INFLUENCE OF LATTICE DEFECTS ON THE ELECTRICAL PROPERTIES OF COLD-WORKED METALS

H. G. VAN BUEREN

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STELLINGEN

I.

De vorm van de door Lifshits afgeleide uitdrukking voor de wisselwerkingskracht tussen twee lichamen met willekeurige complexe diëlectriciteitsconstante suggereert dat deze ook kan worden verkregen uit een beschouwing van de eigentrillingen van het systeem.

E. M. Lifshits, Z. exp. theor. Phys. **29**, 94, 1955.

II.

De door Leech afgeleide formule voor de geretardeerde wisselwerkingskracht tussen twee atomen is onjuist.

J. W. Leech, Phil. Mag. **46**, 1328, 1955.

III.

Conclusies volgende uit overwegingen omtrent de zogenaamde "steric hindering" ter verklaring van het verschil in eigenschappen van verwante legeringen, hebben slechts zeer beperkte waarde. Dit geldt zowel voor substitutionele als voor interstitiële legeringen.

IV.

Volgens Gordon en Nowick zou de „snelle" verkleuring van NaCl-kristallen onder röntgenbestraling samenhangen met reeds vóór de bestraling aanwezige chloorvacatures. Deze bewering is slechts houdbaar indien bovendien wordt verondersteld dat de betreffende kristallen ten minste 0·01 atoomprocent verontreinigingen bevatten.

R. B. Gordon en A. S. Nowick, Phys. Rev. **101**, 977, 1956.

V.

De berekening door Mason van de dislocatiedichtheid in metalen uit de waargenomen mechanische hystereseverliezen bij hoge frequenties is niet juist.

W. P. Mason, Bell System techn. J. **34**, 903, 1955.

VI.

Het voorkomen van een incubatietijd bij de plastische deformatie van germanium en silicium is een mogelijke aanwijzing voor het bestaan van stabiele, relatief gering beweeglijke toestanden van de dislocaties in deze stoffen.

R. G. Treuting, J. Metals **7**, 1027, 1955.

VII.

De bepaling van de dislocatiedichtheid in germanium en silicium uit de telling van het aantal door een bepaalde etsing teweeggebrachte etsputten, dient noodzakelijk gecalibreerd te worden met behulp van een onafhankelijke methode, vóórdat uit de tellingen conclusies mogen worden getrokken.

VIII.

Ter toetsing van de theorie van Brinkman over de vorming van "displacement spikes" tijdens de bestraling van metalen met neutronen of andere nucleonen, zou het aanbeveling verdienen de magnetische weerstandsverandering van dusdanig bestraalde materialen te onderzoeken als functie van de temperatuur tijdens en na de bestraling.

J. A. Brinkman, J. appl. Phys. **25**, 961, 1954;
Dit proefschrift, pag. 86.

IX.

Voor de toepassing van dislocatievrije materialen moet, indien deze in de naaste toekomst ter beschikking komen, in de eerste plaats worden gedacht aan het gebied der halfgeleiders.

X.

Ter verklaring van de interstellaire polarisatie is het niet noodzakelijk het bestaan van langgerekte stofdeeltjes aan te nemen.

L. Davis, Vistas in Astronomy I, Pergamon Press, London 1955, p. 336.

XI

Foto-electrische waarnemingen van de eclipsveranderlijke RZ Cassiopeiae geven aanleiding tot het vermoeden dat de atmosfeer van de heldere component op sterke en onregelmatige wijze wordt beinvloed door de zwakke component. Het is mogelijk dat dit effect verantwoordelijk is voor de variaties van de periode.

R. Szafraniec, Acta Astronomica, Sér b, **2**, 86, 1952;
C. M. Huffer en Z. Kopal, Astrophys. J. **114**, 297, 1951.

XII.

De schildering van het karakter van beoefenaren der exacte wetenschappen door litteratoren van naam werpt vaak een verkeerd licht op de habitus van deze onderzoekers.

XIII.

Het schrijven van populair-wetenschappelijke lectuur door personen die niet actief in de door hen behandelde tak van wetenschap werkzaam zijn, moet ten stelligste worden afgekeurd.

INFLUENCE OF LATTICE DEFECTS ON THE ELECTRICAL PROPERTIES OF COLD-WORKED METALS

PROEFSCHRIFT

TER VERKRIJGING VAN DE GRAAD VAN
DOCTOR IN DE WIS- EN NATUURKUNDE
AAN DE RIJKSUNIVERSITEIT TE LEIDEN
OP GEZAG VAN DE RECTOR MAGNIFICUS
DR. A. E. VAN ARKEL, HOOGLERAAR IN DE
FACULTEIT DER WIS- EN NATUURKUNDE,
TEGEN DE BEDENKINGEN VAN DE FACULTEIT DER WIS- EN NATUURKUNDE TE
VERDEDIGEN OP DINSDAG 10 JULI 1956
TE 16 UUR

DOOR

HENDRIK GERARD VAN BUEREN

GEBOREN TE ROTTERDAM IN 1925

PROMOTOR:
PROF. DR. H. B. G. CASIMIR

CONTENTS

GENERAL INTRODUCTION

The mechanism of plastic deformation of crystalline solids depends primarily on the behaviour of lattice defects, such as dislocations, vacancies and interstitial atoms. The motion of dislocations gives rise to the well-known phenomenon of glide or slip in metals. In order to explain the large plastic deformation of metals under the influence of moderate stresses, not only the motion but also the formation of large numbers of dislocations by the action of the stress must be understood. Motion of dislocations in imperfect crystals is accompanied by the formation of vacancies and interstitials. Thus in a plastically strained metal all three kinds of defects are present. They affect appreciably the physical properties of the material, such as the electrical resistivity, the thermo-electric power and the magnetoresistance, as well as the X-ray diffraction pattern, the density, etc.

