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The atomic and electronic structure stability of 3C-SiC/SiC interface superstructures: A DFT calculation

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We report total energy and electronic structure calculation of SiC/Si interface with unequal atom densities due to apparent lattice matching between them. The result shows several distinctive metastable structures depending on which interface systems are involved. We find that, for a particular interfacial system, the energy differences range between 10-52 meV per Å2 for both Si-C and Si-Si interfaces respectively with 3C-SiC facets having dense surface atoms whilst those of Si being sparse. We find that the interface structures are associated with vacant channels and stabilized by the existence of over-coordinated atoms (floating bonds). We also observed atomic undulation near the Si-C interface pinched at Si substrate to stabilize the interface. We reveal that, the coexistence of floating bonds and dangling bonds (under coordinated atoms) with the transfer of electrons from the dangling bonds to the floating bonds are the microscopic mechanism of the interface stabilization. The calculated interface formation energies indicate that Si-Si is more favorable compared with Si-C. The electronic dispersion structure calculation shows either metallic or semiconducting character due to electron transfer from SiC to Si. The stable structure of SiC(111) on Si(110) shows semi-conducting behaviors while that of the 3C-SiC(111) on Si(111) is metallic and that might be due to the relative electronegativity differences between Si and C atoms.

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