

Multimodal Chemical and Functional Imaging of Nanoscale Transformations Away from Equilibrium

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The key to advancing energy materials is to understand and control the structure and chemistry at interfaces. While much of the dynamic chemistry can be studied on macro-scale systems, there is a lack of means to localize chemical measurements and correlate them to nanoscale structure of the material. Through a unique merger of advanced scanning probe microscopy and mass spectrometry techniques rooted in innovative data processing and control algorithms, we are now able to understand the interplay between chemical and physical functionality at the fundamental length using multimodal chemical imaging. This multimodal imaging transcends existing techniques by providing nanoscale structural imaging with simultaneous quantitative nanomechanical properties and quantitative chemical analysis. In this talk I will discuss how we have developed and used this capability to visualize dynamic material transformations at interfaces, to correlate these changes with chemical composition, and to distil key performance-centric material parameters [1]. One exciting capability is that the AFM can be used to drive materials away from equilibrium at the nanoscale with highly localized electric fields (Figure 1). This allows field confinement effects on localized chemistry in materials to be locally probed, especially at interfaces. This in turn yields direct information on key energy related questions such as electron and ion motion distribution and transport at and between interfaces. We have applied this approach to the study of systems and processes that underlie energy capture, conversion and storage, including photovoltaics and oxide ferroelectrics, which have historically eluded comprehensive understanding of the mechanisms behind the spatially heterogeneous interfacial chemistry and its link to material performance [2]. Overall, I will focus on ways to unlock the mystery of active interface formation through intertwining data analytics, nanoscale elemental and molecular characterization, with imaging; to better grasp the physical properties of materials and the mechanistic physics-chemistry interplay behind their properties [3].

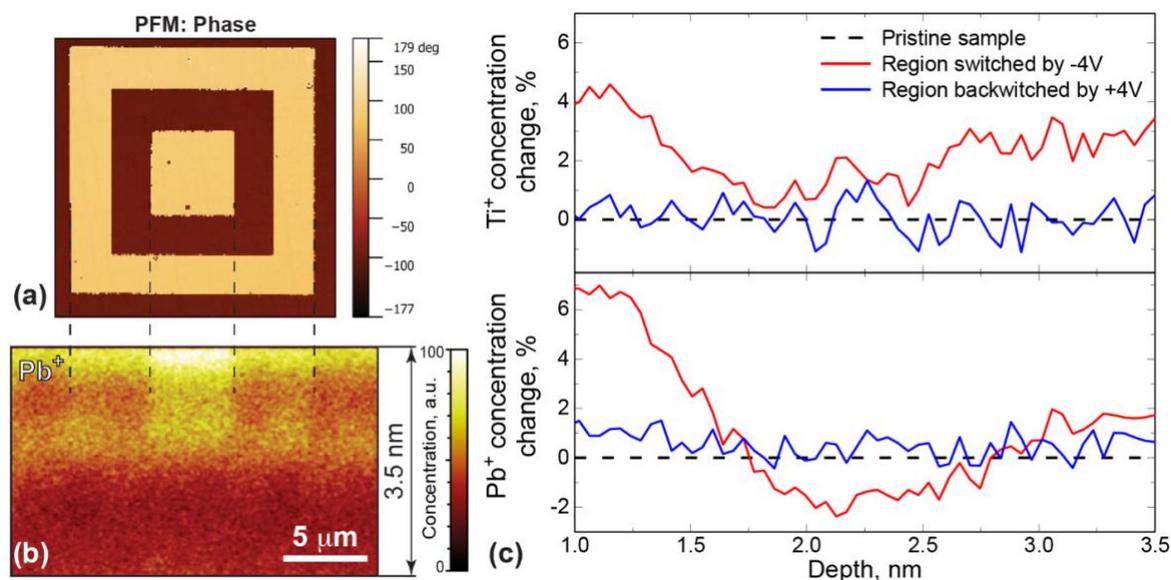


Figure 1. Local chemical changes in the bulk of PZT film, induced by local polarization switching. (a) PFM phase of polled regions; (b) corresponding ToF-SIMS X-Z map of Pb^+ distribution; (c) depth profiles of local concentration changes with respect to the pristine sample of Ti^+ (*top plot*) and Pb^+ (*bottom plot*) within outer square switched by negative bias (*red line*) and middle square backswitched by positive bias (*blue line*).

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- [2] Maksymovych, P.; Jesse, S.; Yu, P.; Ramesh, R.; Baddorf, A. P.; Kalinin, S. V., Polarization Control of Electron Tunneling into Ferroelectric Surfaces. *Science* **2009**, 324 (5933), 1421-1425.
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