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3D visualization of in situ nanoscale dynamics in transmission electron microscopy via self-supervised deep learning

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Background

In recent years, nanomaterials have seen widespread usage in fields as diverse as biomedicines, energy storage and catalysis due to their unique properties. The efficacy of nanomaterials for an application are significantly dependent on their physical and chemical properties. Electron tomography is an invaluable technique, which allows researchers to determine these properties in 3D by reconstructing a series of 2D projections collected at various angles (tilt series).1 However, the 3D spatial properties alone are insufficient to fully characterize nanomaterials and their application. In real world conditions, material properties are rarely static and they change as a result of environmental conditions such as pressure, heat and chemical reactions.2,3 To fully characterize the dynamic behaviour of materials, researchers must move towards 3D volume + time characterizations. Unfortunately, collecting a single tilt series for electron tomography can take about an hour, resulting in loss of temporal information and motion blurring artefacts in the resulting reconstructed volume. Herein, we propose a novel reconstruction method that uses a deep image prior self-supervised neural network (DIP-NN)4 to determine the 3D volume as a function of time. This allows researchers to collect a series of 3D volumes with a temporal resolution of less than a minute.

Methods

To reconstruct a volume time series, 1D slices of the tilt series were used as an input to the DIP-NN. Each slice was mapped to a depth and time coordinate. A 2D orthoslice of the reconstructed volume-time series was predicted for the specified coordinates. To train the network, the orthoslice was forward projected and compared back to the original tilt series. During the reconstruction, the volume-time series is reconstructed slice-by-slice, until the full volume-time series is acquired (Figure 1). Hence, for every 2D image collected in the tilt series a full 3D volume was acquired at the same time of acquisition. This methodology was used to reconstruct simulated nanoparticles with morphological and compositional changes and experimental Au/Ag nanoparticles that were subject to changes in both shape and alloying as a result of in situ heating during electron tomography.

Results

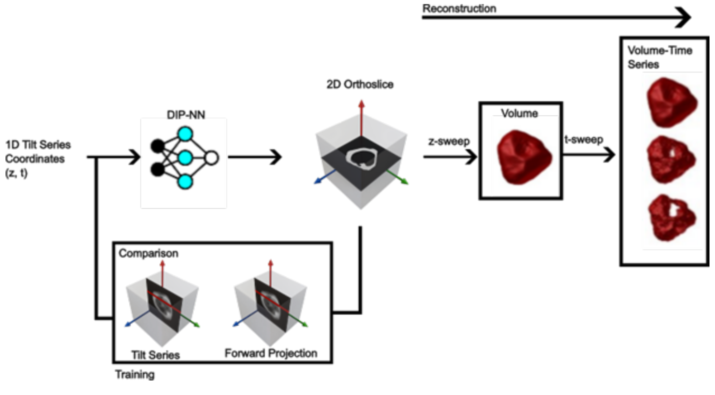
In both the simulated and experimental cases, a significant improvement was observed in temporal resolution compared to conventional tomography. In the simulated case, a set of 100 images in the tilt series was used to reconstruct a set of 100 volumes, where only one would be acquired using conventional electron tomography. In the experimental case, we were able to obtain a frame rate of approximately 1 volume per minute, far outpacing even fast tomography. In both experimental and simulated cases, the reconstruction quality, determined based on the signal-to-noise ratio and the structural similarity index, were comparable to conventional tomography.

Conclusions

Herein, a machine learning method is presented which allows the reconstruction of a series of 3D volumes with a temporal resolution of less than a minute. Unlike supervised machine learning approaches, this method can be trained solely from the acquired tilt series. This method was validated with both simulated and experiment studies on Au and Ag nanoparticles during heating.

Figure 1. DIP-NN algorithm takes in 1D slices of the tilt series using the coordinates for the depth (z) and time (t) to predict a 2D orthoslice of the reconstruction at the same coordinates. For training, this 2D orthoslice is forward projected and compared back to the tilt series. To reconstruct a full volume time series, the 2D orthoslices are stacked slice by slice for every z and t value.

Graphic:



Keywords:

Tomography, Deep Image Prior, Dynamics

Reference:

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