To study the mechanism of plastic deformation of metals, it is therefore useful to direct attention not only to the mechanical properties affected, or to the surface phenomena such as slip line pattern, deformation bands, etc., but also to the general physical properties of the metal.

In this paper the change of electrical resistivity and of magnetoresistivity, caused by plastic deformation, of the monovalent metals copper, silver and gold will be studied, from a theoretical as well as from an experimental point of view. From this study several conclusions will be drawn as to the concentrations, the diffusive properties and the electric scattering power of the various defects formed.

The first chapter is devoted to a discussion of current ideas about the fundamental properties of the defects mentioned and of their occurrence in well-annealed metals. In chapter 2 the behaviour of the defects under stresses exceeding the elastic limit of the metal are discussed and a simple model theory describing the situation in plastically deformed metals is proposed. Theoretical relations are derived between the amount of deformation and the concentrations of the various defects present in the lattice after the deformation. In chapter 3 the change of electrical resistivity of a metal during plastic deformation is discussed and related to the formation of defects. Various experiments are described and their results compared to the theoretical deductions. Chapter 4 deals with the change of resistance of plastically strained metals in a transverse magnetic field. From theoretical considerations it follows that under these circumstances the dislocations can be studied independent of other defects. Chapter 5 is devoted to the study of the thermal recovery phenomena of the electrical properties of deformed metals. Similar recovery phenomena in irradiated and rapidly quenched metals are also considered. Chapter 6 summarizes the conclusions that can be drawn from our investigations.

1. PROPERTIES OF LATTICE DEFECTS

1.1. Dislocations

A complete review of the properties of dislocations cannot be given in this paper; only those aspects to be used in the later sections will be dealt with. For instance, the elastic and dynamic properties of dislocations will not be discussed at all. Detailed accounts on the structure and elementary properties of dislocations can be found in the book of W.T. Read [1]); a fairly complete discussion of the effects of dislocations on the mechanical properties of metals is given by A. H. Cottrell in his monograph [2]), while the mathematical theory of dislocations has been extensively presented by F. R. N. Nabarro [3]). Recently, nearly all these aspects of the dislocation problem have been discussed anew by A. Seeger [4]).

1.1.1. Structure of dislocations

Dislocations were originally introduced into the formal theory of elasticity [5]) by considering a multiply connected body, in which a cut has been made to render it simply connected. By displacing the two cut surfaces, possibly adding or removing some material, and finally joining the surfaces again, a state of strain is obtained which was called a dislocation. In order to ensure everywhere finite and differentiable strains, the relative displacement of the cut surfaces should be compatible with the displacements of a rigid body [5]). According to this condition, the relative displacement of neighbouring points on either side of the cut is given by an expression of the form:

$$\delta u_i = b_i + \sum_j d_{ij}\, x_j, \qquad (1.1)$$

where x_j denote the coordinates of the point, the three constants b_i specify the relative translation of the cut surface and the three constants d_{ij} $(= -d_{ji})$ specify the relative rotation.

A general dislocation is thus described by six constants, or, it can be considered that a general dislocation is in fact built up out of six elementary dislocations, each of them characterized by only one constant, the other five being zero. These elementary dislocations can be illustrated as follows (fig. 1). Consider a hollow cylinder with a cut in its mantle parallel to the axis. A dislocation is formed by displacing the cut surfaces with respect to each other. The six types can be divided into three classes:

(1) Only a translation is present normal to the length direction of the cut. These dislocations are called *edge* dislocations (*b*, *c*).

(2) Only a translation is present parallel to the length direction of the cut. These dislocations are called *screw* dislocations (*d*).

(3) Only a relative rotation of the cut surfaces has been applied. These

dislocations give rise to finite strains at infinity, and do not occur in the ordinary theory of plasticity (*e*, *f*, *g*).

This general concept of dislocations has been applied by J. M. Burgers 6) to the case of glide in solids. He considers an isotropic solid, from which a thin filament of matter in the form of a closed loop has been removed (corresponding to the hole in the cylinders in fig. 1). By displacing the two surfaces of a cap whose edge is formed by the loop, over an amount **b** a dislocation is created, viz. of type (1) or type (2) or a mixture of the two. The strains are largely concentrated around the loop; this is called the dislocation line.

