Capabilities and improvement ability of classical many-body potentials: application to hcp-Zr

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Abstract

Classical interatomic potentials (CIPs) have a low-to-intermediate number of parameters and fixed functional forms that are based on the physical understanding of the chemical bonding (1). Numerically lighter than machine learning potentials, they enable studies not otherwise accessible at the atomic scale, such as uncovering plasticity mechanisms, or validating mesoscale models of alloy mechanical properties (2). Identifying the CIP parameters for a specific material system/physical problem remains a challenging step, knowing that the flexibility of CIPs is limited. A better understanding of the actual capabilities of a given potential type to reproduce some target combination of properties would thus be relevant when selecting, using and/or fitting such a potential. In addition, ways to improve CIPs when their transferability is unsatisfactory are not clearly established.
In this work, we select the case of a many-body central force potential and investigate its ability to reproduce bulk and defect properties in hcp zirconium: hcp is a crystallographic structure for which angular dependence matters, yet simple central force potentials (EAM, FS, etc.) are still widely used in the scientific community for non-fcc metals. We first combine efficient model screening tools to a variance-based sensitivity analysis to establish some of the *intrinsic* limits of this class of CIPs. We recover the known effect of the potential cutoff on the accessible range of c/a ratios and various stacking fault energies (important for both plasticity and irradiation). Interestingly, the influence of CIP parameters is different from one property to another; in particular, vacancy and self-interstitial energetics are mostly affected by two distinct parameters. We therefore propose to use the results of sensitivity analysis to re-optimize existing CIPs and improve their transferability; this process is illustrated by refitting a CIP for the study of small irradiation defects in hcp-Zr. Finally, we discuss the applicability of our approach to (i) more complex interaction models with up to tenth of parameters (MEAM, BOPs, etc.) and (ii) the development of entirely new

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potentials (3).

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