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Machine Learning Based Tracking of Single Nanoparticle Vibrations from a Projected 3D Moiré Lattice

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Machine learning (ML) methods, especially those algorithms based on convolutional neural networks, have been increasingly utilized in the processing and statistical analysis of liquid-phase transmission electron microscopy (TEM) movies. The tasks that have been achieved include the segmentation of nanoparticles (NPs) out of noisy and fluctuating liquid background [1], and "anatomy" of nanoparticle trajectories into fractions of different diffusion modes [2]. In these studies, NPs move in two-dimensions (2D) or assemble into 2D structures, without complications such as vertical feature overlap in the projected TEM images. Meanwhile, recent advancements in controlling NP concentration and interfacial interactions have led to liquid-phase TEM observations of complex 3D lattices composed of NPs [3,4], where multiple lattice layers are collapsed as interlocked NP patterns in projection, poising challenges in analyzing their structure, assigning the NPs in 3D to different layers, and understanding their growth and relaxation dynamics.

Here we demonstrate the training and application of a U-Net neural network to successfully individualize projected and overlapped NPs in a Moiré lattice formed from two hexagonal layers of NPs registered with a misalignment angle. Here the liquid-phase TEM movies were captured on a Hitach 9500 TEM equipped with a Hummingbird liquid holder and Gatan GIF camera. The raw images show complex Moiré patterns, which are hard for humans to manually assign a feature to the NP belonging to a specific layer at nanometer resolution. We established a library of liquid-phase TEM images (>400) simulated from the electron-optics principles of TEM, of Moiré lattices of varying lattice constants, inter-NP spacing, and misalignment angles as the training dataset for a U-Net neural network. The neural network was customized to have two output channels, each corresponding to the NPs belonging to one lattice layer. Using the trained U-Net, we were able to successfully decompose the projected TEM movies into two movies (Fig. 1), each containing only one lattice layer. The individual NP shape and position were determined at nanometer precision, which allows us to further analyze the local vibrations of single NPs at the lattice site, and the analyze of the lattice structure as well as defects (point defects, twin boundaries) in each layer, which are all related to the growth mechanism of the Moiré lattice, and possible applications in their photonic and mechanical properties [5]. We foresee this idea of utilizing ML to decipher 3D structures as a means to understand 3D structures captured as 2D projections, when conventional 3D imaging such as tomography simply does not match with the time scale of dynamics in in-situ TEM imaging [5].

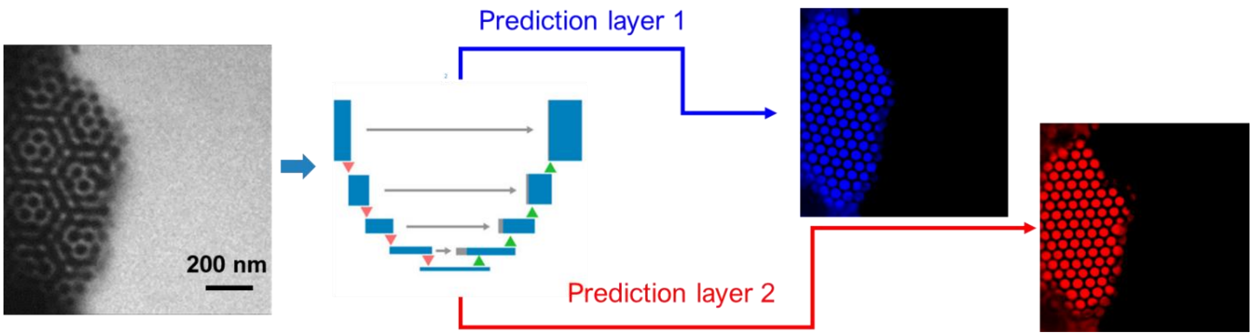

Figure 1. ML based NP tracking from a liquid-phase TEM image of a Moiré lattice. From left to right: a liquid-phase TEM image of an assembled Moiré lattice, schematic of the architecture of U-Net neural network, and the tracked NPs assigned to the two hexagonal lattices overlaying into the Moiré lattice.

References:

[1] L Yao et al., ACS Cent Sci **6** (2020), p. 1421.
[2] V Jamali et al., Proc Natl Acad Sci USA **118** (2021), p. e2017616118.
[3] Z Ou et al., Nat Mater **19** (2020), p. 450.
[4] E Cepeda-Perez et al., Sci Adv **6** (2020), p. eaba1404.
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