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Exploring Local Crystal Symmetry with Rotationally Invariant Variational Autoencoders

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Modern scanning transmission electron microscopy (STEM) is capable of routinely producing atomic resolution images with large fields of view. This is particularly true of annular dark field (ADF) images where low dwell times lead to high quality images without significant drift during the acquisition. Such images can contain thousands of atoms, especially if a focal series is taken. This makes the manual classification of local symmetries near atomic locations a time-consuming process. In this presentation we demonstrate the application of rotationally invariant variational autoencoders (rVAE) to classify different symmetries in atomic resolution ADF images.

The important first step to examine local symmetry is to locate (and possibly identify) each of the atomic locations in the image or image stack. This process is carried out using a suitably trained deep fully convolutional neural network (DCNN) which also carries out semantic segmentation of the image [1, 2]. In this process pixels are either categorized as associated with an atom or part of the background. An example of this segmentation process is shown in Fig. 1 where a single frame from a stack of images of $Sr_3Fe_2O_7$ is shown. Once the segmented image is found the position of each atomic column is determined to subpixel accuracy. These atomic locations are then used to define a stack of sub-images. The size of the sub-images is chosen to highlight the local symmetries around the atomic site. These must be determined on a case-by-case basis and depend on the magnification of the image and the nature of the symmetries we wish to determine.

The stack of sub-images is then used to train the rVAE. It is not the intention of this presentation to discuss the details of the rVAE algorithm, but rather the practical application of this methodology to material science systems. A more detailed discussion of the underlying principles may be found in reference [3] and its included bibliography. For our purposes, it is sufficient to say that once the rVAE is trained, it can be used to encode the data set (or in some cases, similar data sets) to provide information that is not readily obvious from the original real space images. In this case, the encoding of

the sub-images provides information about relative rotation of the sub-images and a number of "hidden" or latent variables. Other implementations may also encode information about off-sets of the sub-images, though those are not included here.

Shown in Fig. 2 are the encoded angle and two latent spaces obtained by encoding sub-images of 40-pixels from Fig. 1. The encoded angle and first latent space reflect the layered structure of $Sr_3Fe_2O_7$ while the second latent space reflects the thickness variation across the field of view. In this presentation, the interpretation of these results, and the importance of selecting a sub-image size commensurate with the image features will be discussed. In addition, application to other systems will also be shown [4].

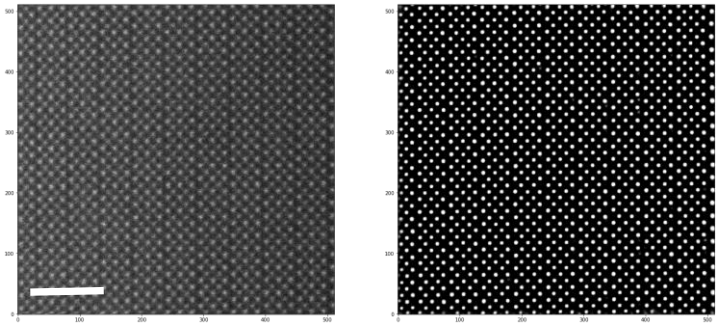

Figure 1. Left: A single frame from a stack of images of $Sr_3Fe_2O_7$. The scale bar is 2 nm. Right: The semantically segmented image.

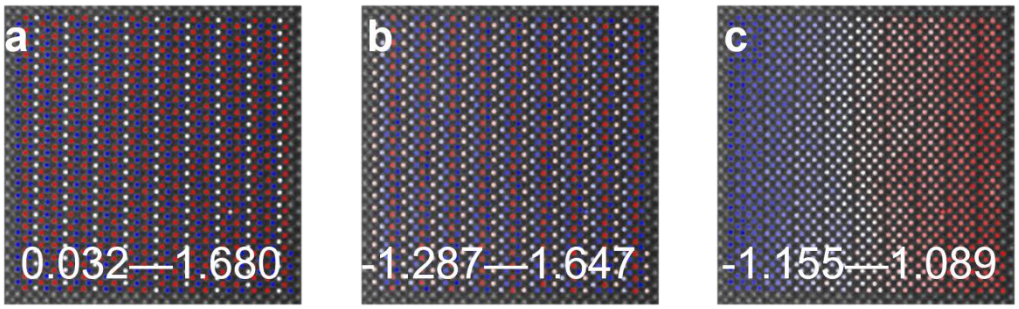

Figure 2. a The encoded angle of the sub-images from Fig. 1 for a 40-pixel sub-image size. **b**, **c** the latent spaces obtained using the rVAE analysis. Images adapted from ref. [3] under Creative Commons Attribution 4.0 International License http://creativecommons.org/licenses/by/4.0/.

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