Insights on the disordered nature in amorphous-based anode materials from Electron Pair Distribution Function

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In the field of material science, the ability to determine structures at high spatial resolution is paramount for understanding their properties. While traditional X-ray and electron diffraction techniques have been successful in determining crystalline structures, the need for new techniques is evident. Conventional methods fall short in providing detailed structural information for disordered structures, such as those found in nanostructured and amorphous materials, making our research on the disordered nature of anode materials all the more significant.

The pair distribution function (PDF) method based on X-ray and neutron diffraction is widely employed for providing quantitative information in amorphous materials [1]. Nonetheless, understanding medium-range structural order in amorphous materials is non-trivial, where the position of atoms cannot be assigned by any equation based on translation vectors. Electron Diffraction (ED) related PDF (ePDF) in Transmission Electron Microscope has the advantage of investigating ordering locally. However, ePDF-based analyses may be affected by dynamical effects, altering the scattering intensities.

This work aims to expand the developed methodology to battery materials research by employing electron diffraction data to obtain PDF coupled with low-loss electron energy loss spectroscopy [2]. This will enable us to delve into the role of volume expansion during lithiation in silicon-carbon-based anode materials, which is a crucial aspect of the electrode's functioning.

Keywords:

S/TEM, ePDF, EELS, batteries

Reference:

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