Although many of the physical properties of materials are strongly dependent on the structure's atomic disorder, direct measurement of such disorder can be difficult, especially where the materials are nanostructured or as thin films. However the small (nm-sized) probe available in a TEM, together with the sensitivity of electron diffraction intensities to even small atomic displacements makes it an ideal method to analyse the disorder in modern materials.

One of the major difficulties for accurately simulating electron diffraction patterns from disordered structures is the need to include dynamical scattering. Using GPU processing, a version of the multislice code has been developed to allow these dynamical simulations to be performed in a time-effective manner [1]. This has enabled a number of studies to be performed on different materials systems that exhibit disorder and lattice vibrations.

The first of these described here is on TIPS-pentacene, a high performance organic semiconductor [2]. Here a lattice vibration arising from a transverse displacement of the conductive pentacene molecule was determined from electron diffraction patterns (shown in Figure 1a) together with a refinement of the ensemble of pentacene fragment displacements (shown in Figure 1b). This provided direct evidence in support of molecular dynamics simulations, which allowed interpretation of the reported transport properties. This has led to the investigation of a family of related pentacene derivatives, such as TMTES-pentacene, with additional significant lattice vibrational modes. An example of the more complex diffuse scattering in this material is shown in Figure 1c, with a dynamical simulation shown in Figure 1d).

Another disordered system under study is lithium vanadate [3]. This is a layered oxide into which lithium ions can intercalate, making it a candidate material for high density lithium ion battery electrodes (replacing the current graphite electrodes that offer very poor stored charge density). There are a number of static disorder mechanisms occurring in the material (a typical electron diffraction pattern is shown in Figure 2a), involving both the vanadium oxide lattice as well as the lithium distribution through the material. Preliminary simulations to identify these different diffuse features (for example in Figure 2b) show how this approach will be used to describe the complete structure of this material.


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Fig. 1: Electron diffraction patterns indicating diffuse scattering from a) TIPS-pentacene with b) dynamical scattering simulations. c) Experimental diffraction from TMTES-pentacene with d) scattering simulations.

Fig. 2: a) Experimental diffraction pattern recorded from lithium vanadate parallel to [010], b) dynamical simulations of the diffuse streaks (indicated by dotted lines) found in this pattern.