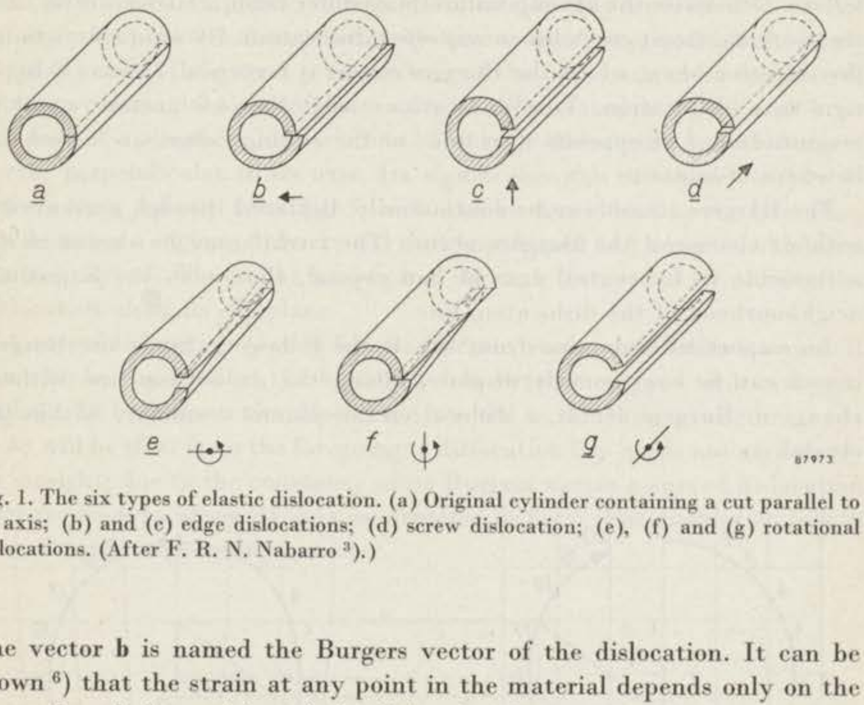

Fig. 1. The six types of elastic dislocation. (a) Original cylinder containing a cut parallel to its axis; (b) and (c) edge dislocations; (d) screw dislocation; (e), (f) and (g) rotational dislocations. (After F. R. N. Nabarro 3).)

The vector **b** is named the Burgers vector of the dislocation. It can be shown 6) that the strain at any point in the material depends only on the vector **b** and the position of the dislocation line; it is independent of the form of the cap.

Frank 7) introduced the dislocation concept in a way especially suited to crystalline solids built on a spatial lattice. In an ideal crystal, the atoms are situated at places

$$\mathbf{r} = l\mathbf{a} + m\mathbf{b} + n\mathbf{c} \, . \tag{1.2}$$

In reality, ideal crystals do not exist, and (1.2) describes the positions of the atoms only approximately; there are internal vibrations, and various atoms are missing, others occupy interstitial sites, etc. However, comparing actual and ideal crystals, one can try to establish a one to one correspondence between the atoms in both crystals. Regions in the actual crystal where this is possible are called *good* regions; regions where such a correspondence can not be unambiguously established are named *bad* regions. Consider a closed circuit (Burgers circuit) in the real crystal. It is always possible to define an associated circuit in the ideal crystal, which, however, is not necessarily closed. When it is not closed, the Burgers circuit is said to encircle one or more dislocations (fig. 2). When the Burgers circuit runs entirely through good crystal, the associated circuit, if not closed, has necessarily a closing failure which is equal to a lattice vector. One then speaks of a *perfect* dislocation, with a Burgers vector equal to that closing failure. Otherwise the closing failure may differ from a lattice vector, and the Burgers circuit encircles an *imperfect* dislocation. By uniquely defining the direction along which the Burgers circuit is traversed, one can assign a sign to a dislocation. Two dislocations with Burgers vectors equal in magnitude but of opposite directions of the closing failure are called dislocations of opposite sign.

The Burgers circuit can be continuously displaced through good crystal without change of the Burgers vector. The circuit may be shrunk as far as possible to its central core of bad crystal, that is to the immediate neighbourhood of the dislocation line.

An important deduction from this is the following: Since the Burgers circuit can be continuously displaced along the dislocation line without change in Burgers vector, a dislocation line cannot terminate within the crystal.

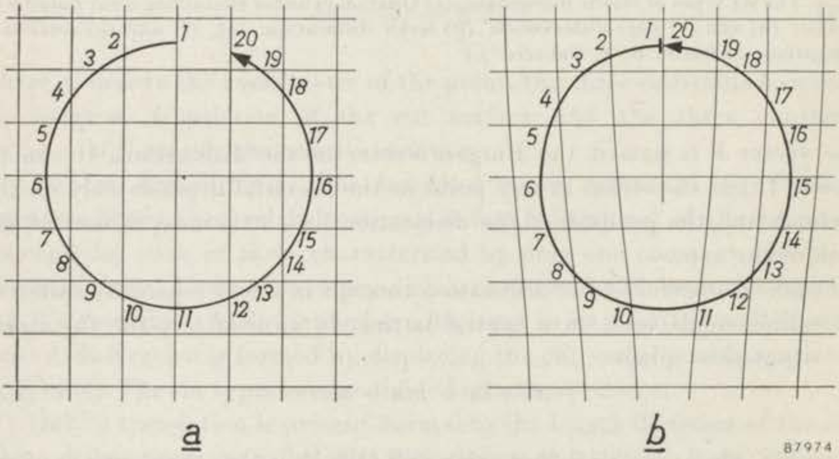

Fig. 2. Ideal (a) and real (b) crystal. The latter contains a dislocation. The Burgers circuit encircling it has an associated circuit in the ideal crystal with a closing failure equal to the Burgers vector of this dislocation. Corresponding intersections of the circuit with lattice planes have been denoted by corresponding figures.

