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Thin nitride films on silicon carbide substrate constitute many technologically important devices, where the nitride/SiC interfaces play particularly important role. In spite of intensive experimental efforts [1-3], the microscopic physics of these intriguing interfaces is mostly unknown. In the case of GaN and SiC, which are partly ionic and partly covalent bonded materials with different degrees of ionicity, the interfacial polarity plays an important role for understanding of the growth process in these materials, and it affects the quality of GaN deposited films. The heterovalent character of these interfaces, together with the piezo- and pyroelectric character of the junction materials, leads to polarization charges and very strong electric fields that could in turn cause changes in atomistic details of the interfaces.

In this work, we present first-principles studies of the first stages of Ga, Al, and N adsorption on the C and Si terminated surfaces of hexagonal SiC, and further the studies on the formed interfaces, 4H-SiC/wz-AlN and 4H-SiC/wz-GaN. In particular, we analyze the formation of interfaces with the wurtzite symmetry and take into account various arrangements of the tetrahedrally coordinated atoms, leading to long or short bonds across the interfaces. Different charge compensation patterns are proposed, which improve the interface stabilities. By studying the atomistic details of the interfaces, as well as the resulting spatial interface total charge density distributions, we can state that the charge compensated interfaces with long bonds between the Si-N, Si-Ga atoms become equivalent to the compensated ones with C-Ga, C-N short bonds, respectively. In addition, we have calculated the formation enthalpies of the interfaces, valence band offsets, induced interface charges, and resulting electric fields.

The present studies shed light on the physics of heteropolar SiC/nitride interfaces and provide microscopic details of interfaces' morphology together with theoretical predictions of important parameters that are a prerequisite for reliable modeling of relevant for devise design phenomena, such as the charge and spin transport across the interface and the thermal boundary resistance effect.

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