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Electron channelling based crystallography

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Abstract

Electron channelling occurs when the incident electron beam is parallel to the atom columns of an object, such as a crystal or a particular crystal defect. Then, the electrons are trapped in the electrostatic potential of an atom column in which they scatter dynamically. This picture provides physical insight and explains why a one-to-one correspondence is maintained between the exit wave and the projected structure, even in case of strong dynamical scattering. Moreover, the theory is very useful to invert the dynamical scattering, that is, to derive the projected structure from the exit wave. Finally, it can be used to determine the composition of an atom column with single atom sensitivity or to explain dynamical electron diffraction effects. In this paper, an overview of the channelling theory will be given together with some recent applications.

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1. Introduction

It is well known that high-resolution transmission electron microscopy (HRTEM) images often show a one-to-one correspondence with the configuration of projected atom columns when a crystal is viewed along a zone axis, i.e., parallel to these columns. This correspondence is present if the distance between adjacent columns is not too small and the resolution of the electron microscope is sufficient. From this, it has been suggested that for crystals viewed along a zone axis with sufficient separation between the columns, the complex wave function at the exit face of the crystal mainly depends on the projected structure, i.e., on the type and position of atom columns. The physical reason for *local* dynamical diffraction is the channelling of the electrons along the atom columns parallel to the beam direction [1–4]. Due to the positive electrostatic potential of the atoms, a column acts as a guide or channel for the electron within which the electron can scatter dynamically without leaving the column. This channelling effect is schematically represented in Fig. 1.

A simple intuitive way to understand electron channelling is to consider each atom as a thin lens as shown in Fig. 2. The lens is even a perfect lens if the shape of the electrostatic potential is parabolic. By passing successive lenses, the electron wave is focussed at periodic distances. The period is called *extinction distance* [5]. It is a function of the *average mass density* of the columns, which in turn is a function of the atomic number of the atoms and the repeat distance of the atoms in the column. Note that when the crystal thickness is equal to the extinction distance, the exit wave is equal to the entrance wave. Then, the effect of the column in a sense disappears. This effect is called dynamical extinction. Note also that for certain thicknesses, the focussing effect of a light column at the exit face can be stronger than that of a heavy column. Therefore, light columns can be visualized in the presence of heavy

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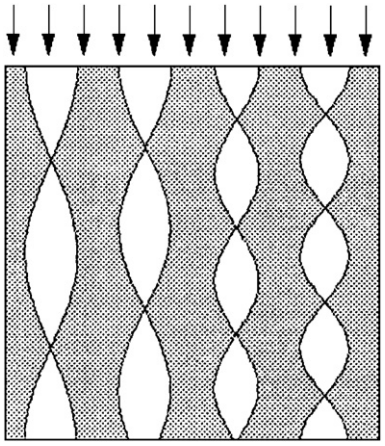

Fig. 1. Schematic representation of electron channelling.

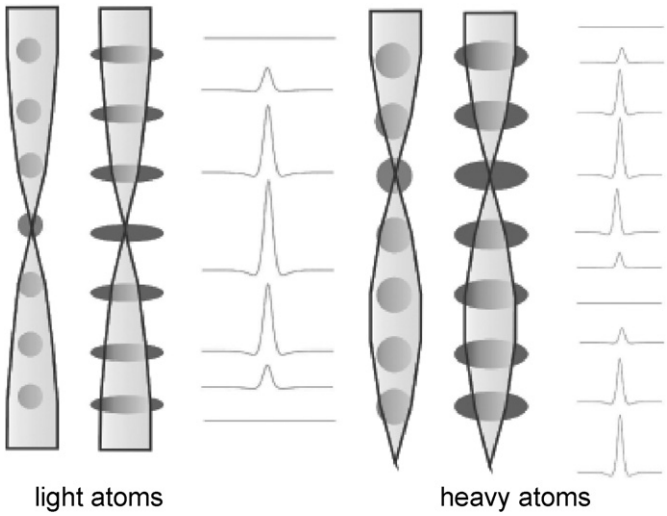

Fig. 2. Each atom in an atom column is considered as a thin lens. By passing successive lenses, the electron wave is focussed at periodic distances. When the crystal thickness is equal to the extinction distance, the exit wave is equal to the entrance wave.

columns. This is an advantage of electron diffraction as compared with X-ray diffraction.

In X-ray diffraction, the interaction between the photons and the crystal is weak so that single scattering dominates and the kinematical theory is valid. In this theory, the diffracted wave is the Fourier transform of the electron density or, in case of crystals, the electrostatic potential. In the classical multislice theory [6], on which many simulation programs are based, the electron wave is also expanded in Fourier series. Physically, this corresponds to describing electron diffraction in terms of plane waves in the direction of the Bragg reflections. In principle, the plane wave basis is a complete basis so that, in mathematical terms, it is always correct to use such an expansion. However, when the interaction of the electron with the crystal is very strong, as is the case in the channelling condition, one needs a very large number of plane waves in order to describe the peakiness of the focussed electron wave so that the advantage of the plane-wave picture is lost and physical insight in the scattering process is obscured. The channelling theory combines ease of calculation with physical insight. For example, in case of a crystal with only one type of columns and a thickness of exactly one extinction distance, it is known from the channelling theory that the exit wave is approximately equal to the entrance wave as if there is no crystal. In the diffraction pattern, it can be seen that the intensity of all the Bragg reflections disappears as if all diffracted electrons have been scattered back to the central beam. This is difficult to understand in terms of diffraction of plane waves, but simple in the channelling theory.

Another basis that is often used to describe electron scattering is the basis of Bloch waves, which are the eigenstates of the electron wave in a periodic potential such as a crystal. These Bloch waves form a complete set of basis functions. However, in terms of Bloch waves, it is difficult to understand that channelling also occurs in an isolated column without the need for a periodic crystal. The channelling theory, on the other hand, is also valid for an isolated column. In principle, electron scattering in an isolated column could also be described using a Bloch wave (or even a plane wave) expansion. This could be done by repeating the column artificially over a large distance so as to avoid overlap of the electron waves. However, this procedure has to be considered as a mathematical rather than a physical approximation. If one deals with a real crystal in which the distance between the columns is sufficiently large, the physical periodicity then plays the role of the mathematical periodicity in the sense that it does not influence the scattering of the electron inside the column.

The importance of channelling to interpret HRTEM images has often been ignored or underestimated. This is probably due to the fact that in the past electron diffraction was often described in reciprocal space. Reciprocal space is particularly useful when a small number of diffracted beams is involved. However, most HRTEM images of crystals are taken in zone axis orientation, where the projected structure is simplest, but the number of diffracted beams is largest. Therefore, a simple real-space channelling theory is believed to yield a more useful and intuitive, albeit approximate, description for dynamical diffraction. Furthermore, this theory allows one to intuitively interpret HRTEM images and diffraction patterns, even for thicker crystals.

2. Channelling theory

In this section, the basic results of the channelling theory will be described in mathematical form. The details of this theory may be found in Refs. [7–10].

When an electron propagates through a crystal, this electron feels the mean projected potential $eU(x,y)$ of the