# Section 1: Linear Perfect Crystal Theory

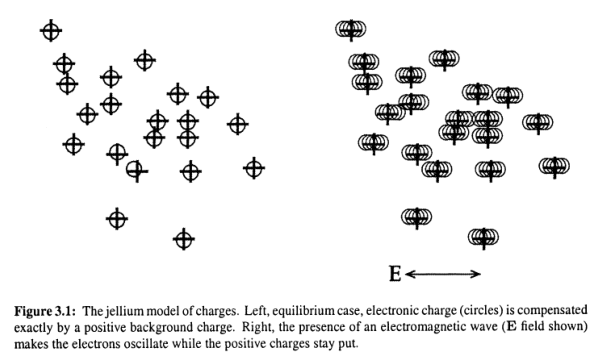
Assume the transverse gauge , then the Maxwell equation is equivalent to

Here, the and are respectively the current density and transverse current density.

In quantum mechanics, one can determine the charge density based on the electric static potential and the kinetic energy. In classical picture, it is not possible to determine amd from first principle. One instead must use a density of positive background charges and a model that maintains an equilibrium electron density in a consistent manner.

The common model of electrons in harmonic potentials is only good for resonant cases but not if multiple Fourier components of the periodic electron density come into play.

In this analysis, we focus on the cases where the X-ray photon energy is much higher than electron binding energies. To handle this case, we use the “jellium model” where we have a mobile electron cloud and a rather static positive charge background .



The background charge density contributes much less than the electron charge to the elastic scattering. However, when compared with non-linear scattering from , the contribution from elastic scattering from is not negligible. It should also be noted that the spin contribution is much weaker than the charge in each case. Therefore, the study of the spin-X-ray scattering effect is challenging.

## Perfect Lattice, Fourier and Block Sums

Assume that the electron charge density, without the influence of the external electric field is

Because is a real function (electron charge distribution function), . Assume that the crystal has inversion symmetry, then one also has . Therefore, if it is a inversion-symmetric crystal, we can choose the origin such that

Define . Then the is the structure factor usually used in the crystallography literatures where is the volume of the unit cell.

The vector potential is real-valued, and therefore we decompose it into two complex conjugate Bloch waves:

The is therefore called as the Bloch base vector. In the same way, we decompose the scalar potential function:

Here the is defined to allow for the phase difference between scalar and vectorial potential.

The current density is defined as:

The velocity is determined through the Lorentz equation. According to the equation (2.19),

Here, the is the Lorentz invariant phase.

The first two terms are the superposition of an oscillatory motion due to the electric field and the initial momentum. The third term is the longitudinal motion due to the Lorentz force. The fourth term is the momentum in the field coupled to the electron and the fifth term gives the nonlinear coupling of the field to the electron.

Under the assumption that the initial momentum of the electron is , then the linear term becomes:

Therefore

The extra term is added phenomenologically to account for the absorption. If is zero, then and are complex conjugate to each other.

The term associated with is a longitudinal current. It can also be expressed in terms of . This term is usually smaller than the first term by a factor of . It will be ignored for the rest of this section.

## System of Linear Equations

By changing the indexes with and , one change the expression into

With this expression, we analyze the Maxwell equation:

This results in:

Therefore, we can simplify this expression through:

Take an integral with for

Replace with to simplify the expression a little bit:

Here we have assumed that .

We do the same thing to the other half:

Try to get rid of multiple of harmonics with integration:

Therefore:

Exchange the symbol and , one gets:

If one replaces with , then .

With this, we finally obtain the same set of equations as those from the book:

## The Dispersion Surface

Assume that is never satisfied for any , in this case, the equation is reduced to:

When there is one reciprocal lattice satisfying the Bragg condition, the eigen-function of the equation for and is:

Where:

Assume that:

Define, with respect to the two points and , the difference is:

Then with respect to the two points and , the solution roughly forms a hyperbola, called dispersion hyperbola (ignoring the absorption):

A diagram of a cone with lines and letters

Description automatically generated with medium confidence

In my opinion, the key challenge in analyzing this figure is to realize that, if you treat the figure with different accuracy for different components in this figure, you will end up with a different functionality of the plot.

For example, the direction and the exact location of the , will be different for different crystal orientation and photon energy and polarization. These effects are minor. If you do not care too much about accuracy. One can ignore these minor contributions and follow the procedure presented here. However, if one is very determined to get the accurate value of and shown in this plot, one cannot really use the argument shown here. The accuracy is too bad. One should notice; however, the equation is correct. To obtain the Pointing vector and the group velocity, one just follows the equations given in the book. The value will be very close to the ones shown in the figure, which is a first order approximation. (For those who want to have a more accurate result, even though the first order approximation is very accurate in a general sense, it will surely be not accurate enough for your verification of your applications. Usually, your application requires exact solutions rather than first order approximation. More often than expected, you are relying on the effects that are ignored in the first order approximation.)