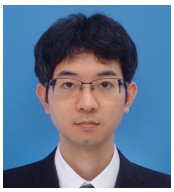
Materials development, Mechanical design

Quantitative atomistic simulation of structural materials using machine-learning interatomic potentials

Department of Mechanical Science and Bioengineering, Graduate School of Engineering Science

Professor Shigenobu Ogata Researchmap https://researchmap.jp/read0185246?lang=en

Assistant Professor Shuhei Shinzato Researchmap https://researchmap.jp/3201?lang=en



Abstract

We develop machine-learning interatomic potentials (MLIPs) trained on quantitative first-principles electronic-structure data (density-functional theory; DFT) and combine them with GPU acceleration to provide an atomistic simulation platform that remains accurate at the multi-million-atom scale. The platform enables pre-experimental, quantitative prediction of properties under extreme environments—such as hydrogen exposure and high temperature—clarifies structure–property relationships, and reveals atomistic details of deformation and fracture. It covers a broad range of structural materials, including high-entropy alloys, steels, conventional alloys, and ceramics, and treats the coupled behavior of dislocations, cracks, interfaces, and solute atoms within a single, consistent framework.

Background & Results

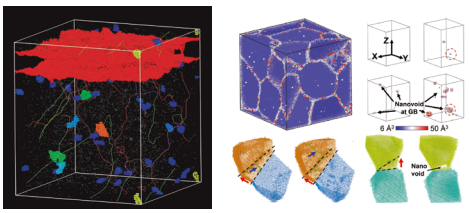
Designing, developing, and safely deploying next-generation structural materials in extreme environments requires atomistic simulation—alongside advanced characterization—to uncover causal mechanisms. In real materials containing multiple elements and operating in diverse chemical environments, where dislocations, cracks, interfaces, and interstitial or substitutional solutes interact in complex ways, quantitative prediction demands platforms that can track millions of atoms over long times. However, atomistic simulations based on first-principles electronic-structure calculations, while highly accurate, suffer from computational cost that scales roughly with the cube of system size, which limits application to realistic scales. Conversely, classical molecular dynamics using empirical interatomic potentials can handle large systems but cannot robustly describe bond rearrangement or changes in electronic structure, which constrains quantitative predictability.

To resolve this, we designed a neural-network-based MLIP tailored to structural materials by training on energies, forces, and stresses from first-principles calculations and combined it with GPU-based parallelization. The resulting platform preserves first-principles-level accuracy while approaching classical-MD efficiency, enabling million-atom models in which multiple lattice defects and solutes interact dynamically. Using the method, we visualized and quantified the interactions of hydrogen with dislocations and grain boundaries and clarified elementary processes underlying hydrogen embrittlement. In high-entropy alloys, we predicted the formation of chemical ordering during heat treatment and assessed its consequences for strength and ductility. For ceramics, we quantified plastic deformability and elucidated the atomistic mechanisms of plastic deformation and fracture. Together, these results provide new insights that directly inform experimental design and process optimization.

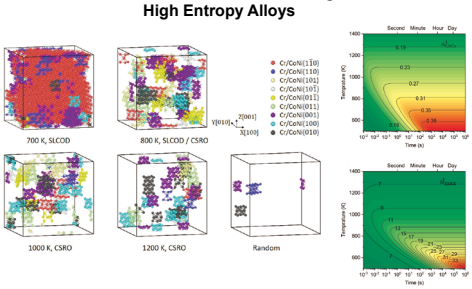
Significance of the research and Future perspective

Building high-accuracy, high-efficiency MLIPs breaks the long-standing accuracy–efficiency trade-off that has separated first-principles simulations and classical molecular dynamics, achieving their coexistence in practice. As a result, the approach enables reliable observation of material behavior and acquisition of quantitative data under conditions that are difficult to measure experimentally; pre-experimental prediction of properties in previously unexplored compositions and data-driven design of new structural materials; and tuning of processing routes to realize optimal properties. These capabilities are expected to accelerate the development of next-generation structural materials for extreme service environments. The methodology also promotes closer integration of simulation with measurement, creation of standardized materials databases, and broader industrial application.

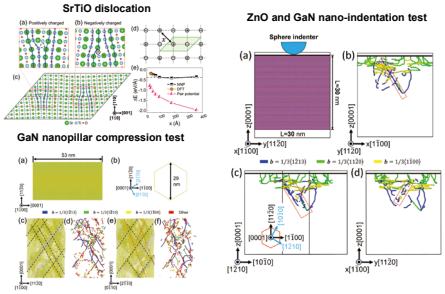
Hydrogen Embrittlement of Fe and Steel



Diffusion and Chemical Ordering in High Entropy Alloys



Plastic Deformation of Ceramics



Patent

Treatise

Meng, Fan-Shun; Shinzato, Shuhei; Matsubara, Kazuki et al. A neural network interatomic potential for the ternary α-Fe-C-H System: Toward million-atom simulations of hydrogen embrittlement in steel. JOM. 2025, 77, 8101-8117. doi: 10.1007/s11837-025-07721-4

Hossain, Rana; Ogata, Shigenobu. Unveiling kink band formation mechanism in MAX phases. Communications Materials. 2025, 6, 51. doi: 10.1038/s43246-025-00766-7

Zhang, Shihao; Li, Yan; Suzuki, Shuntaro et al. Neural network potential for dislocation plasticity in ceramics. npj Computational Materials. 2024, 10, 266. doi: 10.1038/s41524-024-01456-7

Li, Yangen; Du, Jun-Ping; Shinzato, Shuhei et al. Tunable interstitial and vacancy diffusivity by chemical ordering control in CrCoNi medium-entropy alloy. npj Computational Materials. 2024, 10, 134. doi: 10.1038/s41524-024-01322-6

Meng, Fan-Shun; Shinzato, Shuhei; Zhang, Shihao et al. A highly transferable and efficient machine learning interatomic potentials study of α-Fe-C binary system. Acta Materialia. 2024, 281, 120408. doi: 10.1016/j.actamat.2024.120408

URL https://tsme.me.es.osaka-u.ac.jp/index.html

Keyword atomic and molecular simulation, machine learning, structural materials