

1.72: Modulated crystal structure

A *modulated crystal structure* is a density (or atom arrangement) that may be obtained from a density (or atom arrangement) with space-group symmetry by a finite density change (or finite displacement of each atom, respectively) that is (quasi)periodic. A function or a displacement field is periodic if it is invariant under a lattice of translations. Then its Fourier transform consists of δ -peaks on a reciprocal lattice that spans the space and is nowhere dense. A quasiperiodic function has a Fourier transform consisting of δ -peaks on a vector module of finite rank. This means that the peaks may be indexed with integers using a finite number of basis vectors. If the modulation consists of deviations from the basic structure in the positions, the modulation is *displacive* ([displacive modulation](#)). When the probability distribution deviates from that in the basic structure the modulation is occupational.

See also

Model for a displacively modulated crystal structure. The basic structure is two-dimensional rectangular, with lattice constants a and b , the modulation wave vector is in the b -direction, the wavelength of the periodic modulation is λ such that λ/b is an irrational number.

Contributors

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