A dislocation line can branch. Taking the Burgers circuit through good crystal and large enough to encircle the branches, its Burgers vector remains constant as the circuit is displaced past the branchpoint. Thus the vector sum of the Burgers vectors of the branches is equal to the Burgers vector of the unbranched dislocation. Along an unbranched dislocation the Burgers vector has everywhere the same modulus and direction.

From the above general considerations it follows that dislocations in crystals are linear defects characterized by two vector quantities, namely a unit vector denoting the local direction of the dislocation line and the Burgers vector, which measures the resultant displacements of the atoms.

In the theory of plastic deformation, one is only interested in lattice defects which cause a strain that tends to zero at infinity, and therefore only types (1) and (2) of page 4 (or a mixture of the two) have to be considered. These two principal types of dislocation are illustrated in figs 3 and 4 for the case of a simple cubic structure. The edge dislocation has its Burgers vector perpendicular to its axis. Its significance for the theory of plastic deformation follows from fig. 3, as it can be considered as the boundary line between a region of the crystal that has slipped and a region which has not yet slipped. Slip can be propagated through the crystal by moving the dislocation along its slip plane.

A screw dislocation (fig. 4) has its Burgers vector parallel to its axis. It can also be regarded as the boundary line between slipped and unslipped regions. In both cases the slip vector is equal to the Burgers vector.

As will be clear from the foregoing, a dislocation line needs not necessarily be straight; due to the constancy of its Burgers vector a curved dislocation changes its type along its axis, as depicted in fig. 5. For most of its length it is of mixed edge-screw character.

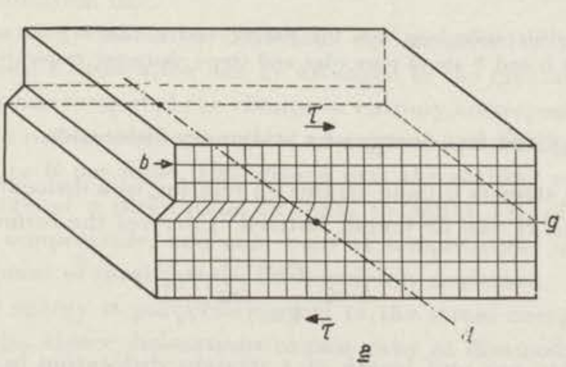

Fig. 3. Perspective diagram of an edge dislocation that has progressed halfway through a crystal. The dotted line *d* is the dislocation axis; the drawn lines represent atomic planes. The Burgers vector **b** is perpendicular to the axis. To complete the shear, the dislocation must move along the slip plane *g* in the direction of **b**.

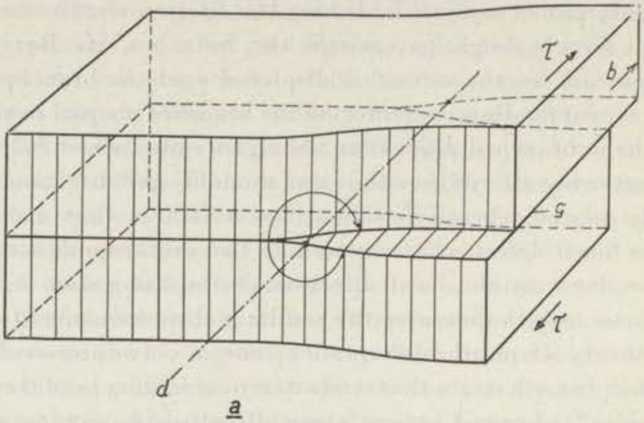

Fig. 4. Perspective diagram of a screw dislocation that has progressed halfway through the crystal. The letters have the same meaning as in fig. 3. To complete slip, the dislocation has to move over the slip plane *g* perpendicular to its Burgers vector **b**.

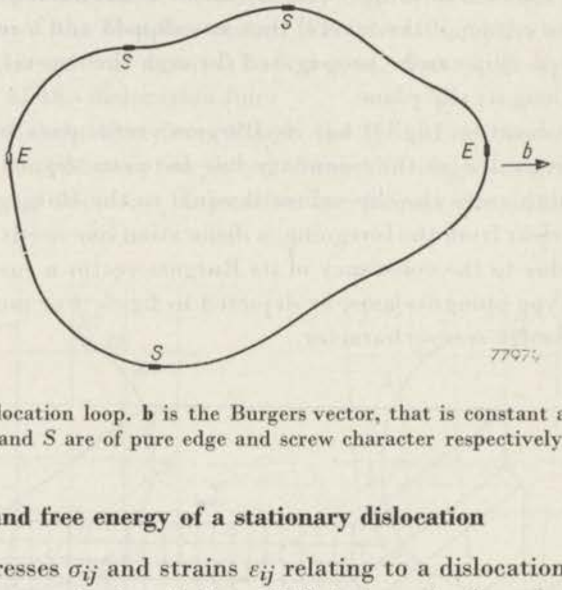

Fig. 5. Closed dislocation loop. **b** is the Burgers vector, that is constant along the loop. Only the parts *E* and *S* are of pure edge and screw character respectively.

