Determining Diffusion Characteristics of Nanoparticles in Liquid Phase TEM Using Deep Learning

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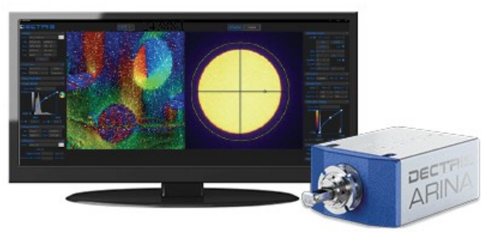
DECTRIS

ARINA with NOVENA

Fast 4D STEM



DECTRIS NOVENA and CoM analysis of a magnetic sample.

Sample courtesy: Dr. Christian Liebscher, Max-Planck-Institut für Eisenforschung GmbH.
Experiment courtesy: Dr. Mingjian Wu and Dr. Philipp Pelz, Friedrich-Alexander-Universität, Erlangen-Nürnberg.

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Meeting-report

Determining Diffusion Characteristics of Nanoparticles in Liquid Phase TEM Using Deep Learning

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The motion and dynamics of nanoscale particles and macromolecules in liquid environments are of paramount importance across scientific disciplines. Liquid phase transmission electron microscopy (LPTEM) enables real-time observation of such dynamics at nanometer scales. Thus, there has been a lot of interest recently in developing LPTEM as a single-particle method. However, the collected trajectories from LPTEM movies are typically short, and as such identifying their underlying mechanism and quantifying their diffusion characteristics (e.g., anomaly exponent, diffusion coefficient) of motion using canonical statistical tests become challenging. Addressing this challenge has led to the development of supervised deep-learning algorithms to identify the underlying mechanism of motion. [1-3]. The state-of-the-art algorithms are capable of identifying ideal stochastic models that are best matched to the experimental data by classifying the trajectories into discrete classes such as Brownian, Fractional Brownian Motion (FBM), and Continuous Time Random Walk (CTRW). Yet, the majority of real experimental trajectories are a mixture of different anomalous diffusion types and different levels of anomaly (e.g., sub-diffusivity) [1, 4, 5]. In such cases, we aim to understand not only the classes present but the contribution from each class as they contain information about the physics of the environment at different regimes of length and time scales.

In this study, we introduce a new supervised deep learning framework designed to determine the contribution of anomalous diffusion classes and their anomalous exponents in single particle trajectories from LPTEM. Unlike traditional methods that output the probability of a trajectory belonging to a discrete diffusion class, our model outputs a continuous mixing ratio of the diffusion classes and their corresponding anomalous exponents. We employed a dilated convolutional deep neural network architecture trained on a large and diverse dataset of simulated trajectories representing a mixture of behaviors with different anomalous exponents. We applied the model to a comprehensive LPTEM dataset containing trajectories of gold nanorods dispersed in water, moving near silicon nitride membrane of liquid cell across a range of conditions. Notably, the model effectively discerns the mixing factors corresponding to the contribution from classes such as FBM and CTRW within the trajectories, along with estimating the true anomaly exponent values characterizing each component's behavior. Our findings reveal nuanced time-dependent diffusion dynamics of gold nanorods, indicating transitions between FBM and CTRW regimes in time influenced by the surrounding environment.

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