doi:10.1017/S1431927617001209
Microsc. Microanal. 23 (Suppl 1), 2017

A Framework to Learn Physics from Atomically Resolved Images

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The acquisition of atomically-resolved images of solid-state crystalline materials is now almost routine, due to tremendous advances in scanning transmission electron microscopy as well as scanning tunneling microscopy. However, the key step of translation from acquired imaging data to actual, tangible knowledge of the physical system requires consistent integration of experimental data with modeling. In most cases (if even attempted), this is still done in ad-hoc fashion with direct comparisons made between simulations and experiment, and a general framework remains elusive.

Here, we present a generalized framework for physics extraction, i.e., knowledge, from atomically resolved images, and show its utility by applying it to a model system of segregation of chalcogen atoms in an $FeSe_{0.45}Te_{0.55}$ superconductor system. We emphasize that the framework can be used for any imaging data for which a generative physical model exists. Consider that a generative physical model can produce a very large number of configurations, not all of which are observable. By applying a microscope function to a sub-set of this generated data, we form a simulated dataset on which statistics can be computed. The model optimization then proceeds via a comparison of the simulated data with the experiment, through a similarity metric termed statistical distance [1], i.e.

$$s = \arccos\left(\sum_{i=1}^{k} \sqrt{p_i}\sqrt{q_i}\right)$$

where p_i and q_i are the probabilities of finding outcome i in the measurement of systems P and Q, respectively, with the total of k possible outcomes. As an example, we attempt to model the segregation of the chalcogen atoms in an $FeSe_{0.45}Te_{0.55}$ superconductor by only considering the nearest-neighbor interactions between the Se and Te atoms. An STM image was acquired on a cleaved single crystal sample as seen in Fig. 1; the atoms displaying higher intensity correspond to Se and the atoms of lower intensity correspond to Te, as discussed in a previous publication [2]. Atomic position and type identification allows transformation to a coordinate system consistent with that of the $FeSe_{0.45}Te_{0.55}$ crystal lattice.

Based on the simple solid solution model of a single layer of interacting atoms of Se and Te, we use Monte Carlo simulations given the bulk composition value to generate equilibrium configurations that can be matched with the experimental data. One key difference in our approach is that we analyze the statistics of the resulting configurations from the model, comparing it with experiment via the statistical distance metric, and then reoptimizing the parameters of the model. This ensures that all the available information from the atomic image is used, as opposed to more trivial matching methods that generally lead to loss of information on configurations. The interaction model can be then optimized to reproduce this statistical information, which is collected in the form of histograms of different atomic configurations, as shown in Fig. 1.

This method can be used for any atomically resolved imaging data so long as a generative model exists, and thus allows knowledge extraction. This is especially important both because such a framework does not yet exist, but also as the knowledge gained e.g., interaction parameters between atoms, adatoms or vacancies, potential barriers for diffusion, etc. are often very difficult to compute from first principles methods. Further improvements can be foreseen, including the use of Bayesian inference for unbiased model selection, which can also provide uncertainty quantification [3].

References:

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[3] This research was sponsored by the Division of Materials Sciences and Engineering, BES, DOE (RKV, SVK). This research was conducted at and partially supported (SJ) the Center for Nanophase Materials Sciences, which is a US DOE Office of Science User Facility.

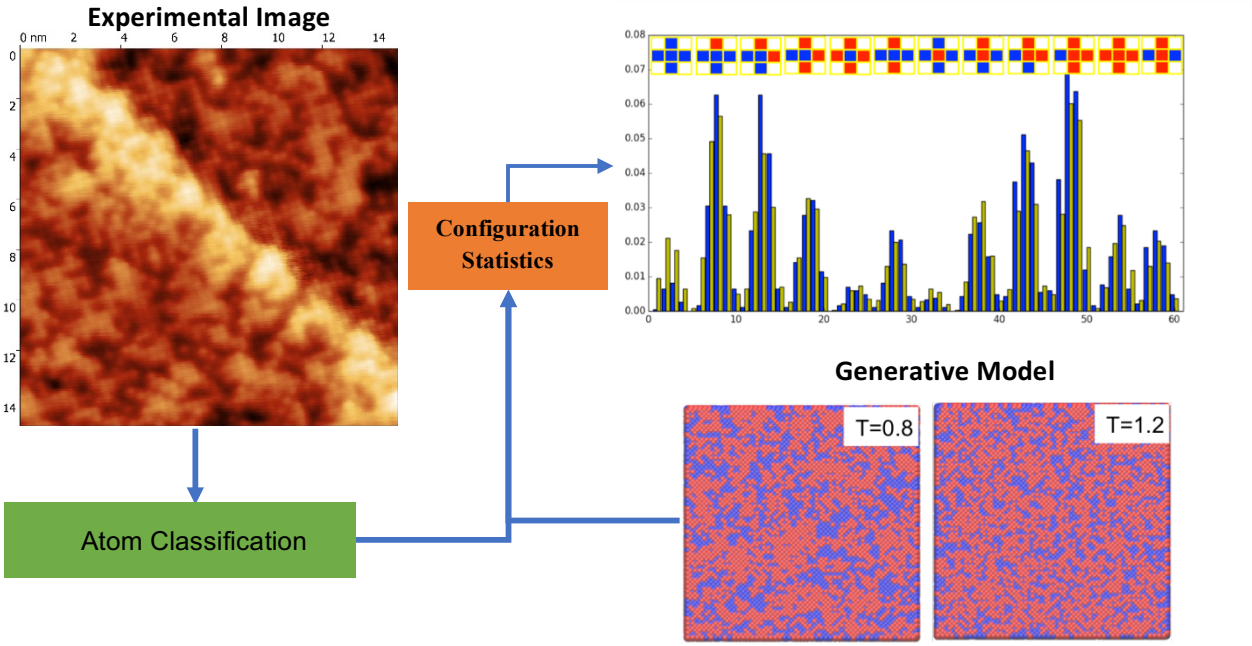

Figure 1. Framework for extraction of knowledge from atomically resolved imaging data. An atomically resolved image is acquired, e.g. via scanning tunneling microscopy, in this case, of $FeSe_{0.45}Te_{0.55}$. After classification of all atomic positions and types in the image, configuration statistics are generated. A generative model (e.g. interacting solid solution model, with only nearest neighbor interactions) is used to simulate data, and the statistics from the simulated data are compared via statistical distance. T refers to different temperature (parameters) used in the simulation.

https://doi.org/10.1017/S1431927617001209 Published online by Cambridge University Press