Ab initio calculation of mobility degradation caused by Si-vacancies in SiC/SiO_2 channels

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Introduction: Due to its wide bandgap, silicon carbide (SiC), in particular the 4H polytype, is a promising material for power semiconductor applications as it allows to build devices with higher breakdown voltages and lower losses than Si. However, SiC suffers from electron scattering caused by defects at the SiC/SiO_2 interface [1] or within the SiC channel which results in a lower channel mobility as compared to bulk SiC and a high specific ON-state resistance [2].
In this work, we present a method to create realistic SiC/SiO_2 interface structures using a reactive force field as well as (tight-binding) density functional theory DFT(B). We then investigate the influence of defects on the transport properties, focusing on Si-vacancies close to the interface [3]. These defects usually come from the transfer of Si atoms into the SiO_2 oxide layer. Finally, the mobility of the constructed structures is calculated. We demonstrate that these defects can be passivated and the carrier mobility partly restored.

Method: The chosen simulation approach is illustrated in Fig. 1(a). It consists of two main steps. *1) Layer-by-layer technique:* As the goal is to examine the influence of Si-vacancies, defect-free SiC/SiO_2 interfaces should be created. For that purpose, silicon oxide (SiO_2) is grown on top of a 4H-SiC cell by depositing Si and O atoms in a layer-by-layer fashion (Fig. 1(b)). After each step, annealing with a reactive force field [4,5] is performed. In the end, the obtained structure is further relaxed with DFT(B) [6]. Defects, such as Si-vacancies, can finally be inserted at different positions.
2) Mobility calculation: Using DFT, the Hamiltonians and the overlap matrices of the produced "devices" are calculated and subsequently passed to a quantum transport solver [7] to calculate the electrical current flowing through them. The dR/dL method [8] allows to determine the defect-limited mobility by calculating the resistance of channels with different lengths.

Results: The layer-by-layer technique proposed above allows to create practically defect-free interfaces as shown in Fig. 2(a). A Si-vacancy was introduced here close to the SiC/SiO_2 interface. The corresponding density-of-states is plotted in Fig. 2(b). Defect states around the conduction band are clearly visible.
Channels with Si-vacancies and after their passivation with nitrogen highlight the influence of the defects on the transport properties. In particular, Fig. 3(a) shows that the transmission function turns on at lower energies after passivation.
Mobility values for both structures were extracted with the dR/dL method. The results are given in Fig. 3(b). A significant improvement from 68.6 cm^2/(Vs) to 130.9 cm^2/(Vs) is observed when going from the defective to the repaired channel.

Conclusion: To investigate the influence of defects on the carrier transport of SiC/SiO_2 channels, we have developed a layer-by-layer deposition scheme and have used the resulting structures to calculate the mobility through a channel with Si-vacancies. Although nitrogen passivation enhances the mobility value, it is still far from its bulk counterpart (900 cm^2/(Vs)), leaving room for further improvements.

References: [1] S. Iwase et al. Phys. Rev. B 95, 041302(R) (2017). [2] Y. Deng et al., J. Electron. Mater. 35, 618–624 (2006). [3] J. Cottom et al., J. Appl. Phys. 124, 045302 (2018). [4] A. P. Thompson et al., Comp Phys Comm 271, 10817 (2022). [5] D. A. Newsome et al., J. Phys. Chem. C, 116, 30, 16111–16121 (2012). [6] T. D. Kühne et al. J. Chem. Phys. 152, 194103 (2020). [7] M. Luisier et al. Phys. Rev. B 74, 205323 (2006). [8] K. Rim et al., IEDM, 1175775 (2002).

