Molecular modeling and multiscaling issues for electronic material applications

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Molecular modeling and multiscaling issues for electronic material applications provides a snapshot on the progression of molecular modeling in the electronics industry and how molecular modeling is currently being used to understand material performance to solve relevant issues in this field. This book is intended to introduce the reader to the evolving role of molecular modeling, especially seen through the eyes of the IEEE community involved in material modeling for electronic applications. Part I presents the role that quantum mechanics can play in performance prediction, such as properties dependent upon electronic structure, but also shows examples how molecular models may be used in performance diagnostics, especially when chemistry is part of the performance issue. Part II gives examples of large-scale atomistic methods in material failure and shows several examples of transitioning between grain boundary simulations (on the atomistic level)and large-scale models including an example of the use of quasi-continuum methods that are being used to address multiscaling issues. Part III is a more specific look at molecular dynamics in the determination of the thermal conductivity of carbon-nanotubes. Part IV covers the many aspects of molecular modeling needed to understand the relationship between the molecular structure and mechanical performance of materials. Finally, part V discusses the transitional topic of multiscale modeling and recent developments to reach the submicronscale using mesoscale models, including examples of direct scaling and parameterization from the atomistic to the coarse-grained particle level.