Characterization of Multi-Functional Materials at the Atomic-Scale: New Approaches to In-Situ Microscopy

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The last few years have seen a paradigm change in the way we characterize materials, with unprecedented improvements in both spatial and spectroscopic resolution being realized in current transmission electron microscopes (TEM). When multi-modal X-ray and electron imaging is combined with density-functional theory (DFT) calculations, the effects of defects, dopants or strain at grain boundaries or interfaces can now be directly determined and correlated to electronic/thermal transport properties. While spatial and energy resolutions better than 60 pm and 10 meV have been reported, aberration-corrected TEM has also enables a large variety of in-situ experiments at close to atomic resolution. Using this approach, the intercalation of multi-valent ions into cathode materials, the dynamics of vacancies, and the interactions between gases and nano-particles can now be directly observed, to only mention a few examples.

Here, I will demonstrate how in-situ multi-modal characterization and DFT modeling can be used to unravel the fundamental structure-property relationship of grain boundaries in photovoltaic CdTe devices or the intercalation of Mg-ions in transition metal oxide cathodes. I will further introduce a novel approach to measuring temperature and thermal expansion in nano-scale materials using electron microscope. I will also show how our recent development of graphene-based liquid cells now enables the direct characterization of biological materials and solid-liquid interfaces at close to atomic-resolution. I will conclude by discussing my vision for the future of high-resolution transmission electron microscopy, including monochromated electron-sources, new data processing approaches for low-dose microscopy as well as operando multi-modal methods combing x-ray and electron scattering.