

Full-Band Device Simulator with Real-Space Treatment of the Short-Range Coulomb Interactions for Modeling 4H-SiC VDMOS Devices

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4H-SiC has been widely used in many power electronic applications because of the extremely high critical electric field and good electron mobility. For example, 4H-SiC possesses a critical electric field ten times higher than that of Si, which allows high-voltage blocking layers composed of 4H-SiC to be approximately a tenth of the thickness of a comparable Si device. This, in turn, reduces the device on-resistance and power losses while maintaining the same high blocking capability.

Unfortunately, commercial TCAD tools like Sentaurus and Silvaco are based on the effective mass approximation, while most 4H-SiC devices are operated under high electric fields, so the parabolic-like band approximation does not hold anymore. Hence, to get more accurate and reliable simulation results for these devices, full-band analysis is needed. The first step in the development of a full-band device simulator is the calculation of the band structure. In this work, the empirical pseudopotential method (EPM) is adopted. We follow the approach of Ng [1] who utilizes genetic algorithm to get to a proper set of EPM form factors that match density functional theory (DFT) results. The 4H-SiC band-structure used in this work is shown in Figure 1.

Acoustic, non-polar optical phonon and polar optical phonon are relevant scattering mechanisms for this material system [2]. Impurities are introduced into the model as discrete dopants. Coulomb scattering is treated in real space using the particle-particle-mesh (P³M) approach [3] and represents the major novelty of this work. Proper treatment of the Coulomb interactions is essential for power electronic applications because of the high carrier densities. Bi-CGSTAB method is used for the solution of the 3D Poisson equation.

For proof-of-concept of the methodology adopted here, a 3D resistor is simulated first [4]. From the resistor simulations, the low-field electron mobility dependence upon Coulomb scattering in 4H-SiC devices is extracted. The simulated mobility results agree very well with available experimental data [5], which is clearly seen from the results presented in Figure 2. An anisotropy of mobility along different crystal orientation is also observed. The ratio between [0001] and [1120] direction is found to be between 1.25-1.75. The field dependence of the carrier drift velocity, compared with experimental data from Ref. [5], is shown in Figure 3. The observed excellent agreement validates further the adopted theoretical model. Next, a 3D VDMOS is simulated, a schematic of which is shown in Figure 4. The electron distribution and the potential profile of the VDMOS device are shown in Figure 5. The output characteristics of the VDMOS device are shown in Figure 6. From the results presented we may conclude that, due to its comprehensive nature, the developed tool can serve as a basis for future investigation of 4H-SiC power devices.

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