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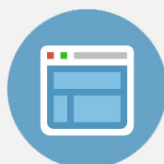
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Can we make the SiC–SiO₂ interface as good as the Si–SiO₂ interface?

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A simple analysis based on the bulk valence and conduction densities of states was employed to estimate the interface-state densities for interfaces between the three most common SiC polytypes (3C, 4H, and 6H) and SiO₂. We found that all polytypes had comparable conduction-band interface-state density with silicon dioxide as Si, being higher for the valence band. The conduction-band interface-state density should be higher for 4H-SiC than for 6H-SiC for both the C- or Si-terminated interfaces. On the contrary, the valence-band interface-state density can be either higher or lower for 4H-SiC compared to 6H-SiC according to which atom, C or Si, terminates the interface. The trends suggested by the above model are in agreement with recent mobility measurements in SiC-based field-effect transistors. © 2001 American Institute of Physics. [DOI: 10.1063/1.1399009]

Silicon carbide could replace silicon in metal–oxide–semiconductor field-effect transistors (MOSFETs) for specific applications that entail high temperatures and/or high voltages. However, the SiC–SiO₂ interface does not have the desirable properties that characterize the Si–SiO₂ interface: the electron mobility in 4H-SiC layers adjacent to the interface is about two orders of magnitude smaller than that in the bulk.^{1–5} The density of states (DOS) at the interface between SiC and SiO₂ is found to be much higher than the corresponding DOS at the Si–SiO₂ interface.^{1–5} Moreover, different polytypes show unusual mobilities with respect to their bulk counterparts. In particular, the *n*-channel mobilities for inversion MOSFETs are higher for 6H-SiC than for 4H-SiC, even if 6H-SiC has lower bulk carrier mobility. Some authors⁶ have suggested that there is a broad interface-state density centered about 2.9 eV above the valence band edge for the different polytypes. This would explain the low inversion channel mobility in 4H-SiC with respect to 6H-SiC: the band gap is larger for 4H-SiC (about 3.3 eV) than for 6H-SiC (about 3 eV), thus involving these interface states in carrier scattering in the 4H polytype more than in the 6H polytype. The presence of these states is generally attributed to carbon clusters and near-interfacial defects in the oxide layer.⁷ Indeed, theoretical investigation has confirmed that the emission of CO molecules during SiC oxidation can lead to carbon cluster formation.⁸

Much effort has been devoted to improvement of the interface quality between SiC and its native oxide. Promising processes for the reduction of the interface-state density are reoxidation,^{9,10} NO annealing,¹¹ or annealing in ammonia.¹² These processes should remove carbon from the interface^{9,10} or passivate carbon-cluster gap states by N incorporation.^{11,12} However, even with these postoxidation processes, the DOS at the SiC–SiO₂ interface is still larger than the corresponding one at the Si–SiO₂ interface. It is certainly possible that the correct processing to completely avoid carbon-related defects has not been found yet. However, let us assume that we can completely eliminate the effects of C-cluster defects at

the interface. In this case, can we expect that the SiC–SiO₂ interface will have the same *intrinsic* properties as the Si–SiO₂ interface, e.g., the same interface-state density?

We suggest in this letter that all polytypes could provide comparable *intrinsic* conduction-band interface-state density with SiO₂ as Si does, the valence-band interface-state density being higher for all polytypes. Also, we find that the conduction-band interface-state density should be higher for 4H-SiC than for 6H-SiC if the interface is either C or Si terminated. On the contrary, the valence-band interface-state density is either higher or lower for 4H-SiC compared to 6H-SiC according to which atom, C or Si, terminates the interface. We arrive at these conclusions by means of a simple Koster–Slater-type¹³ of model that allows us to relate the existence and/or the energy position of interface states to some essential bulk features of the constituent materials and interface-bonding parameters.¹⁴ From this model the existence of an interface state at the SiC/SiO₂ interface is determined by¹⁴

$$1 - V_{\text{SiC}}G_0^{\text{SiC}} - V_{\text{SiO}_2}G_0^{\text{SiO}_2} - (\tilde{V}_{\text{SiC/SiO}_2} - V_{\text{SiC}}V_{\text{SiO}_2})G_0^{\text{SiC}}G_0^{\text{SiO}_2} = 0, \quad (1)$$

where V_{SiC} and V_{SiO_2} are potentials that describe the perturbation that the interface induces on the bulk properties of each semiconductor, and $\tilde{V}_{\text{SiC/SiO}_2}$ is a potential that couples the interface layers.¹⁴ G_0^{SiC} and $G_0^{\text{SiO}_2}$ are retarded Green's functions of SiC and SiO₂, respectively. For the case at hand, Eq. (1) can be further simplified as follows. The SiO₂ conduction-band (valence-band) edge is several eV higher (lower) than the corresponding edge in SiC or Si. Any contribution from $G_0^{\text{SiO}_2}$ can be thus neglected to first order. The existence of interface states is thus determined by the simple Koster–Slater relation $1 - V_{\text{SiC}}G_0^{\text{SiC}} = 0$. In this form, the model has been used with success to explain general trends in defect state formation in semiconductors.¹⁵

