Reinforcing materials modelling by encoding the structures of defects in crystalline solids into distortions cores

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A perfect crystal is a purely theoretical concept. Real-world crystals contain imperfections, also called defects. Identification and characterization of defects provide the crucial information for interpretation of simulations and experiments that bridge the gap between atomic- and micrometer-scales. But what is actually a concept of defects at the atomic scale? How to define the spreading of the defect within the crystalline lattice and to understand its impact on the energy landscape of materials? In this study, we try to answer these questions using machine learning (ML) methods and introduce a novel concept of the distortion scores of local atomic environments to reinforce the methods of atomic-scale materials modeling.

The distortion score of local atomic environments [1] describes a statistical distance from a reference structure, which, for example, can be a perfect crystal structure. Based on these distortion scores, we identify structural defects as atoms-outliers deviating from the reference structure. This score facilitates automatic localization of defects and enables their stratified description, which allows to distinguish the zones with different levels of distortion within the structure. The high sensitivity of the present approach to atomic displacement allows to detect the patterns produced by the of the elastic strain field around defects.

Beyond the localization of defects in the structure, the proposed concept of distortion scores has many advanced applications ranging from the surrogate concept for the energy per atom to the selection of the relevant structural information for the quantitative evaluation of energy barriers from the mean force. Moreover, this concept can serve for design of robust interatomic ML potentials and high-throughput analysis of their databases.

In perspective, this approach can be further extended for amorphous structures as well for interpretation of multivariate data provided by experimental techniques where the atomic coordinates are provided, such as atom probe tomography and transmission electron microscopy.

[1] A.M. Goryaeva *et al*. Nature Comm. **11**: 4691 (2020)