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The scattering of electrons by edge dislocations in Al

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Abstract. A new scheme is proposed to describe the scattering of electrons by deformations due to lattice defects. It is based on the assumption that these deformations are quite homogeneous on an atomic scale with the consequence that the potential seen by the electrons is quite similar to that obtained from self-consistent band-structure calculations for homogeneously deformed lattices. As a first example the scattering by the dilatation field of an edge dislocation is treated. The electrical resistivity is evaluated by solving the Boltzmann equation, taking into account the shape of the Fermi surface and the anisotropy of the scattering probability. Experimental and theoretical values of the electrical resistivity due to edge dislocations in Al are found to be in qualitative agreement showing that the scattering by the dilatation is the dominant mechanism in the case of edge dislocations. As was stated by Watts we find the anisotropy relation $\rho_\perp/\rho_\parallel < 1.5$. That means that edge dislocations have a non-zero component of electrical resistivity $\rho_\parallel$ along the dislocation line.

1. Introduction

Despite great efforts in the last 40 years the electrical resistivity produced by dislocations is still not satisfactorily explained for non-free-electron metals (Ziman 1964, Watts 1987). Because the displacement field of these defects is multi-valued and at certain planes even discontinuous across the missing plane of atoms most of these investigations are based on the concept of the deformation potential (Bardeen and Shockley 1950) according to which only the strain field produced by the dislocation causes the electron to be scattered. Far more crude is the assumption that the wave-functions of the conduction electrons are approximated by plane waves, which is only correct if the ions of the crystal are approximated by a positive background. With these simplifications the conduction electrons are scattered by the potential

$$V_{\mathrm{def}}(r) = [n_0/N(E_\mathrm{F})]\Theta(r) \tag{1.1}$$

which can easily be derived from the requirement that the highest occupied energy levels must be equal in an inhomogeneously strained metal (Landauer 1951). Here n_0 is the electronic density of the undeformed crystal and $N(E_\mathrm{F}) = \frac{3}{2}n_0/E_\mathrm{F}$ is the density of states at the Fermi level. $\Theta(r)$ is the dilatation produced by the dislocation. Thus the conduction electrons suffer no scattering by the shear components of the strain tensor with the consequence that within the framework of linear elasticity screw dislocations do not produce any electrical resistivity. A more refined treatment by Hunter and Nabarro (1953), which goes beyond equation (1.1), could not even qualitatively explain the increase of the electrical resistivity observed after cold work. The discrepancy is approximately a factor of 30 for Cu, Ag, Au and Al. Investigations beyond the theory of linear elasticity (Seeger and

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Stehle 1956, Seeger and Bross 1960) could considerably reduce the discrepancy but still suffer from the fact that they are based on the free-electron approximation. Therefore, new investigations of the problem that benefit from the great progress achieved in the electron theory of solids are desirable.

In the present paper a conceptionally new method to treat the scattering of Bloch electrons by deformation is developed. It is based on the fact that the strain field in the deformed crystals varies weakly on an atomic scale apart from the core of the defect. This means that over the range of a large number of atomic cells the strain field may be considered to be homogeneous. In such a region the potential seen by the electrons is quite similar to the potential obtained from self-consistent band-structure calculations with the same lattice deformation. Screening effects produced by the redistribution of the electrons are taken into account at least globally by this treatment. In a similar way as in the scheme of Hunter and Nabarro, not the displacement, but the strain, is considered as the origin of the perturbation potential. Thus rigid translations of the lattice will have no effect. No ambiguity will occur if the displacement field is of the order of a lattice vector or is multiple valued, as is the case for edge dislocations where the displacement increases by a lattice vector around a closed circuit which is threaded by the dislocations. We believe that this kind of scattering is even more effective in the case of non-vanishing dilatation than the scattering caused by the redistribution of the electrons to equalize the Fermi energy given by equation (1.1). In crystals deformed by pure shears it is the sole origin of the scattering.

As long as we restrict ourselves to first-order perturbation theory (the Born approximation), the scattering amplitude $\langle n'k'|V_{\text{per}}|nk\rangle$ of a deformed crystal may be obtained by the superposition of the contributions due to the nine components of the distortion tensor. This will considerably reduce the numerical work. However, we may go beyond first-order perturbation theory as self-consistent band-structure calculation can be performed for any arbitrary deformation of a crystal.

In the present paper the new concept is first applied to the scattering of electrons by the dilatation produced by an edge dilocation in Al. It is based on self-consistent calculations using the MAPW formalism (Bross 1964, Bross *et al* 1970, Bross and Eder 1987) which allows us to treat the Bloch states $|nk\rangle$, which are the basis for calculating the scattering amplitude $\langle n'k'|V_{\text{per}}|nk\rangle$ on the same level as the perturbation potential. This is very important since V_{per} shows strong variation near the nuclei. When analogous calculations for uniaxially strained crystals and crystals with pure shear are available the scattering by the full strain field of an edge dislocation or of a screw dislocation will also be investigated.

The outline of the present paper is the following. In section 2 the r-dependent deformation potentials are defined, based on investigations of periodic crystals with different lattice parameters. This information is used in section 3 to determine the scattering amplitude $\langle n'k'|V_{\text{per}}|nk\rangle$ for a crystal that is inhomogeneously strained by lattice defects. In first-order perturbation theory this amplitude is found to factorize in a magnitude completely defined by band-structure calculations and the Fourier transform of the distortion field. In section 4 an explicit expression for an edge dislocation in an FCC crystal is derived. In contrast to the continuum approach, the conduction electrons are found to suffer a change of the momentum parallel to the dislocation line. Section 5 deals with the solution of the Boltzmann equation, taking into account completely the asphericity of the Fermi surface and the anisotropy of the scattering. Kohlers' (1948, 1949a, b) variational principle will be used. Finally in section 6 preliminary investigations for edge dislocations are described with results quite close to the experimental ones.

