

Modulation: ordering disorder on a higher dimension

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The unit cell defines the smallest building block of the crystalline structure such that when translation symmetry is applied in a , b and c lattice directions the whole of the crystal can be built. Disorder occurs when atoms or molecules are shifted rotated or occupationally absent as compared to their neighbors within the unit cell in such a way that translational symmetry in the 3 lattice directions is ruined. When these shifts are not random, but instead have an ordered periodicity that can be defined by an atomic modulation function we observe diffraction in reciprocal space. This diffraction appears as a projection on the 3 reciprocal lattice directions that does not have the same periodicity as the basic unit cell.