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An Ergodic Approach to the Interaction of Energetic Electrons and Single Crystals

BY HANS C. H. NIP, R. L. DALGLISH AND J. C. KELLY

Materials Irradiation Group, Department of Physics, The University of New South Wales, Sydney, 2033, Australia

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With some exceptions, recent publications indicate that the compatibility of the special wave-mechanical and classical treatments of the interaction of very energetic ($\geq 5 \times 5^5$ eV) electrons and single crystals is not obvious. We present a qualitative argument that shows that, even if the interaction of the electron and the single crystal may be described completely by particle mechanics, the experimentally measured parameters can still display wave-mechanical effects. The observation of classical or wave-mechanical effects depends on the ability to detect electrons with similar distinct classical trajectories.

Introduction

During the last decade appreciable interest has been focused on the lattice-directed trajectories of positive and negative particles (Lindhard, 1965; Datz, Erginsoy, Liebfried & Lutz, 1967; Goland, 1967; Palmer, Thompson & Townsend, 1969; Nip, 1969; Chadderton, 1970; Berry, 1971). The classical theories of channelling and blocking (Lindhard, 1965) of heavy positive particles have been supported extensively by experimental results and the classical approach has received widespread acceptance and application. On the other hand, for light beta-particles, an interesting discussion has developed regarding the applicability of particle mechanics to the experimental conditions under consideration (Goland, 1967; Palmer, Thompson & Townsend, 1969; Chadderton, 1970). The successful application of electron diffraction theory to the experimental conditions encountered in the electron microscope is well-known and obviously any classical treatment in analogy with Lindhard's model, should be contained by the wave-mechanical diffraction treatment. We consider here the partial success of the diffraction and particle models in the interpretation of these high-energy experimental observations of directional penetration anisotropy. The special wave-mechanical treatment of the 'channelling-like' experiments has so far only achieved *qualitative* agreement with the main experimental features; the particle-mechanical treatment however, shows good quantitative agreement with the main experimental features. We develop guide lines to decide which model to choose for a particular experiment. The argument illustrates the compatibility of both treatments.

A brief survey of the models

The interaction of *positive* beta-particles and a single crystal has been considered in terms of the well-established classical Lindhard model for heavy particles, and recently an analogous model for the directional effects of energetic *negative* beta-particles in single crystals has been suggested (Nip, Hollis & Kelly, 1968). In this classical model, the well-localized electron finds potential minima at the lattice sites and an electron emitted from a substitutionally implanted source or backscattered from a lattice atom can 'weave' in a nearly planar motion along a low-index row (*cf.* Berry, 1971, Fig. 14*a*). An electron emitted from an interstitially sited source or inserted by an external beam will however, be 'blocked' by the potential maximum centred at the axis of the optical channel and may be trapped into a helical motion about a row adjacent to the channel. The discrete nature of the scattering points in the atomic row, *i.e.* the discontinuity of the potential minimum, strongly influences the classical trajectories (Nip & Kelly, 1970). Hence the continuum wall approximation to the interaction potential (Lindhard, 1965) is not applicable to weaving and the periodicity along the row is an important parameter in the theoretical study of the model. On the other hand, for initially interstitially moving electrons, the continuum wall approximation is valid for the largest part of the aligned motion and relativistic equations of motion of the electron in the channel can be obtained. Care should however be taken as possible effects of the row periodicity may be overlooked (Nip & Kelly, 1971). So far, the weaving motion has defied exact analytical treatment and only the results of a computer simulation have been published (Nip, 1969; Nip & Kelly, 1970). These results agree well with the available experimental data (Astner, Bergstrom, Domeij, Eriksson & Persson, 1965; Uggerhøj, 1966; Uggerhøj & Andersen, 1968; Tomlinson & Howie, 1968). For blocking, most experimental results predicted by the model have been reported and the quantitative agreement with the available data is good (Uggerhøj & Andersen, 1968; Tomlinson & Howie, 1968; Kreiner, Bell, Sizmann, Harder & Hüttl, 1970; Nip, Dalglish, Chang & Kelly, 1971). Computer simulation results also indicate fine structures in the angular distribution upon emission and the possibility of

similar effects in the energy spectrum of the emitted particles.

Special wave-mechanical treatments of this 'channellinglike' interaction of energetic electrons and single crystal foils in terms of a preferential excitation of Block waves with anomalous absorption coefficients (Howie, 1966, 1967), and special multi-beam calculations neglecting absorption effects (De Wames, Hall & Chadderton, 1967; De Wames & Hall, 1968; Pathak & Yussouff, 1970, 1971) have been published. These wave-mechanical models have been reviewed recently (Chadderton, 1970). There is good qualitative agreement between most of the above mentioned experimental data and the predictions of both types of special wave theories. The inclusion of still more beams in the calculations makes the theoretical result approach the experimental values but the differences remain appreciable. However, some fine structures have been predicted successfully by these wave models and are as yet unexplained by the classical model (Uggerhøj & Frandsen, 1970).

