Monitoring Structural dynamics Using In Situ Electron Microscopy

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Monitoring Structural dynamics Using In Situ Electron Microscopy

T. Frontiers of in-situ materials characterization - from new instrumentation and methods to imaging aided materials design

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Abstract

Development and tailoring of new materials and solutions within chemistry, electronics, and pharmaceuticals require a deeper understanding of atomic-scale structure as well as structural changes induced during use in real-world operating conditions. Such materials find uses in the energy sector where, advanced nanomaterials are used in for example energy storage, power-to-X catalysts. In pharmaceuticals, tailored materials can be used in controlled drug release and as therapeutic carriers. A core challenge in characterizing such materials is how do to obtain detailed atomic-resolution images of systems and devices under real-world conditions, without affecting them by the imaging process? State-of-the-art transmission electron microscopy techniques can obtain sub-angstrom spatial resolution and high spectroscopic and temporal resolution datasets of devices operating in gas or liquid environments. However, making these observations relevant to real world applications requires minimization of electron beam effects and reliable analysis of data acquired under low electron dose rate conditions. Minimizing electron dose rate during data acquisition reduces the impact of imaging but at the cost of a reduced signal to noise ratio of the acquired data. The result is often that the data becomes noisy and that features become unrecognizable to the naked eye. An automated data analysis approach which has gathered significant traction over the last decade is machine learning and convolutional neural networks.

Well-trained networks, where noisy data is included in the training set. have shown promising performance, even on data acquired *in situ*. Using well-trained convolutional networks, we have successfully identified the dynamic atomic column positions in a gold nanoparticle imaged in 4.5 Pa carbon monoxide at 300°C [1, 2]. Analyzing sequences of such frames reveals the dynamic nature and structural variations due to changes in the local environmental conditions. Data analysis by means of convolutional neural networks has also proven efficient for analyzing images of low-Z materials with poor contrast. Using a convolutional network trained on synthetic data, the dynamic nature at the surfaces of graphene sheets as well as the structural tension in the vicinity of a hole in a graphene sheet could be mapped. The data was acquired at low acquisition times and summed to obtain images which could be analyzed with high accuracy [3, 4].

In this paper, we will discuss approaches to observing dynamic phenomena on nanostructures such as catalysts and 2D materials *in situ* using transmission electron microscopy.

References:

[1] P. Liu, J. Madsen, J. Schiøtz et al., J. Phys.: Mater. 3 (2020), 024009.

[2] P. Liu, T. T. Wu, J. Madsen et al., Nanoscale 11 (2019), 11885-11891.

[3] J. Madsen, P. Liu, J. Kling et al., Advanced Theory and Simulations 1 (2018), 12.

[4] J. Madsen, P. Liu, J. B. Wagner et al., Adv. Struct. Chem. Imag. 3 (2017), 14.