Data mining atomically resolved images for material properties

This challenge is driven by efforts in Scanning Transmission Electron Microscopy to expedite materials data analysis, and generate insight into physics and chemistry of 2D materials irradiated by the electron beam.
Scanning transmission electron microscopy (STEM) and associated spectroscopies are well established, robust imaging tools that have proved to be powerful in visualization of structure and functionality of materials with atomic resolution.1 2 The ultimate goal of localized imaging and spectroscopy is to observe and quantitatively correlate structure-property relationships with functionality – by evaluating chemical, electronic, optical and phonon properties of individual atomic and nanometer-sized structural elements.3 Historic improvements in the underlying instrument hardware and data processing technologies has allowed determination of atomic positions with sub-10 pm precision4, 5 which enabled the visualization of chemical and mechanical strains,6 and order parameter fields including ferroelectric polarization7-10 and octahedral tilts.11-15 Ideally, complete studies have to be performed as a function of global stimuli, such as temperature or uniform electric field applied to the system, as well as local stimuli that are induced by additional electron probe interactions.16-18 Furthermore, this technical combinatorial instrumentation challenge is exacerbated by a wealth of extracted information at both global and local scales necessitating a drastic improvement in capability to transfer, store and analyze multidimensional data sets.

In this challenge, contestants will be supplied with a short atomically resolved movie, 49 individual frames, which illustrate MoSe2 film evolution under the electron beam. We are interested in the motion of the Mo and Se atoms captured throughout the movie. The positions of the atoms and their trajectory will serve as inputs to a Density Functional Theory simulation to reveal the details of the beam-matter interaction, as well as material reconstruction and vacancy formation mechanisms associated with beam induced stress.

Challenge

1. Identify all atom centers in a single frame, with a robust scaleable algorithm capable of identifying all atomic centers in all movie frames. Deliverables: A matrix of X, Y positions for every atomic center in Frame 1, and/or A 3D matrix of X, Y positions for every atomic center in all frames.
2. Identify and label every atomic center common to all frames. Deliverables: A matrix of X, Y locations for atomic centers that can be found in all 49 frames. Each center needs to carry a unique identifier allowing the same atomic to be referenced in any of the 49 frames.
3. Create a vector map of atomic motion for each of the uniquely identified atomic centers common to all 49 frames. Create a graphic that captures trajectories for all atomic centers common to the movie. Deliverable: A vector array of X, Y positions for each uniquely identified atomic center throughout all the movie frames. A graphic illustrating full 49 frame trajectory for one, some, or all atomic centers.
4. Molybdenum and Selenium have different intensities in the image. Selenium atoms are ~8% brighter than the Molybdenum. Furthermore, in an ideal crystal, the locations of Mo and Se atoms in any hexagon in the image are rigidly defined in what can be defined as “upwards and downwards facing triangles,” see Figure 1, of Mo and Se atoms. In this challenge we are interested in identity of the labeled atoms common to all frames. Identity can be determined from intensity, crystallographic orientation, or both. Deliverable: A vector array of X, Y positions for each uniquely identified atomic center throughout all the movie frames, labeled as either Mo, Se, or Unknown. A graphic illustrating full 49 frame trajectory for one, some, or all atomic centers for either Mo, or Se species.

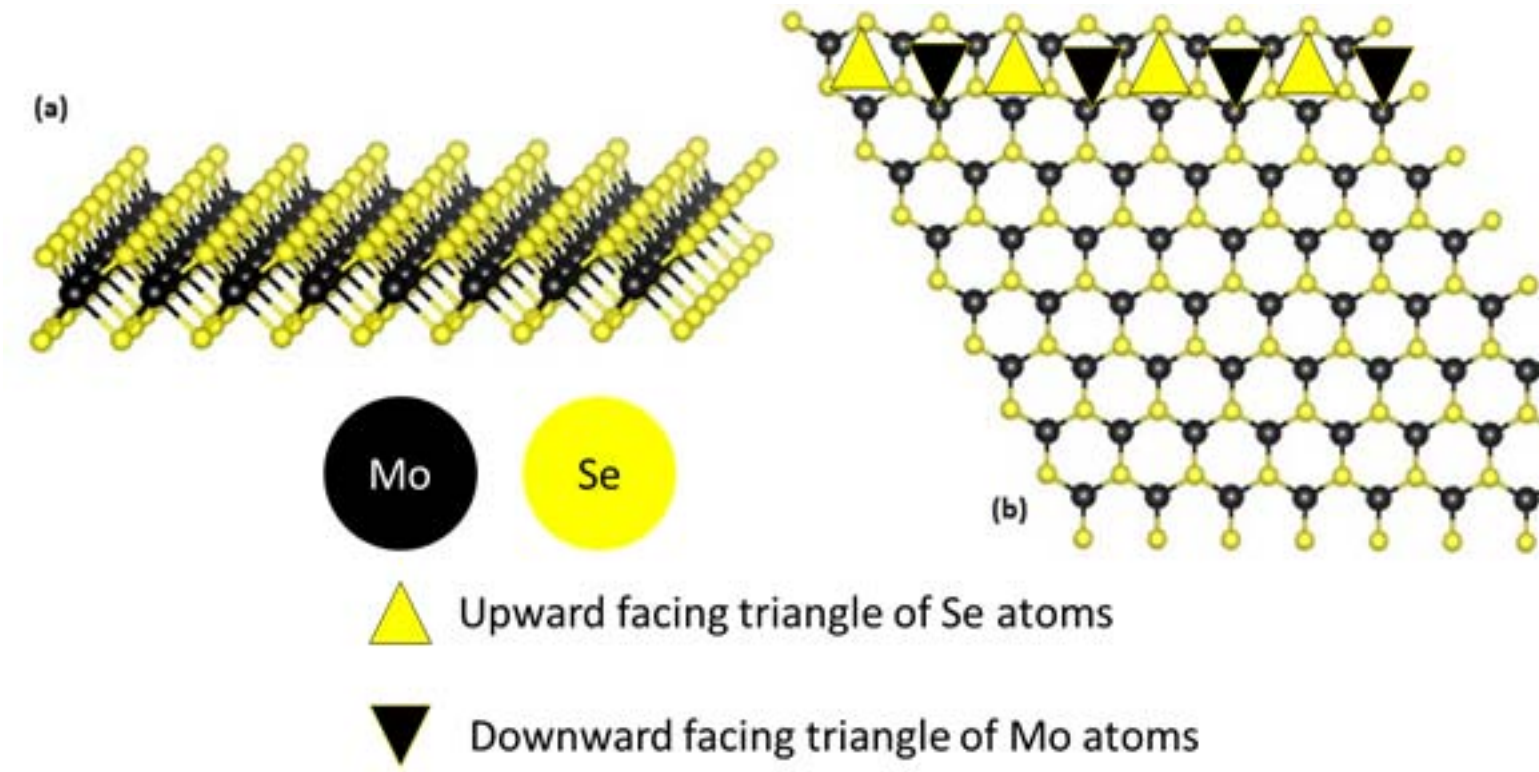

Figure 1. (a) Structure of a hexagonal MoSe2 monolayer. Mo atoms are in black and Se atoms are in yellow. (b) A hexagonal MoSe2 monolayer seen from above.

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