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Computational approach to understand the dynamics of interfacial phenomena

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Materials research is closely related to the interfacial phenomena. For example, thin film structures are frequently governed by the initial period of deposition when the intermixing or epitaxial misfit occurs. The physical and chemical properties of hybrid (composite) materials are also governed with the interfacial properties. However, the interfacial properties are not sufficiently characterized by only the experimental analysis approach. Owing to the rapid increase in computing power and successful development of the computation methodology, molecular level simulation has driven new paradigm of materials research. Increased predicting power of the ab initio calculation combined with molecular dynamics approach can now guide the experimental research.

I will present the computational approaches to understand the interfacial structure evolution in various materials systems. Kinetics analysis of the atomic intermixing behavior on the surface could lead to the fundamental understanding of the asymmetric intermixing phenomena observed in many metallic systems: local acceleration of the deposited atoms near the surface provides an explanation of the puzzling phenomenon of the significant intermixing under low energy deposition conditions such as thermal evaporation or molecular beam epitaxy [1]. Interfacial properties of oxide/Si is crucial for nano-scale CMOS devices. Stress evolution of Si nanowire were investigated by employing reactive molecular dynamics simulation, which is in contrast to the theory of self-limiting oxidation where rigid mechanical constraint of the Si core was assumed. This computational research extended our understanding of the mechanical response in nano-meter scale materials: the Si core of the thinner Si-NW was deformed more with surface oxidation, resulting in a lower compressive stress at the interface. These results explain the experimental observation of full oxidation of very thin Si-NWs [2]. Effect of atomistic interfacial irregularity on the electron transport of Si-NW was also discussed [3]. Finally, I will introduce the recent effort to build a web-based materials design platform. This platform will become an essential research infrastructure where researchers or developers can perform the required elaborate simulation with relatively low entrance barrier to computational research.

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