

酸化物固体材料のハイスループット力場構築と分子動力学シミュレーション：深層地震機構解明へ向けて

High-throughput force-field generation and molecular dynamics simulation of oxide solid materials: towards the study of deep earthquake

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Molecular dynamics (MD) method is a powerful simulation tool for studying atomistic mechanisms of phenomena that cannot be directly observed by means of microscopic experiments, and thus it is widely used in a variety of scientific field such as solid mechanics, fluid dynamics, organic/inorganic chemistry, macro-molecule folding, and even in economics. In MD, we simulate the motions of atoms by solving the Newton's equation of motion with using approximate interatomic potentials. The reliability of the simulation results is dependent on the accuracy of the interatomic potentials. Thus a lot of effort has been devoted to develop the interatomic potentials for Coulombic, covalent, metallic, dispersion interactions, etc. Normally one needs to optimize potential parameters to reproduce physical properties of target material and this process requires a lot of work and experience to guess which parameter affects a certain property the most, thus it takes time to start MD simulation of a target material. On the other hand, when applying the MD method to the discovery or screening of battery material candidates that could become huge number since there are tons of combinations of possible elements, we need to construct reliable interatomic potentials of many target materials very quickly and perform MD simulation to study their properties or screen the candidate material. For this purpose, we developed a methodology of producing interatomic potentials for solid-state electrolyte (SSE) materials in a high-throughput manner. In our method, meta-heuristic and/or bayessian approaches are used to optimize the parameters without the information of derivatives of loss function with respect to optimizing parameters. In addition to the optimization method, the potential parameters are optimized for not only the static physical properties such as formation energies, elastic properties, or lattice constants, but also for the distributions obtained from the dynamics simulation using the ab-initio calculation. This makes the potential accurate and robust for the dynamics of ions and it is shown that the optimized potentials well reproduce ionic conductivity obtained by the ab-initio calculations. This method can also be applied to produce the interatomic potential to study the mechanism of deep-earthquakes. We created a potential for Mg-Si-O ternally system that can well reproduce olivine and spinel structures whose phase transformations are considered to be associated to the deep-earthquakes. Some preliminary results of phase transformation under high temperature and high pressure condition are to be discussed in the presentation.

キーワード：分子動力学、シミュレーション、構造相転移、パラメータ最適化

Keywords: molecular dynamics, simulation, structure transformation, parameter optimization