Taking into account the linear relationship between the one-particle Green's function and the DOS, we can discuss the existence of interface states by looking at the DOS of the bulk materials (either SiC or Si) at energies close to the band

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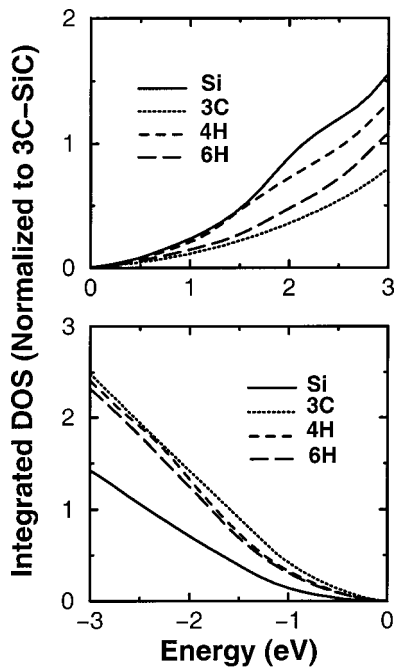


FIG. 1. Integrated DOS (number of states) for Si and three SiC polytypes (3C, 4H, and 6H) for the conduction (upper part) and valence (lower part) bands. All DOSs are normalized to the 3C unit cell volume.

edges. The short-range potential V can be due to any defect or structural and chemical difference between SiC (or Si) and SiO₂ at the interface, and we assume it to be the same for both SiC and Si interfaces. This corresponds to the assumption that the *same* interface quality has been achieved for both semiconductors, i.e., both semiconductor interfaces have the same *type of defects*. This would be the ideal experimental situation. We can now answer the original question. We plot in Fig. 1 the integrated DOS (or the number of states) from the conduction- and valence-band edges for the three most common SiC polytypes (3C, 4H, and 6H) and for Si.¹⁶ For comparison purposes, all DOSs were normalized to the 3C unit cell volume. The DOSs were obtained from the electronic bands calculated self-consistently using the linearized muffin-tin orbital (LMTO) method based on the local density approximation (LDA) in density functional theory.^{17,18} In the energy region relevant to interface-state formation (up to about 2 eV from the band edge) the DOSs for Si and all polytypes are comparable (and even lower for 3C- and 6H-SiC) for the conduction band, while for the valence band the Si DOS is lower than the corresponding DOS for the SiC polytypes. This means that, even if the defects at the Si-SiO₂ and SiC-SiO₂ interfaces are the same, all polytypes will show a higher density of interface states at the valence-band edge and a comparable, if not lower, density of interface states at the conduction-band edge than Si. The model we use is too simple to quantify the differences between polytypes but is sufficient to study qualitative trends of interface-state formation.

With the above model we can now try to understand the differences observed experimentally between 4H- and 6H-SiC polytypes. The interface between these polytypes and SiO₂ is generally grown along the (0001) direction which corresponds to either C- or Si-terminated interfaces.⁹ The interface-state density will thus depend on which atom the

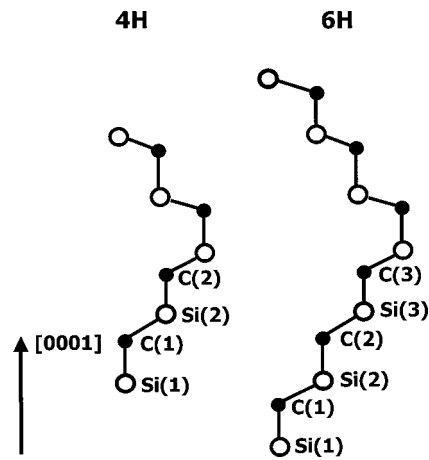


FIG. 2. Inequivalent silicon (open circles) and carbon (closed circles) atoms of the 4H- and 6H-SiC polytypes.