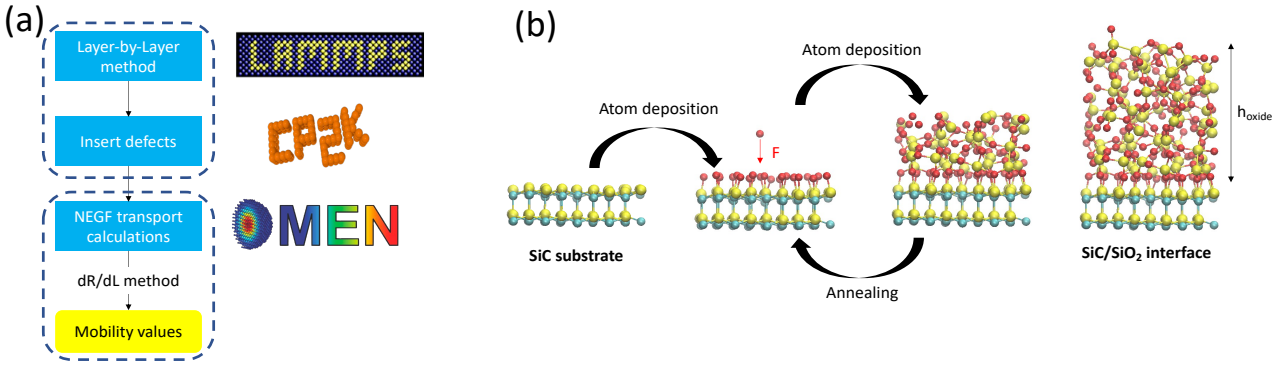

Fig. 1. (a) Illustration of the simulation method to study the transport properties of SiC/SiO_2 channels. A reactive force field is combined with DFT(B) to create realistic interfaces. The resulting Hamiltonian and overlap matrices are passed to an NEGF solver to calculate the mobility with the dR/dL technique. (b) Steps of the developed layer-by-layer procedure to grow SiO_2 onto SiC. Annealing is performed with a ReaxFF force field after the deposition of each atomic layer. Further relaxations of the structure with DFT(B) as implemented in CP2K [6] are not visualized here.

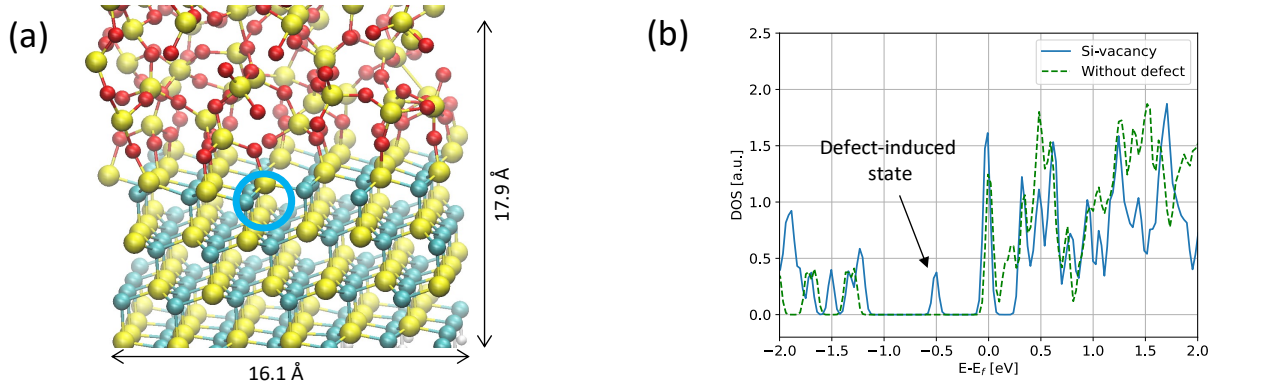

Fig. 2. (a) Exemplary interface structure created with the proposed layer-by-layer deposition technique. The blue circle indicates the location of a Si-vacancy that was introduced on purpose. (b) Density-of-states of the SiC/SiO_2 structure with (solid line) and without (dashed line) Si-vacancy.

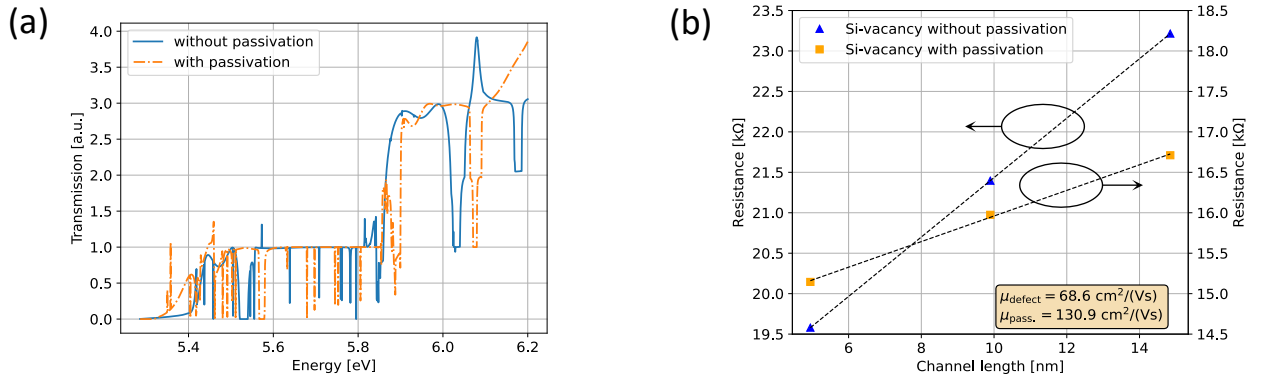

Fig. 3. (a) Transmission function through a SiC/SiO_2 channel with Si-vacancies before (solid line) and after (dashed-dotted line) passivation with nitrogen atoms. (b) Channel resistance as a function of the channel length. Results for the structure with Si vacancies before (triangle) and after passivation (squares) are compared. Lines are guides to the eyes. As expected, a linear resistance increase is obtained. The extracted mobilities with the dR/dL method are reported as inset.