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**Role of Validation and Predictions in Modeling: Specific Examples from Semiconductor Industry**

**Applications**

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With the advent of newer non-Silicon materials, using modeling to estimate properties are becoming necessary for process technology development. Since these materials are integrated as part of larger devices, interfaces and material domains are increasingly modulating properties of materials. Unlike in bulk materials, electronic and thermodynamic properties are difficult to characterize in these material structures as the device sizes overlap with material domains. We will illustrate specific cases from semiconductor processing and property estimation on the importance of verification of models for internal consistency and validation with experimental data. Given the discrepancy of scales between predictions and measurement, techniques need to bridge them. In addition, models that are developed need to be modular with open interfaces for cross-checking and integration across scales as indicated in the recently announced Materials Genome Initiative.

[1] President's initiative on Materials Genome Initiative for Global Competitiveness, June 2011

[2] S. Shankar, B. V. McKoy, W. L. Morgan, "Self-Consistent Modeling of Weakly Ionized Plasmas-Challenges in Quantum and Classical mechanics," Sixth U.S. National Congress on Computational Mechanics, U.S. Association for Computational Mechanics, Dearborn, Michigan, (2001)