interface terminates, C or Si. Therefore, we consider the DOS of both polytypes according to the contributions coming from the different C and Si atoms in the bulk. 4H-SiC has two distinct C and two distinct Si atoms in the unit cell, while 6H-SiC has three C and three Si atoms that are inequivalent in the unit cell (see Fig. 2). The integrated partial DOS coming from inequivalent atoms is shown in Fig. 3 for the conduction band and in Fig. 4 for the valence band. From

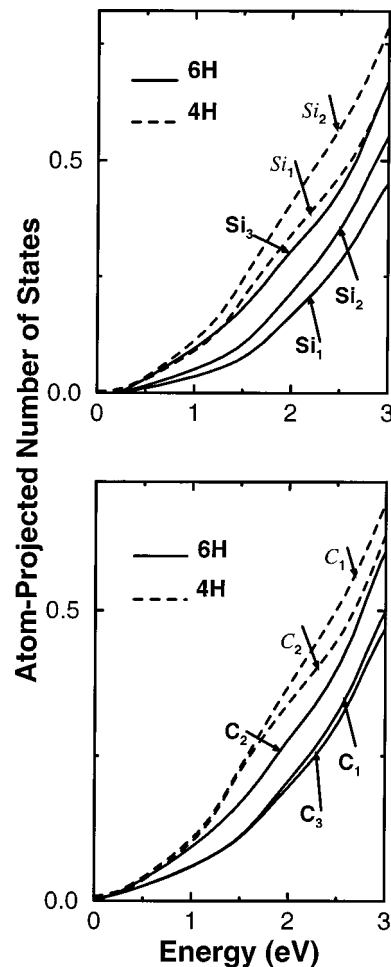


FIG. 3. Partial number of states from different inequivalent silicon (upper part) and carbon (lower part) atoms for the conduction band of the 4H- and 6H-SiC polytypes. Letters in italic indicate the atoms of 4H-SiC.

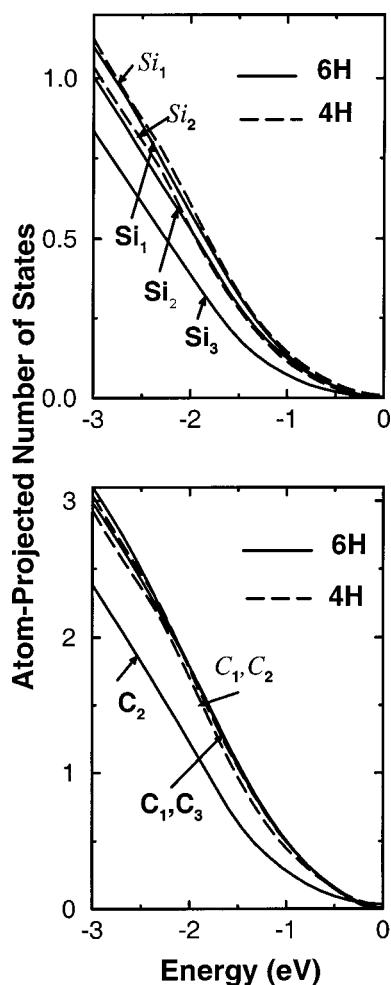


FIG. 4. Partial number of states from different inequivalent silicon (upper part) and carbon (lower part) atoms for the valence band of the 4H- and 6H-SiC polytypes. Letters in *italic* indicate the atoms of 4H-SiC.

Fig. 3, we can thus conclude that, close to the conduction-band edge, the DOS is higher for 4H- than for 6H-SiC whether or not the interface is terminated by C or Si atoms. This would correspond to a higher density of interface states and thus to lower mobility as observed in experiments.¹⁻⁵ On the other hand, for energies close to the valence-band edge the DOS could be higher or lower for 4H-SiC than for 6H-SiC. For example, if the 6H-SiC is terminated by the carbon atom labeled C(2) (see Figs. 2 and 4) and 4H-SiC is terminated by any of its carbon atoms we expect the interface-

state density to be higher for 4H-SiC than for 6H-SiC. The opposite would occur if 4H-SiC terminates with any of its inequivalent C atoms and 6H-SiC terminates with the carbon atom C(3). Indeed, in *p*-doped samples, alternation of interface quality has been observed³ for 4H- and 6H-SiC polytypes that could be explained by the present model. Finally, we can also conclude that, if the interface is terminated by a combination of C and Si atoms, the interface-state density will be given by a combination of different atomic contributions with weights that correspond.

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