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.

$r(n,j) = n + r_j + u_j(n + r_j).$

The modulation function has a Fourier expansion

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

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

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