2. The concept of an r-dependent deformation potential

In the LDA formalism (Hohenberg and Kohn 1964, Kohn and Sham 1965, Sham and Kohn 1965) self-consistent calculations may be performed for a homogeneously deformed crystal. Its deformation is described by the Jacobian $\mathbf{J}$ or the distortion β

$$J_{lk} = \delta_{lk} + \beta_{lk} \tag{2.1}$$

yielding the Eulerian strain tensor (Murnagham 1951)

$$\epsilon_{lk} = \tfrac{1}{2}(J_{jl}J_{jk} - \delta_{lk}) = \tfrac{1}{2}(\beta_{lk} + \beta_{kl} + \beta_{jl}\beta_{jk}). \tag{2.2}$$

Sums upon repeated indices are implicitly assumed throughout this paper. Using the Kohn–Sham (1965) equations the one-particle energy $E_{nk}(\beta)$ as well as the particle density

$$\rho(r, \beta) = \sum_{\text{occ}} |\Psi_{n,\tilde{k}}(r, \beta)|^2 \tag{2.3}$$

are found as a function of β or ϵ. The summation over n and $\tilde{k}$ extends over those one-particle states for which $E_{n,\tilde{k}}(\beta) \leqslant E_F$. In the deformed crystal the wave-vector $\tilde{k}$ and the reciprocal latice vectors are obtained by the affine transformation

$$\tilde{k} = (1 + \beta)^{-1} \cdot k \qquad \tilde{K} = (1 + \beta)^{-1} K \tag{2.4}$$

from the corresponding vectors of the undeformed case.

With regard to the inhomogeneous case considered in the following sections it is useful that the zero level of Coulomb potential is chosen such that the Fermi energy is identical to zero for any value of the distortion:

$$E_F(\beta) = 0. \tag{2.5}$$

Besides $\rho(r, \beta)$ the self-consistent procedure yields the effective one-particle potential $V_{\text{eff}}(r, \beta)$. If the deformation is chosen to be small, e.g. $\|\beta\| \ll 1$, both $\rho(r, \beta)$ and $V_{\text{eff}}(r, \beta)$ may be approximated by a suitably chosen power expansion in β. Restriction to the first non-trival terms gives the identities

$$\rho(\tilde{r}, \beta) = \rho(r, 0) + \beta : \mathbf{P}(r) \tag{2.6}$$

$$V_{\text{eff}}(\tilde{r}, \beta) = V_{\text{eff}}(r, 0) + \beta : \mathbf{W}(r) \tag{2.7}$$

for any pair $\tilde{r}$ and r satisfying

$$\tilde{r} = \mathbf{J} \cdot r. \tag{2.8}$$

Here and in the following : means the trace of a product of two tensors. Definitions (2.6) and (2.7) guarantee that the second-rank tensors $\mathbf{P}$ and $\mathbf{W}$ have the correct translation symmetry with respect to lattice vectors R of the undeformed crystal, as $V_{\text{eff}}(r, \beta)$ and $\rho(r, \beta)$ do not change under a rigid translation by a lattice vector:

$$\tilde{R} = \mathbf{J} \cdot R. \tag{2.9}$$

Note that $\mathbf{W}(r)$ is not a mere partial derivative of $V_{\text{eff}}(r, \beta)$ with respect to β. Rewriting the identities in the following way

$$V_{\text{eff}}(r, \beta) = V_{\text{eff}}((\mathbf{1} + \beta)^{-1} \cdot r, 0) + \beta : \mathbf{W}((\mathbf{1} + \beta)^{-1} \cdot r) \tag{2.10}$$

shows that the first term describes a rescaling of the one-particle potential of the undeformed crystal. In the deformed crystal new physical phenomena are mainly attributed to the tensor $\mathbf{W}$ which plays the role of an r-dependent potential. In the following $\mathbf{W}$ is called the r-dependent deformation potential.

Using first-order perturbation theory it can easily be verified that the change of the one-particle state described by the wave-vectors k and $\tilde{k} = \mathbf{J}^{-1} \cdot k$ in the undeformed and deformed crystal, respectively, is given by

$$E_{n\tilde{k}} - E_{nk} = \beta_{jl} \langle nk | (1/m) W_{jl}(r) - p_j p_l | nk \rangle \tag{2.11}$$

where p is the operator of momentum. Usually the right-hand term is called the band deformation potential for the Bloch state $|nk\rangle$. A similar expression for the energy shift is given by Khan and Allen (1984), but their tensors $\mathbf{X}(r)$ and our $\mathbf{W}(r)$ have a different origin.

As we will see in the next section the present definition of r-dependent deformation potential suffers from the fact that it additionally requires knowledge of the displacement field when we want to describe the scattering of Bloch electrons in an inhomogeneously strained crystal even in the lowest order of the strain. This obvious disadvantage can be avoided by a simple power expansion of $V_{\text{eff}}(r, \beta)$

$$V_{\text{eff}}(r, \beta) = V_{\text{eff}}(r, 0) + \beta : \tilde{\mathbf{W}}(r) \tag{2.12}$$

where $\tilde{\mathbf{W}}$ may be considered as a modified deformation potential. Strictly speaking such a definition is only valid in the limit $|\beta| \to 0$. Otherwise the function $\tilde{\mathbf{W}}(r)$ varies on a subatomic scale as $V_{\text{eff}}(r, \beta)$ and $V_{\text{eff}}(r, 0)$ show different translation symmetry. Using equation (2.8) the relation

$$\tilde{W}_{jl}(r) = W_{jl}(r) - x_l \partial V_{\text{eff}}(r, 0)/\partial x_j \tag{2.13}$$

in the central atomic cell is derived showing $\operatorname{grad} \tilde{\mathbf{W}}(r)$ to be discontinuous at the surface of the atomic polyhedron.

