Consider a cell with real space translation vectors a, b, and c; and reciprocal space translation vectors a^*, b^*, and c^*.

I believe that the static structure factor describes the symmetry of the atoms and spacings *within* the cell related by the translation vectors. Therefore fractional atomic coordinates $x, y, z < 1$, and integer miller indices $h, k, l \geq 1$.

For a simple cubic lattice:

$a = b = c \qquad \alpha = \beta = \gamma = 90^o$

Basis: (0,0,0)
$F(\mathbf{Q}) = f_0(\mathbf{Q}) \exp(0) = f_0(\mathbf{Q})$

We know that for an SC lattice we expect to see diffraction spots corresponding to integer h, k and l; however, non-integer values are forbidden.

Clearly from this calculation,

$F\left(\frac{1}{2}00\right) = F(hkl) = f_0(\mathbf{Q})$

However if I double the cell to dimensions $2a$ x b x c the basis becomes,

Basis: (0,0,0) and (1/2, 0, 0)
$F(\mathbf{Q}) = f_0(\mathbf{Q}) \exp(0) + f_0(\mathbf{Q}) \exp\left[-2\pi i\left(\frac{h}{2}\right)\right]$
$F(\mathbf{Q}) = f_0(\mathbf{Q}) + f_0(\mathbf{Q}) \exp(i\pi h)$

When h is even: $F(\mathbf{Q}) = 2f_0$
When h is odd: $F(\mathbf{Q}) = 0$

Odd integer values of h in the supercell correspond to the $(h/2\ 0\ 0)$ reflections of the simple cubic lattice and this demonstrates they are forbidden.

So I believe what I was trying to say earlier was something like:

To calculate a zero-value for the structure factor, the basis must include the atoms that cause a reflection to be forbidden. This is only true for the integer miller indices of the cell.