1.1.2. Energy and free energy of a stationary dislocation

When the stresses σ_{ij} and strains ε_{ij} relating to a dislocation are known, its strain energy can be found. Cottrell [2]) derives the formula:

$$U \approx \frac{Gb^2}{4\pi a} \log\left(\frac{r_1}{r_0}\right) \tag{1.3}$$

for the energy per unit length of a straight dislocation in a simple cubic lattice with atomic spacing *b*. For an edge dislocation, $a = 1 - \nu$, for a screw dislocation $a = 1$, where ν is Poisson's ratio; *G* is the shear modulus. Additional terms arising from the finite dimensions of the material are left out of account here; r_1 denotes the extent of the strain field of the dislocation, r_0 the radius of a cylindrical region around the axis of the dislocation within which the strains become so large that Hooke's law is no longer valid. If we put r_0 equal to one atomic distance, the strains at the surface of the inner cylinder are already of the order $^1/_4$, which are much to large for ordinary elasticity theory to be applicable. We shall therefore take $r_0 = 10^{-7}$ cm. In an ordinary crystal one may take r_1 to be of the order of 1 cm, thus one has

$$U \approx \frac{4Gb^2}{\pi a} \tag{1.3a}$$

for the energy per unit length. In copper, this energy works out to 5.10^{-4} erg/cm, or about 8 eV per atomic plane perpendicular to its axis for an edge dislocation, and about 5 eV for a screw dislocation.

Various authors have tried to determine somewhat more accurately the energy of dislocations of arbitrary type in various crystal structures. The most recent results have been obtained by Foreman ^{8}); they confirm the values quoted above. The difference in energy between the various types are relatively small, and no conclusion is possible as to what kind of dislocation may be expected to be most probable. The uncertainty is largely due to the unknown energy contained in the dislocation core.

Cottrell ^{2}) has estimated the amount of energy concentrated within r_0, and finds this to amount approximately to $^1/_3\, Gb^3$ per atomic plane, which is of the order of 1 eV and thus not very small compared to the strain energy outside r_0 (therefore it plays an important part when the distinction between two kinds of dislocations is studied). It is an interesting property of a dislocation that about half of its strain energy arises from regions outside 10^{-4} cm from the dislocation line.

The presence of a dislocation increases the disorder of the crystal. On the other hand a dislocation can be arranged in the crystal in various ways. Cottrell ^{2}) has computed the change in entropy corresponding to the introduction of a dislocation in a crystal of unit volume, finding ΔS to be minus a few times R per mole. This means that the entropy contribution to the free energy of a dislocation amounts to about 1% of the strain energy at room temperature, and can, even at temperatures of the order of the melting point of most metals, be completely neglected.

Thus the free energy is practically equal to the strain energy which is positive and large. Hence dislocations cannot exist as thermodynamically stable lattice defects.

1.1.3. Motion of dislocations

Slip is based on the motion of dislocations. The above discussion already yields some insight into the kinematical properties of dislocations. Following Frank [7]), we consider a Burgers circuit anywhere in the (actual) crystal and let a dislocation line move from outside to inside the circuit. The closing failure of the associated path, which may originally have been zero or finite, is then changed by the Burgers vector **b** of the dislocation. Two adjacent ions on the circuit between which the dislocation has passed are thus displaced by an amount approximately equal to **b** relative to each other (the displacement is measured in the actual crystal and needs thus not be exactly equal to **b**).

Let **n** be the unit vector normal to the planar area that has been swept by an infinitesimal segment $d\sigma$ of the dislocation line. Then with this movement a change of volume occurs which, per unit area swept, is equal to (**b**.**n**). If the movement is such that this product is zero, there is no