3. Scattering of Bloch electrons in an inhomogeneously deformed crystal

In this section it is assumed that a slowly varying distortion field $\beta(r)$ strains a crystal inhomogeneously. That means that the change of $\beta(r)$ on the atomic scale can be neglected, $\|a\| \cdot \|\operatorname{grad} \beta(r)\| \ll 1$. A displacement of such behaviour may be caused by lattice defects or long-wavelength phonons. As this assumption is not true for the core of a dislocation or of a point defect such regions must be excluded. In an inhomogeneously strained crystal the wave-vector k is no longer a good quantum number and transitions from the Bloch state $|nk\rangle$ into $|n'k'\rangle$ will occur. For $k' \neq k$ this transition is essentially described by the matrix element

$$\langle n'k' | V_{\text{per}}(\tilde{r}) | nk \rangle = \int \Psi^*_{nk'}(\tilde{r}) V_{\text{per}}(\tilde{r}) \Psi_{nk}(\tilde{r}) \, \mathrm{d}^3\tilde{r} \tag{3.1}$$

where Ψ_{nk} and $\Psi_{n'k'}$ are Bloch functions of the undeformed crystal. $V_{\text{per}}(\tilde{r})$ is the effective one-particle potential of the deformed crystal in the sense of the Kohn–Sham (1965) formalism. The integral has to be performed in the strained crystal. As the deformation is slowly varying it may be divided into atomic cells of varying shape

$$\langle n'k'|V_{\text{per}}(\tilde{r})|nk\rangle = \sum_{\tilde{R}} \int_{V_c(\tilde{R})} \Psi^*_{n'k'}(\tilde{r}+\tilde{R})\, V_{\text{per}}(\tilde{r}+\tilde{R})\Psi_{nk}(\tilde{r}+\tilde{R})\, \mathrm{d}^3\tilde{r} \tag{3.2}$$

where $V_c(\tilde{R})$ is the atomic cell at $\tilde{R}$. Its deformation is approximately described by the distortion $\beta(\tilde{R})$. As a consequence of the inhomogeneous deformation of the whole crystal a bare perturbation is produced which is screened by the conduction electrons. Now our basic assumption is that the resulting one-particle potential might be approximated by the potential of a homogeneously deformed crystal having the distortion $\beta(\tilde{R})$:

$$V_{\text{per}}(\tilde{r}+\tilde{R}) = V_{\text{eff}}[\tilde{r}+\tilde{R}, \beta(\tilde{R})]. \tag{3.3}$$

Using (2.7) we obtain up to terms linear in β

$$V_{\text{per}}[\tilde{r}+\tilde{R}, \beta(\tilde{R})] = V_{\text{eff}}(r+R, 0) + \beta(\tilde{R}) : \mathbf{W}(r+R) \qquad \text{for } \tilde{r} = (1+\beta)\cdot r. \tag{3.4}$$

Note that both functions appearing on the right-hand side (RHS) are periodic with respect to the lattice vectors R of the undeformed crystal.

Using an affine transformation the integration appearing in (3.2) may be expressed by an integration over the atomic cells of the undeformed crystal

$$\begin{aligned}\int_{V_c(\tilde{R})} &\Psi^*_{n'k'}(\tilde{r}+\tilde{R})\, V_{\text{per}}(\tilde{r}+\tilde{R})\Psi_{nk}(\tilde{r}+\tilde{R})\, \mathrm{d}^3\tilde{r} \\ &= \exp[\mathrm{i}(k-k')\cdot R]\{1+\mathrm{Tr}[\beta(\tilde{R})]\} \int_{V_c} \Psi^*_{n'k'}(r+\beta\cdot r+\tilde{R}) \\ &\quad \times [V_{\text{eff}}(r) + \beta(\tilde{R}) : \mathbf{W}(r)]\cdot \Psi_{nk}(r+\beta\cdot r+\tilde{R})\, \mathrm{d}^3 r. \end{aligned} \tag{3.5}$$

For values of $\beta\cdot r$ within the atomic cell both Bloch functions may be expressed by

$$\Psi(r+\beta\cdot r+\tilde{R}) = \Psi(r+\tilde{R}) + (\beta\cdot r)\cdot \mathrm{grad}\,\Psi(r+\tilde{R}). \tag{3.6}$$

Unfortunately for large values of R an analoguous approximation is not allowed for the second term $\tilde{R}$ in the argument of the Bloch functions. Restricting up to terms linear in β we obtain after a straightforward manipulation

$$\begin{aligned}\langle n'k'|V_{\text{per}}|nk\rangle &= \sum_R \exp[\mathrm{i}(k-k')\cdot R]\langle n'k'|V_{\text{eff}}(r-\tilde{R})|nk\rangle_{V_c} \\ &\quad + D_{jl}\sum_R \exp[\mathrm{i}(k-k')\cdot R]\beta_{jl}(\tilde{R}) \end{aligned} \tag{3.7}$$

where

$$D_{jl} = \langle n'k'|W_{jl}(r)|nk\rangle_{V_c} - \langle n'k'|x_j \frac{\partial V_{\text{eff}}}{\partial x_l}(r)|nk\rangle + \int_{\partial V_c} x_j V_{\text{eff}}(r)\Psi^*_{n'k'}(r)\Psi_{nk}(r)\, \mathrm{d}F_l. \tag{3.8}$$

