Semiconductor Device Modeling: The Last 30 Years

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Numerical simulation of semiconductor devices has evolved to a wide and viable research field over more than three decades. The various subjects considered reflect the tremendous progress in semiconductor technology. The term Technology CAD (TCAD) has been coined to describe classical device simulation, which is based on continuum theory and classical transport theory. By solving the continuity equations for electrons and holes self-consistently with the Poisson equation for the electrostatic potential, the operation of various unipolar and bipolar devices can be well understood, both qualitatively and quantitatively [1]. The main drivers for TCAD tool development were silicon integrated circuit technology and silicon power devices. According to the scaling rules of CMOS technology, the doping levels and the electric field strengths in the junctions were continuously increased, which eventually resulted in reliability problems due to hot carriers. To study hot carrier effects theoretically, end of the 1980s Monte Carlo simulation including a numerically tabulated electronic band structure has been introduced. The Monte Carlo method solves the classical Boltzmann equation for the charge carriers and is often considered a reference method for the simpler transport models used in TCAD. The continuous reduction of the supply voltage below three Volts, however, alleviated the hot carrier problem significantly. With the advent of strain engineering in the 1990s the electronic band structure was intentionally distorted by imposing appropriate strain conditions. Full-band Monte Carlo calculations helped to quantify the effect of the band structure changes on the electronic transport properties. For the classical TCAD tools new mobility models have been developed taking the strain dependence into account. With continued down-scaling of the oxide thickness the classical TCAD tools needed to be augmented by quantum correction models which approximate the quantum mechanical charge distribution in the channel. Besides silicon main stream technology, a variety of new semiconductor nano-structures and nano-devices came into the focus of device simulation, but also a variety of new materials. Examples are carbon nano-tubes, graphene, and organic semiconductors, to name a few. Device modeling has entered the field of mesoscopic physics, where quantum mechanical effects such as confinement, tunneling, interference and charging effects determine the characteristics of a device [2]. This extended field of research is commonly referred to as Computational Electronics [3]. Mesoscopic physics still uses concepts from continuum theory, such as band structure, band diagrams, and envelope functions which are wave functions where the lattice-periodic part has been factored out. At the small end of mesoscopic structures the tight-binding method is often used, which is an empirical atomistic method for electronic structure calculation. Specific problems need to be considered on an atomistic level and require so-called *ab initio* methods. An example is the degradation of gate insulators, where *ab initio* calculations give insight into the type of field-induced defects and their kinetics. Another important subject of device modeling deals with electrical devices coupled to some non-electric system, as it is the case for optoelectronic devices, including various types of semiconductor lasers, or thermoelectric devices, but also MEMS and sensor devices for various applications. In summary, it can be concluded that device modeling has evolved to a wide multidisciplinary field. Numerical mathematics, computer science, and various fields from physics such as solid state physics, quantum mechanics, and statistical mechanics, are closely interlinked. Today, Computational Electronics provides a multitude of approaches and tools to cope with the ever increasing number of new semiconductor devices and structures, and the new materials being introduced.

References

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