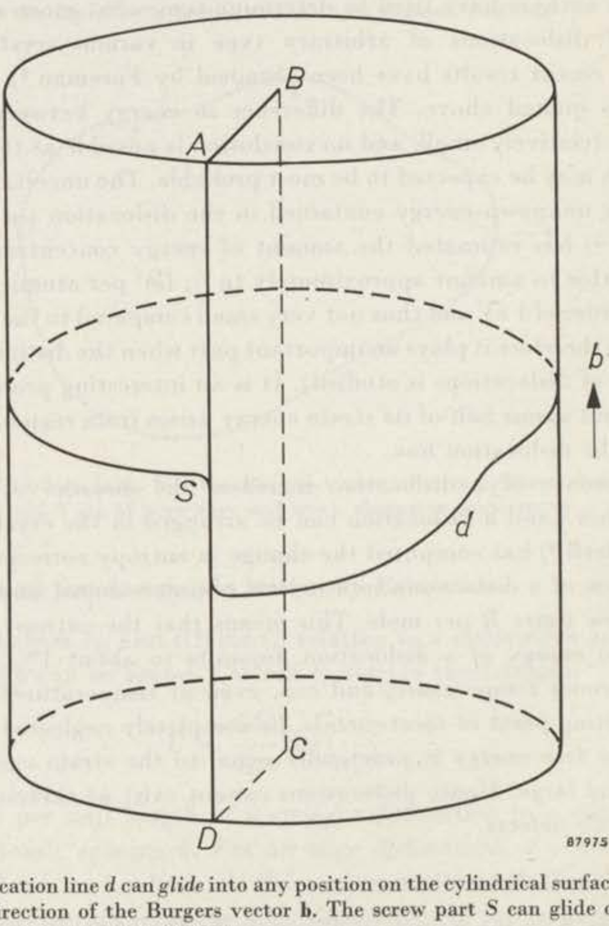

Fig. 6. The dislocation line *d* can *glide* into any position on the cylindrical surface containing itself and the direction of the Burgers vector **b**. The screw part *S* can glide on any plane through its axis, e.g. the plane *ABCD*.

volume change and the dislocation is said to *glide*. Glide motions thus occur when the dislocation line moves in a surface containing itself and its Burgers vector (fig. 6), this is termed its glide surface or slip surface. It is easily seen that all motions of pure screw dislocations are pure glide motions.

For dislocations with some edge character, however, glide motion can occur only on a definite glide plane. From fig. 6 it follows that glide motions are characterized by the property that the projection of the dislocation line on a plane perpendicular to the Burgers vector is invariant in area and shape.

All motions not satisfying this condition necessitate the production of vacancies resp. the transfer of interstitial atoms to lattice sites when $(\mathbf{b}.\mathbf{n})$ is positive, or the production of interstitial atoms resp. the removal of vacancies when $(\mathbf{b}.\mathbf{n})$ is negative. Such motions, when occurring at not too high temperatures, bring about an appreciable change in the free energy of the crystal and are therefore only possible under appreciable forces. They are called *climb* motions. Glide motions on the contrary take place already under very slight forces.

Forces on dislocations

In this study we are not concerned with the elastic and dynamic properties of dislocations. Nevertheless, the concept of the force on a dislocation should be touched upon, as it arises in several connections later on. The force exerted on a dislocation by an elastic stress field $\mathbf{P}$ can be introduced as follows. If a line element $d\sigma$ of a dislocation moves so as to sweep a planar element of area $d\mathbf{n} = d\sigma \times d\mathbf{x}$, than the traction on the element is $\mathbf{n}.\mathbf{P}$, and the work done by the field in this motion is $(\mathbf{n}.\mathbf{P}).\mathbf{b} = (\mathbf{b}.\mathbf{P}).\mathbf{n}. = (\mathbf{b}.\mathbf{P}).(d\sigma \times d\mathbf{x}) = [(\mathbf{b}.\mathbf{P}) \times d\sigma].d\mathbf{x}$. The force $d\mathbf{F}$, exerted by the elastic field $\mathbf{P}$ on the element $d\sigma$ of the dislocation can thus be defined as 3,7):

$$d\mathbf{F} = (\mathbf{b}.\mathbf{P}) \times d\sigma\,.$$

If only a uniform shear stress τ acts in the direction of the Burgers vector, it is easily seen that

$$\mathbf{F} = \tau\mathbf{b} \tag{1.4}$$

per unit length.

We shall now discuss the motion of dislocations in more detail.

1.1.3.1. *Glide motion*

In the presence of an elastic stress field, the component of the force on a dislocation that is acting in the plane tends to move the dislocation in that plane. Such a motion is a glide motion, no volume changes are connected with it. However, still a small force is needed, as naturally in a crystal, when a dislocation is displaced from a symmetrical position to an unsymmetrical one, this displacement is opposed by a force. This force is due to the fact that the atoms near to the slip plane are no longer in equivalent positions on opposite sides of the dislocation. Its magnitude depends on the variation, with the position of the dislocation, of the energy of misfit between the faces of the slip plane. Following Peierls [9]) we assume in a simple cubic lattice with lattice spacing b a sinusoidal relation to exist between the shear stresses acting on the atoms on both sides of the slip plane and the deviations u of these atoms from their symmetrical positions:

$$\tau = \frac{G}{2\pi} \sin \frac{4\pi u}{b}. \tag{1.5}$$

The total energy of misfit of a row of atoms of unit length parallel to the dislocation is

$$E_m = \int b\tau \, du. \tag{1.6}$$

Thus:

$$E_m = \frac{Gb}{4\pi} \int\limits_{u=b/4}^{u} \sin \frac{4\pi u}{b} \, du = \frac{Gb^2}{8\pi^2} \left[1 + \cos \frac{4\pi u}{b} \right]. \tag{1.7}$$

