Bruker / MIT Symposium 2022

ANALYZING MODULATED STRUCTURES IN RECIPROCAL SPACE

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More than the working with most conventional crystals, the investigation of modulated structures involves the detailed and critical analysis of diffraction patterns. These patterns are where modulated structures are first identified, and the subsequent interpretation and indexation of the patterns are critical to a successful structure solution. In this presentation, we will discuss what can be learned from the diffraction data in reciprocal space, especially when we draw on knowledge of the average structure. Topics will include the assignment of the q-vectors, the occurrence of twinning, the determination of space groups, and the anticipation of the form a modulation might take.