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

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

[1]Physikalisches Institut und Interdisziplinäres Centrum für Elektronenmikroskopie und Mikroanalyse (ICEM), Universität Münster, Münster, Germany

dieter.hinderks@uni-muenster.de
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Since modern electron microscopes operate at acceleration voltages up to several hundred kV, a relativistic treatment for simulations is necessary. The focus of this work lies on relativistic scattering processes in crystalline materials (Figure 1).

Beginning from the non-relativistic case we want to build up the necessary theory. Non-relativistic scattering processes in crystalline materials using Bloch waves for the incident electrons have been calculated frequently. Before entering the crystal the incident electrons are expressed as simple plane waves. Inside the crystal the electrons are described using Bloch waves, because of the periodic nature of the periodic potential. After leaving the crystal the electrons are described by a superposition of plane waves to fulfill the boundary conditions. In order to obtain an accurate expression for the wave function of the incident electrons many excited Bloch waves have to be considered. Therefore the calculation of the resulting wave function becomes computationally intensive. The appearance of inelastic scattering processes inside the crystal is considered by using corresponding matrix elements [1].

This work focusses on a fully relativistic description of such scattering processes generalizing the non-relativistic theory outlined above. For high electron energy, the speed of the electrons approaches the speed of light, which makes a relativistic treatment necessary (Figure 2). For a relativistic description the calculation of the matrix elements has to be done considering the Dirac equation

Using the relativistic propagator theory, the scattering matrix can be written as

This notation allows to easily separate the electric and magnetic part in the matrix element. Here and are the wave functions of the excited electrons in the initial and the final state as a function of space-time coordinates, respectively. Moreover, and are scalar and vector potentials depending on space-time coordinates, which are generated by the incident electrons, is one of the Dirac matrices, and is a vector with three components in which every constituent is given by a four dimensional matrix [3].

The excited electron is under influence of the electric and magnetic fields, which are induced by the charge

and the current

which depend on space-time coordinates. The corresponding potentials and are calculated using a Greens formalism. Using this theory with simple plane waves to describe the incident electrons one obtains the differential cross section [2].

As already pointed out, the fast incident electrons have to be described using Bloch waves to consider their movement in the periodic potential. To ensure a fully relativistic treatment the Bloch waves have to be replaced by relativistic Bloch waves [3]

The relativistic character is assembled in four component spinors , is a reciprocal lattice vector, and is the transverse momentum of the incident electrons.

The fourier coefficients of one single Bloch wave depend on the crystal structure and can be determined analoguously to the non-relativistic case. One single Bloch wave leads to a sum over reciprocal space. The full solution for the wave function leads to a sum over different Bloch waves which are excitated at the same time and therefore are weighted with excitation coefficients .

The obtained matrix elements using Bloch waves differ from the matrix elements using simple plane waves [2] basically in additional sums in the matrix elements to consider the Bloch waves.

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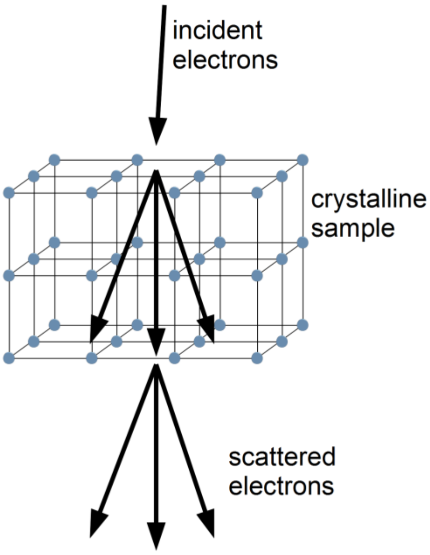

Figure 1. Schematic sketch of the scattering problem. Before entering the crystal the electrons are described as plane waves. Inside the crystalline material the electrons are given as Bloch waves. After leaving the crystal the electrons are described as a superposition of plane waves to satisfy the boundary conditions.

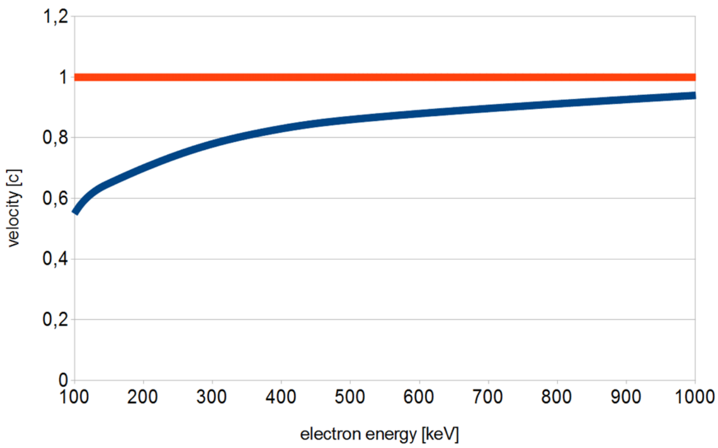

Figure 2. Velocity of the primary electrons in terms of speed of light as a function of their energy.