In deriving equation (3.7) we have assumed that the vector $\tilde{R}$ characterizing the atomic cell in the deformed crystal and its map R in the unstrained crystal differ from one another by an amount of order β. In fact their difference is defined by the displacement field

$$s = \tilde{R} - R \tag{3.9}$$

which can be comparable in magnitude to the lattice spacing. This displacement field survives in the first term of equation (3.8) since it describes how the Bloch functions $|nk\rangle$ and $|n'k'\rangle$ vary in the strained crystal. In the formulation of the r-dependent deformation potential $\mathbf{W}$ there is no way to avoid this term. This may have severe consequences when s is multi-valued or even discontinuous. Provided that s is well behaved and small on an interatomic scale a power expansion in the displacement is possible, yielding

$$\sum_R \int_{V_c} \Psi^*_{n'k'}(r+\tilde{R}) V_{\text{eff}}(r) \Psi_{nk}(r+\tilde{R})\, \mathrm{d}^3 r = D \cdot \sum_R \exp[\mathrm{i}(k-k')\cdot R] s(R) \tag{3.10}$$

where

$$D = -\langle n'k'| \operatorname{grad} V_{\text{eff}} |nk\rangle + \int_{\partial V_c} V_{\text{eff}}(r) \Psi^*_{n'k'}(r) \Psi_{nk}(r)\, \mathrm{d}F. \tag{3.11}$$

This obvious disadvantage can only be avoided by using the concept of the modified deformation potential defined by equation (2.12). Then the deviation of the Kohn–Sham potential from its value in the perfectly periodic lattice is given by

$$-\beta(R) : \tilde{\mathbf{W}}(r). \tag{3.12}$$

As long as we are interested in terms linear in the strain, the matrix element for the transition from the state $|nk\rangle$ into the state $|n'k'\rangle$ is then given by

$$\langle n'k'|V_{\text{per}}|nk\rangle = \sum_R \beta(R) : \int_{V_c} \Psi^*_{n'k'}(r+R) \tilde{\mathbf{W}}(r) \Psi_{nk}(r+R)\, \mathrm{d}^3 r \tag{3.13}$$

where the integral extends over the atomic cell characterized by the lattice vector R in the unstrained crystal. Using Bloch's theorem yields

$$\langle n'k'|V_{\text{per}}|nk\rangle = \langle n'k'|\tilde{W}(r)|nk\rangle_{V_c} : \sum_R \beta(R) \exp[\mathrm{i}(k-k')\cdot R]. \tag{3.14}$$

Note that the RHS of (3.8), apart from the surface integral, is the same as the matrix element in the preceeding equation. Similar to the double-differential cross section for scattering of neutrons, $\langle n'k'|V_{\text{per}}|nk\rangle$ factorizes into two terms that are of completely different physical origin and that are only coupled by the change of the quasi-momentum of the Bloch electrons. Both matrix elements $\mathbf{D}$ and $\langle n'k'|\tilde{W}(r)|nk\rangle_{V_c}$ are completely defined by the Bloch functions, the one-particle potential V_{eff} of the unstrained crystal and the r-dependent modified deformation potential obtained by investigating a homogeneously deformed crystal. The second factor is simply the Fourier transform of the distortion $\beta(R)$. It is solely determined by the deformation of the crystal and independent of the electronic structure. This new formalism does not distinguish between dilatations and pure shear deformation as all elements $\langle n'k'|W_{jl}|nk\rangle$ will be non-zero in a real crystal. In deriving equations (3.7) and (3.14) we have explicitly exluded the case $k' = k$, so they will not merge in the RHS of (2.11).

4. Scattering of Bloch electrons by the dilatation field of an edge dislocation

In this section the new formalism is illustrated by investigating the scattering of Bloch electrons by a non-split edge dislocation in an FCC lattice. As the evaluation of the elements of **D** is rather time consuming we restrict ourselves to the scattering by its dilatation field. In an FCC lattice the Burgers vector b, the unit vector t along the dislocation line and the unit vector n normal to the slip plane are given by

$$b = \tfrac{1}{2}(0, -1, 1) \qquad t = (1/\sqrt{6})(-2, 1, 1) \qquad n = (a/\sqrt{3})(1, 1, 1). \tag{4.1}$$

For simplicity the dilatation field obtained by the theory of linear elasticity for an isotropic medium

$$\mathrm{Tr}[\beta(r)] = \Theta(R) = -(b/2\pi)[(1-2\nu)/(1-\nu)](R\cdot n)/[(R\cdot n)^2 + (R\cdot b^0)^2] \tag{4.2}$$

is used (Kröner 1958). ν denotes Poisson's number and $b^0 = b/\|b\|$.

In order to evaluate the Fourier transform of Θ it is advantageous to use the following primitive vectors for the FCC lattice:

$$a_1 = a(1, 1, 1) \qquad a_2 = \tfrac{1}{2}a(0, -1, 1) \qquad a_3 = \tfrac{1}{2}a(1, 1, 0) \tag{4.3}$$

where a_1 and a_2 define the mesh of lattice points in the plane perpendicular to the dislocation line. As the primitive vector has a non-zero component in this plane

$$a_3 = \tfrac{1}{3}a_1 - \tfrac{1}{2}a_2 + a_{3\|} \qquad \text{with } a_{3\|} = (a/2\sqrt{6})t \tag{4.4}$$

the arrangement of the lattice points is shifted by the vector $\frac{1}{3}a_1 - \frac{1}{2}a_2$ when going from one plane to the next. After six such steps it will look the same again. Therefore, the third side of the parallelepiped introduced to define periodic boundary conditions is chosen to be $6Na_3$. The lattice points within this fundamental domain are defined by

$$R = l_1a_1 + l_2a_2 + (6l_3 + \lambda)a_3 \tag{4.5}$$

where $\lambda = 1, \ldots, 6$ and $-\frac{1}{2}N < l_1, l_2, l_3 \leqslant \frac{1}{2}N$. Using (4.4) R may be decomposed in the following way

$$R = R_\perp + v_\lambda + 6l_3'a_{3\|} \tag{4.6}$$

where

$$R_\perp = l_1'a_1 + l_2'a_2 \qquad v_\lambda = (\tfrac{1}{3}a_1 - \tfrac{1}{2}a_2)\lambda \tag{4.7}$$

are two-dimensional vectors in the glide plane. Here l_1', l_2' and l_3' are integers which may be restricted as l_1, l_2 and l_3 due to the periodic boundary conditions.

