Composite modulated structures of electrode materials for rechargeable alkali-ion batteries

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Electrode materials in rechargeable alkali-ion batteries, that follow a solid-solution mechanism, change composition over very large ranges while maintaining their structure type. This is strongly reminiscent of compositionally and displacively flexible systems that form incommensurate composite structures (see Figure 1) [1].

A number of examples have appeared in the recent literature where materials with potential as rechargeable Na-ion battery electrodes have formed modulated structures in certain composition ranges [2-4]. In the case of Na$_x$VO$_2$ is has been concluded that a modulated structure forms, based on evidence from in-situ X-ray diffraction data [2-3]. With a [3+1] dimensional incommensurate composite structure approach, the mismatch between potential metal-oxide and Na-ion substructures may be linked directly to the overall, apparently non-stoichiometric, composition.

This presentation will review the evidence for modulated structures in battery materials and draw on examples from both our own work and that of others and discuss these in light of a more common occurrence of such structures.

Figure 1: Schematic of electrode, with changing ion concentration, whose structure is best described using a modulation function. Alkali ions are located where the modulation function (vertical centre) has maxima, with the wavelength changing continuously with ion content ($x$).