ReaxFF reactive force field simulations on material growth – building connections between atomistic-scale simulations and experiment

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ABSTRACT

The ReaxFF method provides a highly transferable simulation method for atomistic scale simulations on chemical reactions at the nanosecond and nanometer scale. It combines concepts of bond-order based potentials with a polarizable charge distribution.

Since its initial development for hydrocarbons in 2001[1], we have found that this concept is transferable to applications to elements all across the periodic table, including all first row elements, metals, ceramics and ionic materials[2]. For all these elements and associated materials we have demonstrated that ReaxFF can accurately reproduce quantum mechanics-based structures, reaction energies and reaction barriers, enabling the method to predict reaction kinetics in complicated, multi-material environments at a relatively modest computational expense. At this moment, over 2000 publications including ReaxFF development of applications have appeared in open literature and the ReaxFF code has been distributed around the world and has been implemented in major open-source and commercial computational chemical software packages.

This presentation will describe the current concepts of the ReaxFF method, the current status of the various ReaxFF codes and acceleration methods that allow for microsecond-range predictions. Also, we will present and overview of recent and developing applications to material synthesis, in particular complex material deposition and growth at Al_2O_3 and SiC interfaces related to Ga/Ga-oxide, BN, 2D-chalcogenide and SiC-growth[3-5] using both molecular and atomic precursors.

References

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