Depending on the value of λ, the Fourier transform of Θ may be split into six partial sums

$$\sum_R \exp[\mathrm{i}(k-k')\cdot R]\Theta(R) = \sum_\lambda^6 \sigma_\lambda(k-k') \tag{4.8}$$

where

$$\sigma_\lambda(p) = -\frac{b}{2\pi}\frac{1-2\nu}{1-\nu}\sum_{R_\perp}\frac{R_\perp + v_\lambda \cdot n}{(R_\perp + v_\lambda)^2}\exp[ip\cdot(R_\perp + v_\lambda)]\cdot S(p) \tag{4.9}$$

and

$$S(p) = \sum_{l_3=-N/2+1}^{N/2}\exp[i6l_3(p\cdot a_{3\parallel})] = \frac{\sin[3N(p\cdot a_{3\parallel})]}{\sin[3(p\cdot a_{3\parallel})]}. \tag{4.10}$$

Due to the periodic boundary conditions the RHS is only non-zero when $3(p\cdot a_{3\parallel})$ is a multiple of π. Thus we have

$$S(p) = \frac{\pi}{3|a_{3\parallel}|}\sum_{n=-\infty}^{\infty}\delta\left(p\cdot t - n\frac{2\pi}{a}\sqrt{\frac{2}{3}}\right). \tag{4.11}$$

As the diameter of the first Brillouin zone in the direction of the unit vector is 2.5 times $(2\pi/a)\sqrt{2/3}$ the momentum of the electrons in the direction of the dislocation line can change by the discrete values $n(2\pi/a)\sqrt{2/3}$ with $-5 \leqslant n \leqslant 5$. For this reason we expect a greater variety of scattering processes than in the continuum approximation which leaves unchanged the component of wave-vectors in the direction of the dislocation. This will have the consequence that in the directions of the dislocation line the electrical resistivity will no longer be zero, a fact first pointed out by Watts (1987).

The partial sums σ_λ are not absolutely convergent. In order to obtain finite results, the summation over $R_\perp$ may be limited to the lattice points within a circle of radius R_{max} or by a factor of convergency $\exp(-\mu|R_\perp + v_\lambda|^2)$, which allows a summation analogous to the Ewald technique. In both cases the magnitudes of μ or R_{max} are approximately given by the density of dislocation lines.

$$1/\mu = R_{max}^2 = 1/\pi n. \tag{4.12}$$

Ewald's summation technique in the present case is based on the identity

$$\frac{1}{\|R_\perp + v_\lambda\|} = \int_0^\eta \exp(-t|R_\perp + v_\lambda|^2)\,dt + \int_\eta^\infty \exp(-t|R_\perp + v_\lambda|^2)\,dt \tag{4.13}$$

where $\eta > 0$. The following steps are analoguous to the three-dimensional case yielding finally (Leibfried 1955)

$$\begin{aligned}\sigma_\lambda(p) = -\frac{b}{2\pi}\frac{1-2\nu}{1-\nu}\sum_{n=-\infty}^{\infty}\delta\left(p\cdot t - \frac{2\pi}{a}\sqrt{\frac{2}{3}}n\right)\\ \times\left\{\sum_{R_\perp\neq 0}\frac{(R_\perp + v_\lambda)\cdot n}{(R_\perp + v_\lambda)^2}\exp[ip\cdot(R_\perp + v_\lambda)]\exp(\mu|R_\perp + v_\lambda|^2)\right.\\ + i\frac{2\pi}{V_c}\sum_K \exp(-iK\cdot v_\lambda)\frac{(p_\perp + K)\cdot n}{(p_\perp + K)^2}\left[\exp\left(-\frac{(p_\perp + K)^2}{4(\mu\eta)}\right)\right.\\ \left.\left. - \exp\left(-\frac{(p_\perp + K)^2}{4(\mu)}\right)\right] - \exp(iPv_\lambda)\frac{v_\lambda\cdot n}{\|v_\lambda\|^2}\exp(-\mu v_\lambda^2)[1-\exp(-\eta v_\lambda^2)]\right\}\end{aligned} \tag{4.14}$$

where $V_c = \sqrt{\frac{6}{2}}a^2$ and $\boldsymbol{K}$ is a vector of the two-dimensional reciprocal lattice spanned by the basis vector $(2\pi/3a)(1,1,1)$ $(\pi/a)(0,-1,1)$. η is chosen in such a way that a small number of terms in the sums over $\boldsymbol{R}_\perp$ and $\boldsymbol{K}$ yield the desired accuracy. In the first sum the core of the dislocations is excluded as $\boldsymbol{R}_\perp \neq 0$. The term $\boldsymbol{K} = 0$ in the second sum comes from the far-reaching deformation field and is rapidly varying for $p_\perp \simeq 0$ (forward scattering). For $p = 0$ it is zero but in its immediate vicinity a peak with height inversely proportional to the square root of the density of dislocations occurs.

