

1.35: Displacive modulation

For a *displacively modulated crystal phase*, the positions of the atoms are displaced from those of a basis structure with space group symmetry (an ordinary crystal). The displacements are given by the *atomic modulation function* $\mathbf{u}_j(\mathbf{r})$, where j indicates the j th atom in the unit cell of the basic structure.

$$\mathbf{r}(n, j) = \mathbf{n} + \mathbf{r}_j + \mathbf{u}_j(\mathbf{n} + \mathbf{r}_j).$$

The modulation function has a Fourier expansion

$$u_j(r) = \sum_k \hat{u}(k) \exp(2\pi i k \cdot r), \text{ with } k = \sum_{i=1}^n h_i a_i^*,$$

with finite value of n . If $n=1$, the modulated structure is one-dimensionally modulated. A special case of a one-dimensionally modulated structure is

$$r(n, j)_\alpha = n_\alpha + r_{j\alpha} + A_{j\alpha} \sin(2\pi i q \cdot n + r_j) + \phi_{j\alpha}, (\alpha = x, y, z).$$

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