# Section 3: Extended Takagi-Taupin Theory

## Subsection 3.1: Disturbed Lattice, Fourier and Bloch Sums

Assume that the displacement from the equilibrium positions for each atom can be represented by a smooth field . The new position of the atom is . Then at each location, the local reciprocal lattice can be defined as

If one reads the definition given in the book, one can easily see that this is the proper definition.

In the worst case, there is both atomic lattice deformation and electron cloud modulation. In this case, one needs to consider:

It is convenient for the further development of the theory to model as the sum of distorted Bloch waves, representing optical phonon, excitons, etc.:

In this expression, and is the Bloch wave with and .

One should notice that the phase of the modulation of the phase of the Fourier component of the electron density distribution is defined with respected to the deformed lattice . The reason is that a modification of the electron density within the unit cell is carried along with an overall lattice distortion .

There are quite some interesting properties of the double Fourier expansion. I do not fully understand it at this moment and need to think about it in more details during my third reading of the text. At this moment, I think it does not change too much for my purpose. Therefore, I will skip it at this moment.

The Block base vector and frequency will be admitted, corresponding to the number N of branches of the dispersion surface in the related perfect-crystal diffraction problem. The positive directed part of the modulated multiple block wave is then:

In the below, there are some theories about how to contrast the first order partial differential equation that is equivalent to the Takagi-Taupin theory.