5. Solution of the Boltzmann equation

According to Fermi's golden rule the transition probability for the scattering from Bloch state $|nk\rangle$ into the state $|n'k'\rangle$ in our case is given by

$$W(nk, n'k') = (2\pi/\hbar)|\langle n'k'|V_{\text{per}}|nk\rangle|^2 \delta(E_{nk} - E_{n'k'}). \tag{5.1}$$

For edge dislocations in an FCC crystal this expression is quite anisotropic, i.e. it does not only depend on the absolute value of the change of momentum. Further complications are due to the fact that the Fermi surface of the metals in mind is quite non-spherical. Therefore, it is not possible to solve the Boltzmann equation exactly. Its approximate solution by use of the variational principle is well known. See, for example, Kohler (1948, 1949a, b), Wilson (1953) and Ziman (1960). It is based on the fact that of all functions $X_{nk,i}$ satisfying the equation

$$\frac{V_0}{(2\pi)^3}\frac{1}{2}\sum_n \int X_{nk,i}(X_{nk,i} - X_{n'k',i})W(nk, n'k')\frac{\partial f}{\partial E_{nk}}\,\mathrm{d}^3k$$
$$= \frac{e}{\hbar}\int \operatorname{grad} E_{nk}|_i \, X_{nk,i}\frac{\partial f}{\partial E_{nk}}\,\mathrm{d}^3k \qquad \text{for } i = 1,2,3 \tag{5.2}$$

the solution of the Boltzmann equation gives the left-hand-side (LHS) maximum. Here e is the electronic charge and $f(E_{nk})$ the Fermi–Dirac distribution. As the LHS is simply σ_{ii} the variational procedure approximates the diagonal elements of the tensor of the electrical conductivity from below. As usual the variational principle is solved by the use of a Ritz *ansatz* for the vector function $\boldsymbol{X}_{nk}$. In order to satisfy the translation symmetry in $\boldsymbol{k}$ space we have approximated each component of $\boldsymbol{X}_{nk}$ by a linear combination of suitably chosen monomials expressed in components of grad E_{nk}. In the case of Al to be treated in the next section a satisfactory accuracy is reached by a Ritz *ansatz* of rank 60.

6. Explicit results for edge dislocations in Al

Preliminary investigations of the change of electrical resistivity due to dislocations have been carried out for the case of Al where explicitly self-consistent band-structure calculations were available for different values of the lattice parameter (Bross and Eder 1987). These investigations are based on the MAPW formalism using the warped-muffin-tin approximation. Consequently the effective one-electron potential $V_{\text{eff}}(r)$ as well as the r-dependent deformation potential $\tilde{\boldsymbol{W}}(r)$ are obtained as functions of $|r|$ inside the muffin-tin spheres and are given by a finite series of plane waves in the interstitial. As in the case of Cu where

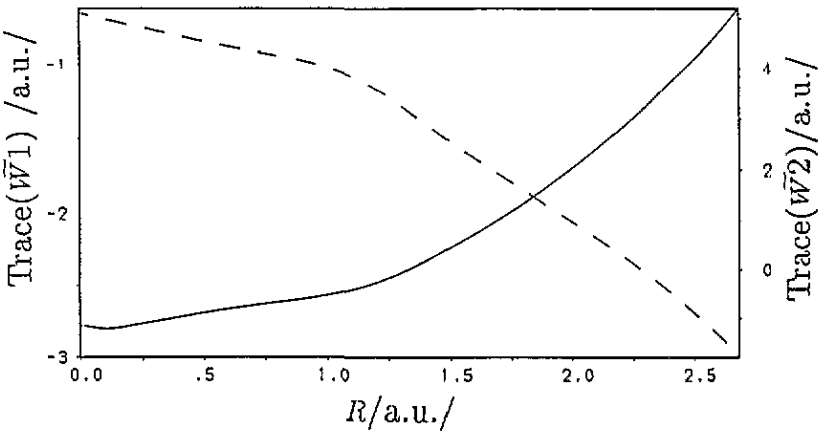

Figure 1. The deformation potential $\tilde{W}$ inside the muffin-tin sphere: full curve, as defined in equation (2.12); broken curve, next term, $\tilde{W}^{(2)}_{jj,ll}$, in the power expansion with respect to β.

full potential calculations have been performed (Fehrenbach and Bross 1993) non-spherical contributions of the potential are expected to have little influence on the present problem.

The value of $\mathrm{Tr}(\tilde{W})$ inside the muffin-tin sphere is plotted in figure 1 (full curve). It shows slowly varying behaviour even near the nucleus at $r = 0$, revealing directly the character of a screened perturbation potential. Its spherical mean value -1.57 Ryd is considerable larger than the width of the occupied conduction band (0.81 Ryd). For comparison the next term in the power expansion in β, $\tilde{W}^{(2)}_{jj,ll}$ (to be summed over repeated indices) is mapped by the broken curve. It is of the same magnitude as the term of first order with the consequence that far from the dislocation line non-linear effects can be neglected. The potential defined by equation (2.10) is plotted in figure 2. It has quite different behaviour. Starting with a rather large value, 64.7 Ryd, it reaches the value -0.15 Ryd at the surface of the muffin-tin sphere. Again the broken curve shows the next term, $W^{(2)}_{jj,ll}$, in the power expansion with respect to β which turns out to be relatively small.

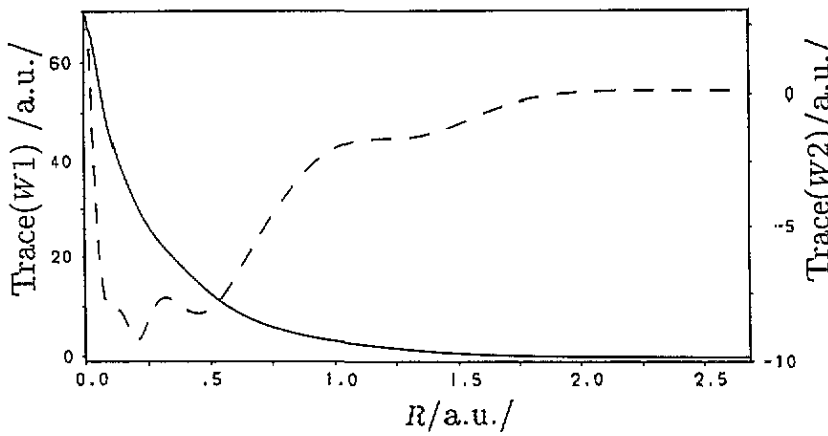

Figure 2. The deformation potential $\mathrm{Tr}(W)$ inside the muffin-tin sphere: full curve, as defined in equation (2.10); broken curve, next term, $W^{(2)}_{jj,ll}$, in the power expansion with respect to β.

