

**(Invited Abstract)**

**TCAD Process/Device Modeling Challenges and Opportunities for the Next Decade**

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Technology CAD process and device simulation tools play a critical role in advanced technology development by giving insight into the relationships between processing choices and nanoscale device performance that cannot be obtained from physical metrology tools alone. TCAD makes its greatest impact when a detailed understanding of the underlying physical mechanisms is tightly coupled within the technology development cycle so that physical insights feed directly into technology directions. This paper highlights progress in modeling over the past decade that has enabled this success and the challenges and opportunities that lie ahead.

The technology development impact of continuum process and device modeling approaches over the past decade has been enabled by insights obtained from atomistic materials and transport modeling coupled with detailed materials characterization. In diffusion modeling, the key role of dopant-defect clustering and extended defect formation has transformed our understanding of dopant transient enhanced diffusion and activation. *ab initio* modeling of defect energetics has complemented TEM imaging of extended defects and electrical measurements of dopant activation to build up a clear physical framework for understanding and engineering ultrashallow junctions. More recently, detailed bandstructure and device transport modeling combined with process simulation has enabled understanding and optimization of stress effects to achieve significant device performance gains in a manufacturable technology. In both of these areas, a hierarchy of physical models has been used to connect a detailed physical description at an atomistic level to computationally efficient models that can be applied to technology analysis and optimization.

Looking ahead to the next decade, the pace of new material introduction is expected to increase dramatically, requiring computational materials science on a broader scale than ever before to guide materials selection and enable technology evaluation. At the same time, continued reductions in device size give an opportunity for direct, atomic-scale modeling of the full device structure to understand the relationship between materials and interface states and device operation. Moving from evolutionary to revolutionary CMOS scaling, TCAD can provide early insight into the fundamental benefits and limitations of alternative device structures. This will require detailed, physically based device modeling tools driven from an understanding of materials structure and properties, taking us beyond the realm of traditional device modeling tools. As we meet these challenges, the opportunity to impact the direction of technology is greater than ever.