The compatiblity of the particle and wave models

The relatively successful application of both models to the experimental results under consideration, has caused some controversy, possibly because the compatibility of the particle- and wave-models is not immediately obvious. An argument which illustrates this compatibility and suggests experimental conditions favouring either model is presented here.

A free electron will have a constant probability distribution throughout space. On detecting the electron, its probability density distribution contracts to a delta-type function whose shape is determined by the uncertainty principles. Assuming that each electron in the projectile beam upon entering the target is 'detected' by the interaction potential of the crystalline target foil, we obtain from $\Delta x \Delta p > h$, that

$$\Delta x \Delta\lambda > \lambda^2. \tag{1}$$

Here Δx is the positional uncertainty of the electron, and $\Delta\lambda$ is the uncertainty in the de Broglie wavelength λ of the electron. If we want to apply a classical two-body model we must make the following assumptions:

(i) the electron interacts with one lattice atom at a time, *i.e.*

$$\Delta x < a_s \tag{2}$$

where a_s is the smallest interatomic spacing in the target and

(ii) the tails of the probability density distribution of the electron do not interfere coherently, *i.e.* the range of coherence δ of the incident radiation is smaller than the separation a_n of the scattering points (Cowley, 1968).

From equations (1) and (2) we easily derive

$$a_s > \lambda^2/\Delta\lambda\,. \tag{3}$$

Similarly, using Cowley's definition of δ, we obtain

$$a_n \gg \lambda^2/\Delta\lambda\,. \tag{4}$$

We can safely assume $a_s \simeq a_n$ and find from the basically identical relations (3) and (4) a necessary condition for the applicability of a classical model of correlated two-body collisions:

$$a \gg \lambda^2/\Delta\lambda \tag{5}$$

where a is a target constant of the order of the interatomic spacing. We have chosen this somewhat elaborate derivation of equation (5) to illustrate its generality. The best experimental conditions (*e.g.* in electron microscopy) give angular resolutions of 10^{-3} radians which, combined with a 4% energy resolution gives the condition for the applicability of such a classical model as

$$a/\lambda \gg 50\,. \tag{6}$$

For a 0·8 MeV electron, $\lambda \simeq 0{\cdot}01$ Å, and with a lattice spacing of the order of 1 Å, condition (6) is not satisfied.

If equation (5) is satisfied, all electron wave-packets are sufficiently localized to be considered to move in classical trajectories through the crystal foil. It is however, extremely difficult to deal quantitatively with such a many-body model other than by statistical mechanics or a computer simulation. However, the following argument might yield some insight into the experimentally anticipated effects. For a random orientation of the crystal with respect to the initial electron beam – and equation (5) satisfied – all electrons must move in statistically similar classical trajectories. Any group of experimentally detected electrons will then form a representative statistical sample of the initial electron beam modulated by the *full* crystal. The various experimental parameters of this statistical sample should thus display the influence of the whole crystal. Moreover, the electrons are indistinguishable and for sufficiently large samples, the Ergodic Theorem will hold. Hence the sample observation of each experimental parameter will relate to the probability distribution of the value of that parameter for a single electron that has experienced the full periodicity of the whole crystal. But such an electron will have traversed a three-dimensionally periodic potential and its spatial distribution *etc.* should be the same as those obtained from the solution of a one-particle Dirac equation for a projectile in a three-dimensionally periodic potential. The solutions of such an equation must be Bloch states, and the mathematical treatment of the interaction of the beam thus is equivalent to the mathematical formalism employed in the wave theory of diffraction. Hence, although the interaction is that of a beam of classical electrons experiencing two-body collisions with the lattice atoms, the experimentally measured parameters will follow a Bloch-formalism. Next, consider the experimental case in which the initial beam is aligned with a simple crys-

tallographic direction. A large fraction of the electrons will travel in the particular lattice-directed mode of blocking before being randomized or trapped in a helical weaving motion along the low-index direction. For a sufficiently thin target, the electrons transmitted and detected near this direction will not form a representative subsample of all possible classical electron trajectories in the crystal and will only display the features associated with their particular trajectories (*cf.* Berry, 1971, Fig. 14*a*). When, however, we move our detector away from the aligned position, the detected electrons will no longer include the 'lattice-directed' subsample. Those detected will have travelled in all classical trajectories through the foil and thus display the wave-mechanical effects as discussed before. Similarly if the crystal thickness is much larger, than the range of lattice-directed trajectories, all detected electrons will have been randomized inside the crystal before transmission.

Conclusion

The statistical many-body treatment of a beam of classical electrons in a single crystal can be related to the wave-mechanical treatment of a projectile in a three-dimensionally periodic potential with the aid of the Ergodic Theorem.

To obtain experimentally 'classical' effects, we must be able to detect a subsample of electrons with similar *particular* classical trajectories without violating condition (5). Any experimental quantity which is directly associated with the statistical treatment of *all possible* classical trajectories will display wave-mechanical effects.

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