The characteristics of the MAPW formalism are as cited by Bross and Eder (1987): each Bloch function is superposed by a rapidly varying part and a linear combination of plane waves with $(k+K)^2a^2/(2\pi)^2 \leqslant 14.85$. As the evaluation of the matrix elements $\langle n'k'|\,\mathrm{Tr}\,\tilde{\mathbf{W}}|nk\rangle$ is quite time consuming the number of plane waves has been restricted by $(k+K)^2(a/2\pi)^2 \leqslant 7.5$ in those contributions which have only slight influence on the final results. The corresponding error is estimated to be less than 5%.

As is common for static defects the scattering of the conduction electrons at the Fermi surface produces the electrical resistivity. According to section 4, in the present case the wave-vectors in the direction of the dislocation line can only change by a multiple of $(2\pi/a)\sqrt{\frac{2}{3}}$. Figure 3 maps the intersection of the Fermi surface with the planes $k = (2/a)\sqrt{\frac{2}{3}}tn$, $n = 0, \ldots, 5$. The closed curves within the first Brillouin zone are the relics of the second zone in the free-electron approximation whereas the small pockets at the corner of the Brillouin zone are hole states, which may be attributed to higher zones. With increasing value of $k \cdot t$ the influence of the latter regions becomes more important. Further details of the parametrization of the Fermi surface used to perform the three-dimensional integrals are desribed by one of the present authors (Häberlen 1988). We only want to mention here that the rapid oscillation of $\sigma_\lambda(k-k')$ near the forward direction was eliminated by a finer mesh of integration.

The final results are depicted in figure 4, showing the tensor of electrical resistivity per density of dislocations. ρ_{xx} and ρ_{yy} are the components of the resistivity in the slip direction and perpendicular to it, respectively, and ρ_{zz} is the component in the direction of the dislocation line. The full curve is the average $\bar{\rho} = \frac{1}{3}\,\mathrm{Tr}(\rho)$; the broken curve, with the scale on the RHS, is the anisotropy relation

$$\alpha = \tfrac{1}{2}(\rho_{xx} + \rho_{yy})/\rho_{zz} \tag{6.1}$$

originally defined by Watts (1987). In contrast to older investigations we get a significant value of the electrical resistivity in the direction of dislocation with the consequence that the anisotropy relation α reaches values between 1.0 and 1.5. Thus our investigations satisfy the criteria derived by an analysis of experimental results according to which a good theory should yield a value α less than about 1.6 (Watts 1987).

The mean value $\bar{\rho}$ has to be compared with the experimental value given by Rider and Foxon (1966). For dislocation densities in the region 1.0×10^9 cm^{-2} and 4.0×10^9 cm^{-2} they have found the value $(18 \pm 1) \times 10^{-20}$ Ω cm^3 at 4.2 K which is larger by a factor of two than our value. As was stresed by Watts (1989) other measurements suffer from the fact that the dislocation densities are underestimated. After having corrected this Watts obtained values closer to our results. Considering the approximations which we have made in the present investigation it is quite remarkable that our results are so close to the experimental ones.

7. Outlook

Within the framework of our concept a far better agreement is to be expected by considering

(i) the influence of all elements of the tensor of distortion and
(ii) higher terms in the power expansion of β.

