Quantitative Techniques and Image Simulation in TEM/STEM, SEM and Diffraction

IM2.P069
Calculations of elastic and inelastic scattering processes of relativistic electrons in oriented crystals

D. Hinderks[1], H. Kohl[1]

[1]Westfälisches-Wilhelms-Universität, Physikalisches Institut, Münster, Germany

dieter.hinderks@uni-muenster.de

Many modern electron microscopes operate at acceleration voltages up to several hundred kV. The accelerated electrons thus reach velocities approaching the speed of light. Therefore the scattering processes have to be treated relativistically. We focus on inelastic scattering in crystals.

In a non-relativistic treatment a periodic potential is used to describe the crystal. The periodic potential of a crystal provides Bloch waves as solutions of the Schrödinger equation. The scattering process is mathematically described using matrix elements between product states of such Bloch waves multiplied by the objects wave function [1].

We have extended this non-relativistic treatment to relativistic electrons. The Schrödinger equation is replaced by the relativistic Dirac equation. For a periodic potential the solution of the Dirac equation provides us relativistic four component Bloch waves (Fig. 1). Spin-up and spin-down electrons are described by two different four components of this wave function (Fig. 2). Inserting the periodic potential and Bloch wave ansatz into the Dirac equation we obtain equations which allow us to calculate the excitation coefficients and the Fourier coefficients of the wave function using a matrix diagonalization. Due to the four component wave functions we thus obtain four equations to calculate this coefficients. But only one of these equations yields a nontrivial solution, which is needed to diagonalize this matrix.The formalism is similar to the non-relativistic case. Using Fermis golden rule and separating the coordinates of the incident electron from those of the atom electrons, We can view the incident electrons as a perturbation which leads to a transition of the atomic electrons from an initial to a final state. In our approach we use the relativistic propagator theory where the atomic electrons are seen under the influence of a scalar and a vector potential generated by the fast incident electrons via their charge and current. Therewith we obtain an expression for the scattering matrix in first order Born approximation (Fig. 3).Retardation of the electro-magnetic field is automatically included in this relativistic treatment. This approach has previously been used for relativistic plane waves [2]. In our formalism we substitutione the plane waves by Bloch waves for crystalline materials. Consequently we have to evaluate the matrix elements considering different sums over reciprocal space and the different single relativistic Bloch waves.

1. A. Weickenmeier and H. Kohl, Phil. Mag. B60 (1989) 467.
2. R. Knippelmeyer et al.,Ultramicroscopy 68 (1997) 25-41.

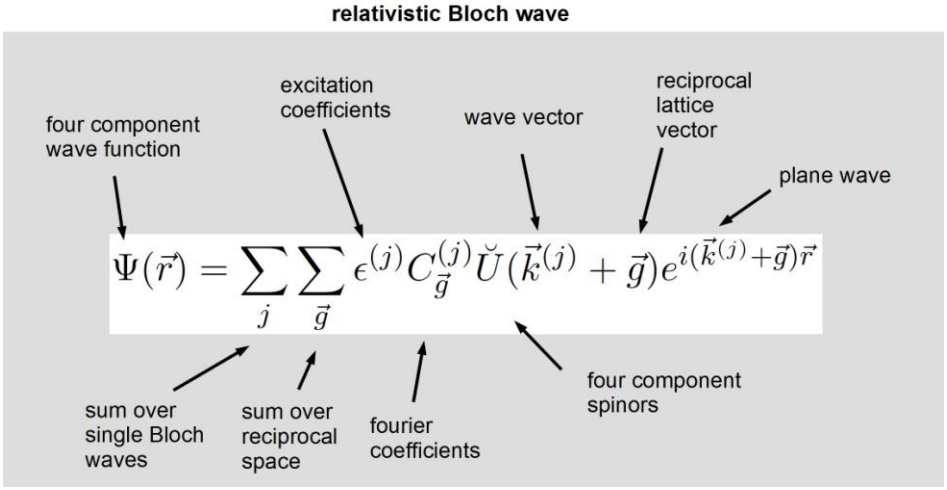

Figure 1. Relativistic Bloch wave.

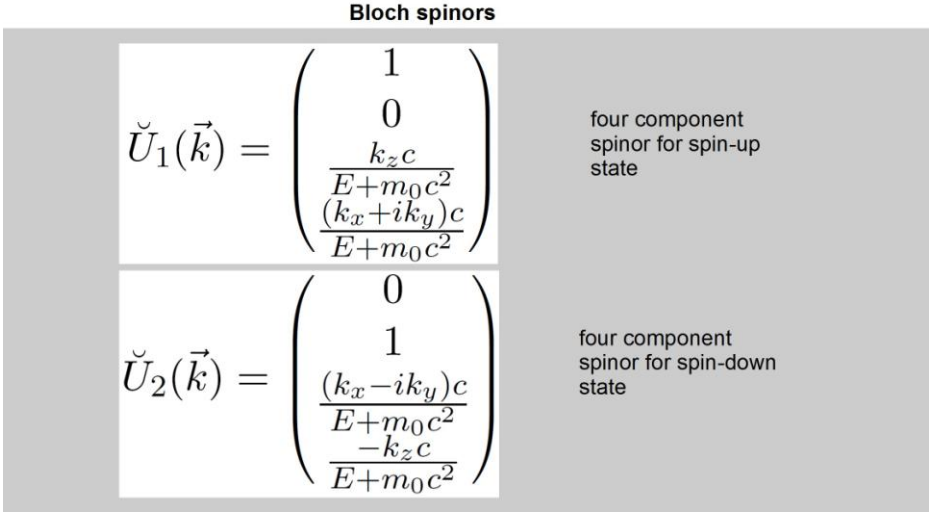

Figure 2. Bloch wave spinors.

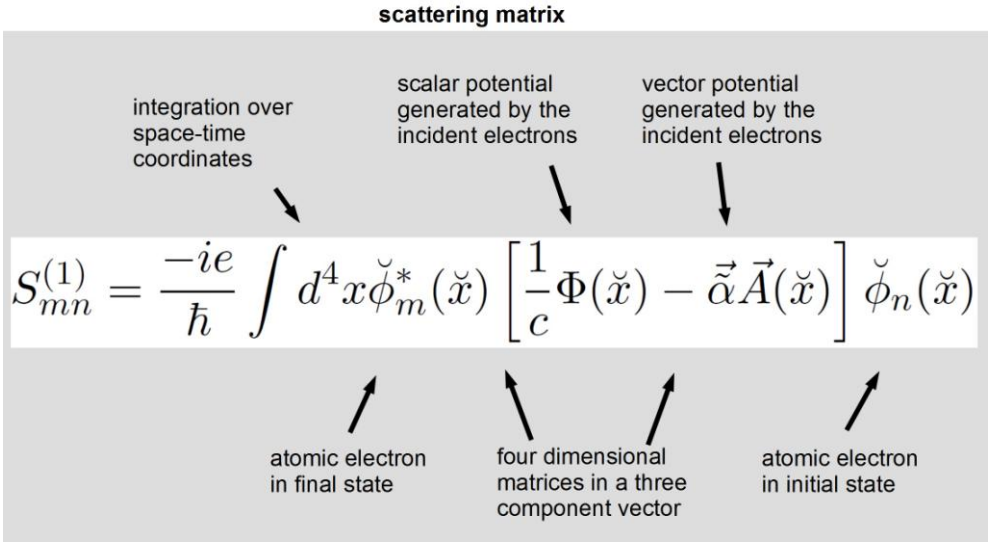

Figure 3. Scattering matrix.