Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A1] Symposium A-1

Chair: Anton Van der Ven(University of California Santa Barbara, United States of America)
2018年10月29日(月) 13:30 ～ 15:00 Room6

[SY-A1]Uncertainty Quantification for Classical Effective Potentials

○Sarah Longbottom, Peter Brommer (School of Engineering, University of Warwick, UK)

Effective potentials are an essential ingredient of classical molecular dynamics (MD) simulations. Little is understood of the errors incurred in representing the complex energy landscape of an atomic configuration by an effective potential containing considerably fewer parameters. The probabilistic sloppy model method [1] has been implemented in the *potfit* force matching code [2]. This introduces uncertainty quantification into the interatomic potential generation process. Uncertainties in the effective potential are propagated through MD to obtain uncertainties in quantities of interest, which are a measure of the confidence in the model predictions.

We demonstrate the technique using three potentials for nickel: two simple pair potentials, Lennard-Jones and Morse, and a local density dependant EAM potential. A sloppy model fit to DFT reference data is constructed for each potential to calculate the uncertainties in lattice constants, elastic constants and thermal expansion. These can be used to show the unsuitability of pair potentials for nickel. In contrast, with EAM we observe a decreased uncertainty in the model predictions. This shows that our method can capture the effects of the error incurred in the potential generation process without resorting to comparison with experiment or DFT, which is an essential part to assess the predictive power of MD simulations.

Further work is in progress to create a new potential, with uncertainty quantification, for silicon heterostructures. The potential is tailored to describe thermal transport in specific morphologies which are of interest as thermoelectric devices [3, 4].

[1] S. L. Frederiksen, et al., Phys. Rev. Lett., 93(16), 2004.
[2] P. Brommer, et al., Modell. Simul. Mater. Sci. Eng., 23(7), 2015.
[3] H. Karamitaheri, et al., J. Appl. Phys., 113(20), 2013.
[4] H. Karamitaheri, et al., J. Appl. Phys., 115(2), 2014.