Determination of structures from defined nanocrystalline regions by scanning nanobeam diffraction tomography

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Crystallography is intrinsically limited by its reliance on signal averaged over large collections of perfectly ordered molecules within a single crystal lattice or even across multiple crystals. This is limiting when crystals contain severe disorder pathologies or are beam sensitive. Recent advances in electron diffraction have reduced the minimum size of crystals useful for structure determination to 100s of nms[1–3], overcoming many of these limitations. Scanning nano-beam diffraction has been applied to the study of nanomosaicity within a single micron-scale crystal[4], illustrating the benefit of scanning nano-beams for structure determination. We demonstrate that scanning a sub-10nm electron probe over a peptide nanocrystal at multiple orientations yields a collection of patterns that represent a full tilt series across reciprocal space. Use of a direct electron detector allows meaningful intensities to be extracted from sparse, individual diffraction patterns; this reduced data is sufficient for phasing by molecular replacement and compares favorably with data collected by selected area diffraction. Scanning nanobeam diffraction can be collected from regions of a crystal as small as 40nm, allowing for the fine sampling of specific areas within a single crystal. This approach has implications for circumventing polycrystallinity, reducing radiation damage and accessing the ensemble of structures present within a crystal.

References

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