

Aperiodic crystallography from 3-dimensional electron diffraction using kinematic and dynamical approaches

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Aperiodic structures are fascinating due to their unique way of creating a long-range ordering of atoms, ions, or molecules. Beyond producing hypnotic diffraction patterns, aperiodic materials appear across various research fields, showcasing a wide array of properties. To fully understand local crystal chemistry and the associated physicochemical properties, it is essential to characterize and take into account the modulations present in these structures. However, solving the structures of such materials remains a niche within crystallography, primarily accessible through single-crystal X-ray diffraction (SCXR). For crystals that do not meet the criteria for SCXR analysis, three-dimensional electron diffraction (3D ED) techniques have proven effective in addressing crystallographic challenges for sub-micrometric scale samples that conventional X-ray diffraction cannot reach, sometimes revealing even finer details than X-ray methods, such as chirality and improved contrast for light atoms [1-2]. In the realm of aperiodic crystallography, 3D electron diffraction is particularly well-suited for detecting and characterizing the symmetry and structure of modulated structures. This suitability arises from the sensitivity of electron diffraction to weak, subtle features in reciprocal space, along with the dynamical effects that enhance the intensity of satellite reflections. Over the last decade, substantial and continuous advancements in 3D ED data acquisition, data reduction, and the application of the dynamical theory of diffraction in structural refinement are gradually bridging the gap between single-crystal X-ray diffraction and 3D ED, making 3D ED an increasingly self-sufficient technique [3]. The unique aspects of aperiodic crystallography achieved through 3D ED will be illustrated with examples of incommensurately modulated samples, including minerals [4], biominerals [5], intermetallics [6], and long-period stacking ordered materials [7] (Fig. 1).

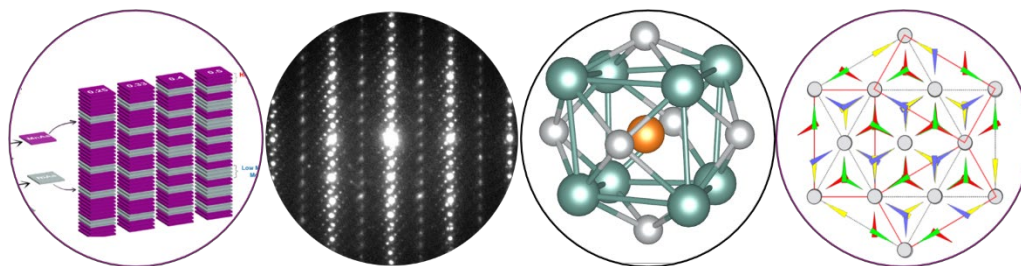


Figure 1. examples of modulated compounds solved from 3D ED

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