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Novel CBED Methods for Structure Analysis

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In modern electron microscopes, with field emission sources and good condenser optics, the electron beam can be focussed into a probe less than a nanometre in diameter. With the addition of an aberration corrector, the probe size can be further reduced to less than an Ångström. Such small probes enable diffraction and spectroscopic data to be obtained selectively from within individual nanoparticles. Because the probe is focussed, the diffraction data manifests itself as a convergent beam electron diffraction (CBED) pattern. Each disc provides a two dimensional map of the intensity of the scattered beam versus the orientation of the incident beam. As such, the CBED pattern contains a wealth of information about the specimen and well established methods exist for extracting this information to determine space groups, bonding, lattice parameters, Debye-Waller factors, strain, dopant-site occupancy and other structural parameters [1].

In this paper, we consider novel scattering geometries in CBED that enable access to specific and important structural information in convenient and practicable ways.

One such powerful geometry is that of 3 beam diffraction, whereby only 2 diffracted beams come near the Bragg condition simultaneously (Fig. 1). Under such conditions, for centrosymmetric crystals, both the phase and the magnitude of the three structure amplitudes are determined uniquely by the distribution of scattered intensity in the 3 beam CBED pattern [2,3]. In particular, the phase (specifically, the three-phase invariant) can be determined by inspecting the pattern and the magnitudes can be determined from three distances measured on these patterns (Table 1). The experimental conditions under which these results can be exploited will be discussed quantitatively.

Another advantageous geometry is that which excites a quasi-zone axis arrangement of lower order Laue zone (LOLZ) reflections. Here the crystal is oriented such that the Ewald sphere is tangential to the plane of reciprocal lattice points beneath the zero order layer. The resulting two dimensional array of CBED discs contain striking lines of contrast (Fig 2) which can be understood in terms of the interaction of a near systematic row of zero order Laue zone reflections with a LOLZ dispersion surface [4]. That is, the lines in each disc provide a map of sections of the dispersion surface, with each line being linked with a specific eigenvalue associated with the dynamical interaction of the LOLZ reflections. The sensitivity of these lines of contrast to specific structural information, such as information about the structure in the direction parallel to the incident electron beam, will be discussed. Examples of how this contrast could be applied experimentally to obtain structural information from small specimen volumes will be presented.

References
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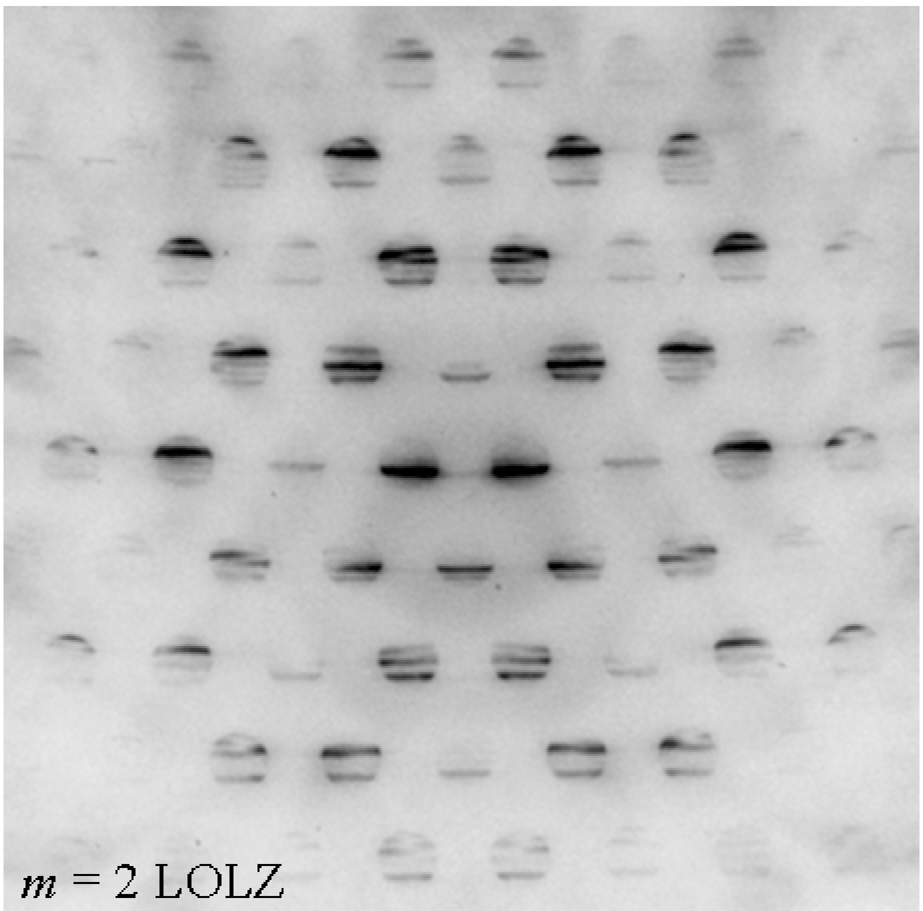

FIG. 1. Experimental LOLZ CBED pattern of $Ba_3Ti_2RuO_9$ showing lines of contrast in each disc associated with the dispersion surface generated by dynamical lower layer line interactions.

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