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Anharmonic thermo-elasticity of tungsten from accelerated Bayesian adaptive biasing force calculations with data-driven force fields

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The elastic properties of tungsten, a ubiquitous material in future energy systems, are investigated up to its melting temperature by means of a data-driven approach. The proposed workflow combines machine learning of the force field and enhanced sampling of the crystalline structure. While the machine learning force field achieves the accuracy of ab initio calculations, its implementation in sampling methods is often limited due to its high computational cost, which is commonly a few orders of magnitude larger than that of traditional potentials. To overcome this limitation, we propose a fast and robust Bayesian sampling scheme aiming at estimating the fully anharmonic free energy of crystalline solids with the help of an improved adaptive biasing force method. This method performs a thermodynamic integration from a harmonic reference system, wherein zero frequencies associated with the periodic boundaries are screened off. The proposed sampling method drastically improves the speed of convergence and overall accuracy. We demonstrate the efficiency of the improved method by calculating the second order derivatives of the free energy, such as the elastic constants, which are performed almost 100 times faster than with the standard methods. The proposed method enables the prediction of the elastic properties of tungsten in the range of temperatures that cannot be investigated experimentally, from 2100 K to the melting temperature. The accuracy and numerical efficiency of the proposed strategy open up many avenues for the reliable prediction of finite-temperature properties of materials, such as the relative stability of structural defects and elastic constants.

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