Let the distance of the centre of the dislocation to the nearest position of symmetry be ab, where a is variable. Then we can describe the relative positions of the atoms on both sides of the slip plane approximately by

$$u = \frac{b}{2\pi} \operatorname{arc\,tan} \frac{x}{\zeta},$$

where $x = (a + {}^1/_2 n)b$; $n = 0, \pm 1, \pm 2, \ldots\ldots$, and $\zeta = qb/2(1 - \nu)$, where q is a factor depending on the exact form of the law of force (1.5) between the atoms. It is unity for a pure sinusoidal law, and may be 5 in actual cases; ζ is a measure for the *width* of the dislocation. Summing (1.7) over all these positions, the misfit energy can be shown to depend on a as [3])

$$E_m = \frac{Gb^2}{2\pi(1-\nu)} \, e^{-4\pi\zeta/b} \cos 4\pi a. \tag{1.8}$$

By differentiating (1.8) we find for the force on a dislocation preventing its movement:

$$F = \frac{2Gb}{1-\nu} \, e^{-4\pi\zeta/b} \sin 4\pi a. \tag{1.9}$$

According to (1.4) the theoretical critical shear stress acting in the glide plane needed to move the dislocation is

$$\tau_{cr} = \frac{F_{\max}}{b} = \frac{2G}{1-\nu} \, e^{-4\pi\zeta/b}. \tag{1.10}$$

The magnitude of this stress depends very sensitively on the width of the dislocation and thus on the exact form of the shear stress function (1.5) and on the crystal structure. In actual crystal lattices ζ can be decreased in the ratio: lattice spacing in a direction perpendicular to the slipplane to lattice spacing in the glide direction (= Burgers vector). This can give an appreciable effect in τ_{cr}, especially when slip occurs on close-packed planes. It has not yet been possible to make a reliable estimate of ζ (see e.g. Foreman, Jaswon and Wood [10])) and hence the theoretical critical shear stress to move a dislocation cannot be computed even to the order of magnitude. However, it is certainly several orders of magnitudes smaller than the theoretical critical shear stress of a perfect crystal, which is of the order of $G/10$ [11]).

It is this property of dislocations, viz. the low theoretical value of the shear stress needed to move them across their glide plane, which makes these lattice defects so important in plastic flow. The observed critical shear stress for plastic deformation of actual metal single crystals is of the order of 10^{-5} to 10^{-3} G, thus much smaller than the theoretical critical shear stress of a perfect crystal. Polycrystalline materials show a higher critical shear stress, yet always much smaller than this theoretical value (except in some cases of especially hardened materials). This discrepancy can only be explained by the fundamental assumption that slip takes place by glide motion of dislocations.

In actual cases, the motion of dislocation is not only hindered by the "fundamental" Peierls force discussed above, but to a large extent by the presence of other lattice defects in the crystal. As Seeger [12]) has pointed out, the Peierls force may nearly always be neglected compared to these other influences, except maybe at very low temperatures. Leibfried [13]) has indicated however, that even then the Peierls force is easily overcome by the thermal vibrations and the zero point vibrations of the lattice.

However, the conclusion that dislocations are relatively very mobile lattice defects remains valid, also when the influence of other lattice defects is taken into account (see also chapter 2).

During glide motion a dislocation can reach considerable velocities. The ultimate velocity limit is that of sound in the metal, but dislocations cannot reach this limit because of the large energy dissipation that occurs by reason of the interaction with the lattice vibrations (generation of heat or sound waves). An exact treatment of this problem has not yet been possible. Associated with a moving dislocation is a *kinetic energy*, arising from the atomic motions constituting the dislocation motion. This energy increases with the dislocation velocity, particularly because the width of the dislocation decreases. This decrease in width is similar to the relativistic contraction of a yard stick, the width tending to zero as the velocity approaches its upper limit. The kinetic energy becomes comparable to the elastic energy of a stationary dislocation at speeds of the order of one tenth of the velocity of sound, which will therefore be the order of magnitude of the actual velocity limit of dislocations.

1.1.3.2. *Climb motion*

Motion of a dislocation out of its glide plane necessitates a change of volume, as explained above. Such motion is illustrated in fig. 7. With a dislocation of not pure screw character (for a pure screw dislocation each lattice plane through its axis is a glide plane) is associated an extra half-plane of atoms, as can also be seen from fig. 3. The motion of the dislocation outside its glide plane is accompanied by a change of the dimensions of this half plane. That is to say, some of the atoms belonging to the half plane have to disappear somewhere in the lattice, or new atoms have to be added to it. The transport of atoms through the lattice has to take place by *diffusion*.

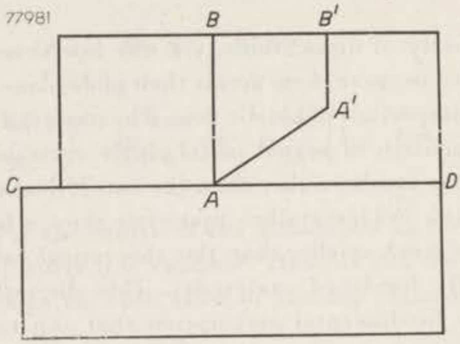

Fig. 7. Climb motion of a dislocation of not pure screw character (axis perpendicular to the plane of drawing). When the dislocation axis moves from A to A', the extra half-plane BA becomes $B'A'$, that is, it becomes shorter. Some atoms have therefore to diffuse away. (After A. H. Cottrell[2]).)