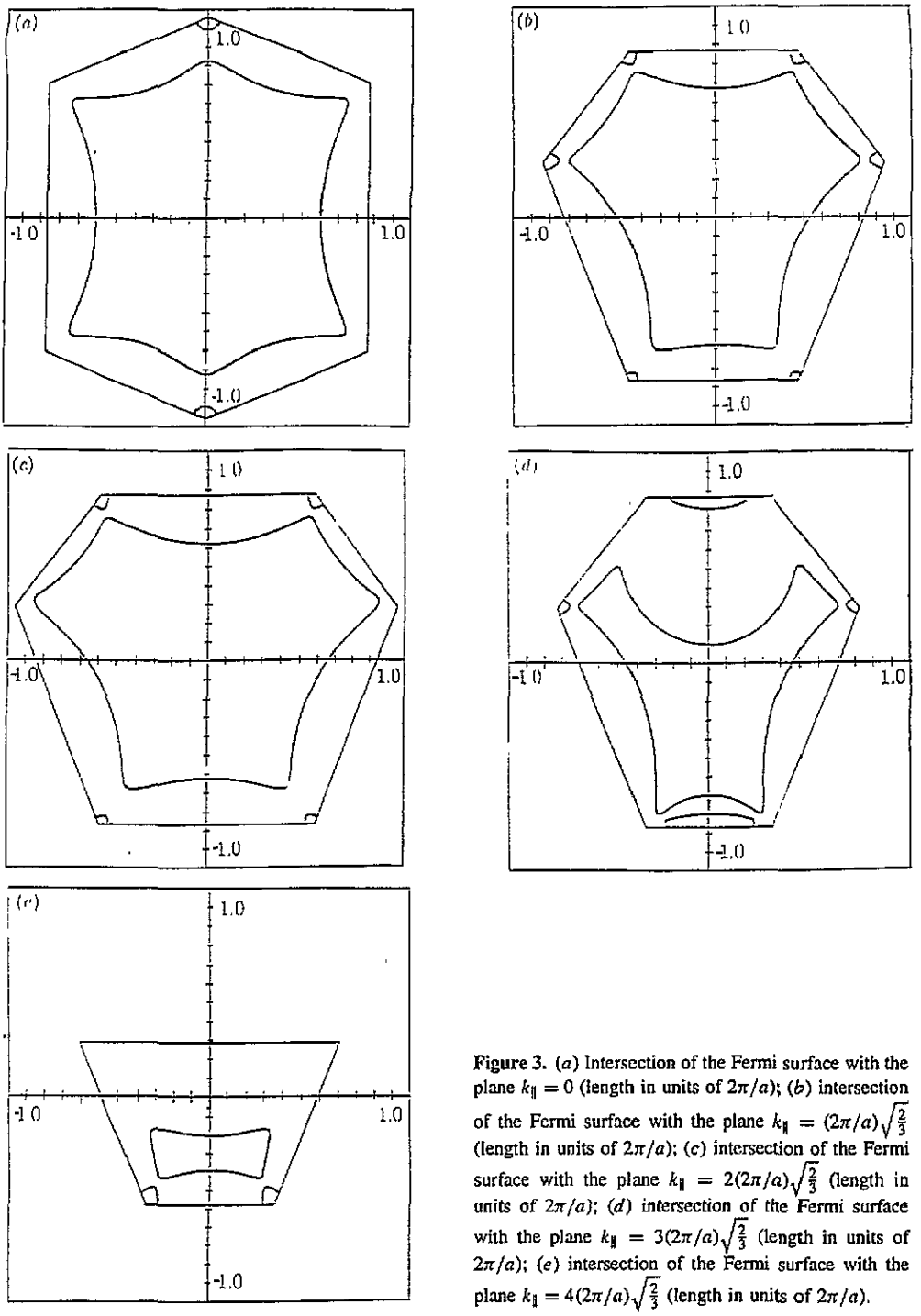

Figure 3. (*a*) Intersection of the Fermi surface with the plane $k_{\parallel} = 0$ (length in units of $2\pi/a$); (*b*) intersection of the Fermi surface with the plane $k_{\parallel} = (2\pi/a)\sqrt{\frac{2}{3}}$ (length in units of $2\pi/a$); (*c*) intersection of the Fermi surface with the plane $k_{\parallel} = 2(2\pi/a)\sqrt{\frac{2}{3}}$ (length in units of $2\pi/a$); (*d*) intersection of the Fermi surface with the plane $k_{\parallel} = 3(2\pi/a)\sqrt{\frac{2}{3}}$ (length in units of $2\pi/a$); (*e*) intersection of the Fermi surface with the plane $k_{\parallel} = 4(2\pi/a)\sqrt{\frac{2}{3}}$ (length in units of $2\pi/a$).

Certainly the scattering of the conduction electrons by the core of the dislocation will increase the electrical resistivity (Harrison 1958, Brown 1967, 1977a, b, 1978a, b, Watts 1988). In our treatment this core region may be chosen to be quite small compared to the

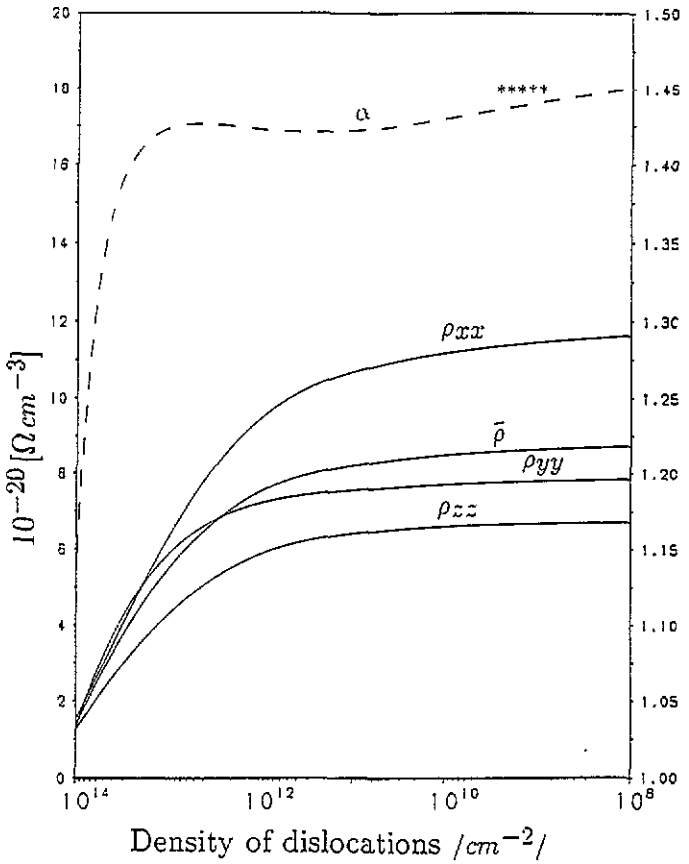

Figure 4. Change of the electrical resistivity due to edge dislocations (scale on the LHS) and the anisotropy relation α (scale on the RHS). All components of the electrical resistivity are in units of 10^{-20} Ω cm^3. ****, experimental values according to Rider and Foxon (1966).

volume covered by the dislocation. The remaining pertubation potential will be localized at the dislocation line but it is questionable whether this contribution may be approximated according to the ideas proposed by Brown. The influence of the topological singularity around the dislocation as described by Kawamura (1978a, b, 1982), Yosida and Kawamura (1979) and Teichler (1981, 1985) may have an influence, but even the magnitude of this effect is not known.

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