Relativistic calculations of elastic and inelastic electron scattering processes in crystals using the Dirac equation

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Since modern electron microscopes work with acceleration voltages of about 200 to 400 kV, relativistic effects arise. For simulations a relativistic treatment is necessary. We report on calculations of relativistic scattering processes in crystalline materials (Figure 1).

Non relativistic calculations have already be done in which the transmitted primary electron is described using Bloch waves [1] and the material is described by a periodic atomic potential. This scattering problem can be solved using the Schrödinger equation. The periodic potential yields Bloch waves as resulting wave functions. Nevertheless the calculations are complicated, because the excitation of the different Bloch waves depends on the actual scattering geometry.

Inelastic scattering processes will be considered by calculating adequate matrix elements [1]. We extend the non relativistic treatment to a fully relativistic description of these scattering processes. In many modern electron microscopes the accelerated electrons have an energy of a few hundred keV. For electrons accelerated to an energy of 200 keV the velocity is about 70 percent of the speed of light (Table 1). At these velocities a relativistic treatment is indispensible.

The solution of the relativistic scattering problem for elastic scattering is based on the corresponding procedure of non relativistic scattering. However, the Schrödinger equation has to be replaced by the Dirac equation,

$$(-i\hbar c\vec{\boldsymbol{\alpha}}\vec{\nabla} + \boldsymbol{\beta} m_0 c^2 + V)\Psi = E\Psi\ .$$

Alpha and Beta contain 4x4 matrices describing two spin states and antiparticle states. Alpha is a three component vector. Each component represents a matrix. The potential V describes the periodic potential of the crystal. By splitting the Dirac equation into two parts and using dual spinors the equations form becomes similar to Schrödinger like equations [2]. For a periodic potential we obtain Bloch wave like wave functions and we can make an ansatz for the wave function as follows,

$$\Psi(\vec{r}) = \sum_j \varepsilon^{(j)} u_k^{(j)}(\vec{r}) U(\vec{k}) e^{i\vec{k}\vec{r}}\ .$$

Similar to the non relativistic solution, in the relativistic treatment the wave function contains a periodic part u(**r**) and excitation coefficients epsilon for the Bloch waves. U(**k**) is a spinor with four components. Now the relativistic part is concentrated in the function U(**k**).

The periodic functions u(**r**) are comparable to the non relativistic solution with Bloch waves

$$u_{\vec{k}}(\vec{r}) = \sum_{\vec{g}} c_{\vec{g}} e^{i\vec{g}\vec{r}}\ .$$

These functions u(**r**) depend on the location of the electron and also on the wave vector. $c_{\mathbf{g}}$ are the fourier coefficients and the last part describes a simple plane wave.

Using this notation allows to employ calculation methods of the non relativistic problem and extend them to the actual scattering problem. The relativistic problem is concentrated in the new function U as described. With this approach the Dirac equation for this scattering problem can be solved and the wave function will be determined. Using this wave function allows for example the calculation of diffraction patterns or in combination with relativistic matrix elements the effect of inelastic scattering in crystalline materials can be considered.

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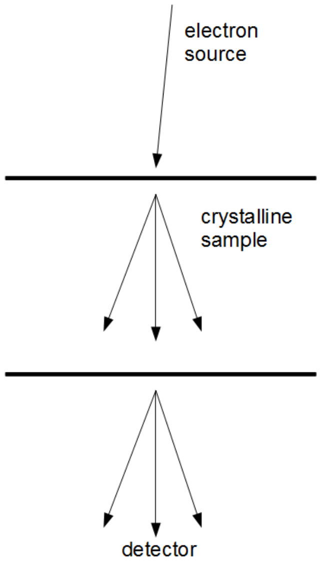

Figure 1. Schematic illustration of the regarded scattering problem. Outside the crystal the electrons are seen as plane waves. Inside of the crystal the electrons are treated as excited Bloch waves. In the calculations the boundary conditions have to be included.

Acceleration voltage	Velocity
80 kV	0.41 c
100 kV	0.55 c
200 kV	0.70 c
300 kV	0.78 c
400 kV	0.83 c
500 kV	0.86 c
1000 kV	0.94 c

Table 1. Velocity of the primary electrons in parts of the speed of light at different acceleration voltages [3].