This does not seriously impede climb as a possible form of motion, if the temperature of the crystal is high enough for diffusion to take place as rapidly as is needed to maintain the structure during the motion. However, for most metals at room temperature or below, diffusion is a slow process and the climbing dislocation leaves in its wake a sheet of vacancies or interstitial atoms. With climb of dislocations therefore an *activation energy* is associated, either for diffusion or for formation of defects, or for both.

The reverse process is the absorption of vacancies or interstitial atoms at dislocations, thereby causing the dislocation to climb. This process also occurs only appreciably at fairly high temperatures, and is manifested e.g. in the phenomenon of polygonization.

Consider a segment $d\sigma$ of a dislocation line. Let the distance travelled by the dislocation be $\mathbf{dx}$. The change of volume associated with this motion is equal to

$$\Delta V = \mathbf{b} \cdot (\mathrm{d}\sigma \times \mathbf{dx}) , \tag{1.11}$$

which can also be written as:

$$\Delta V = \mathbf{dx} \cdot (\mathbf{b} \times \mathrm{d}\sigma) . \tag{1.12}$$

From these formulae it can be inferred that the change of volume, that is to say the number of vacancies or interstitial atoms left in the wake of a dislocation of unit length, per unit area travelled is proportional to

$$b \sin \alpha \cos \beta , \tag{1.13}$$

where α is the angle between Burgers vector and dislocation line and β is the angle between the direction of motion and the normal to the glide plane.

The climb motion, or as it is also called the *unconservative* motion of dislocations does occur not only when absorption of vacancies or interstitials takes place, but also after two dislocations on different glideplanes have intersected each other. Then in each of the two dislocations a *jog* is formed, the magnitude and direction of each being given by the Burgers vector of the other dislocation (see for a detailed treatment the book [1]) of Read). This jog can be considered as a short piece of dislocation. According to the theorem of the conservation of the Burgers vector (section 1.1.1) the Burgers vector of the jog is the same as that of the dislocation in which it occurs. Suppose now that one of the crossing dislocations (Burgers vector $\mathbf{b}_1$) undergoes a glide motion (for instance under the action of a shear stress), and the other dislocation (Burgers vector $\mathbf{b}_2$) is fixed. Then, after crossing, the jog formed in the moving dislocation will have to move together with the dislocation to which it belongs. In general it will then perform an unconservative type of motion. The glide plane of the jog is defined as the plane through its axis, that is a line parallel to the Burgers vector $\mathbf{b}_2$ of the fixed dislocation, and its own Burgers vector, that is the Burgers vector $\mathbf{b}_1$ of the moving dislocation. The direction of motion, given by the vector $\mathrm{d}\mathbf{x}$, is such that for the element (considered straight) of the moving dislocation $\mathrm{d}\sigma_1$ in which the jog occurs, the condition:

$$\mathrm{d}\mathbf{x} \,.\, (\mathbf{b}_1 \times \mathrm{d}\sigma_1) = \mathrm{d}\sigma_1 \,.\, (\mathrm{d}\mathbf{x} \times \mathbf{b}_1) = 0 \tag{1.14}$$

is fulfilled. The condition for glide motion of the jog reads however:

$$\mathrm{d}\mathbf{x} \,.\, (\mathbf{b}_1 \times \mathbf{b}_2) = \mathbf{b}_2 \,.\, (\mathrm{d}\mathbf{x} \times \mathbf{b}_1) = 0 \,. \tag{1.15}$$

The second edition can be fulfilled together with the first one when either $\mathrm{d}\mathbf{x} \times \mathbf{b}_1 = 0$, that is when the moving dislocation has pure edge character, or when $\mathbf{b}_2$ lies in the glide plane of the moving dislocation. In general, however, $\mathbf{b}_2$ has a component normal to the glide plane of the moving dislocation and the latter has not pure edge character; the jog will then leave a trail of vacancies or interstitial atoms.

Thus, for example, two crossing screw dislocations ($\mathrm{d}\mathbf{x} \times \mathbf{b}_1$ is a maximum) that are mutually perpendicular acquire jogs which on further movement leave a trail of vacancies or interstitials that are spaced only one atomic distance from each other (maximum efficiency of jog formation).

In the general case of two dislocations of arbitrary character crossing under an arbitrary angle, the efficiency of vacancy formation (or interstitial formation) of the jogs formed can be found as follows. According to (1.12) the volume change due to the motion of the jog in the moving dislocation is given by

$$\Delta V_j = \mathbf{b}_2 \cdot (\mathbf{dx} \times \mathbf{b}_1)\,. \tag{1.16}$$

Now $\mathbf{dx}$ can be taken perpendicular to $d\sigma_1$, for the only physically interesting component of motion of the dislocation line is that perpendicular to itself, the component parallel to the line being of no interest. Thus it is found from (1.16) that the efficiency of defect formation is given by

$$e \sim (\mathbf{b}_1 \cdot d\sigma_1) \times (\mathbf{b}_2 . \mathbf{n}_1)\,, \tag{1.17}$$

where $\mathbf{n}_1$ stands for the unit vector normal to the glide plane of the moving dislocation. This formula confirms the conclusions already reached in the discussion above: jogs in moving edge dislocations ($\mathbf{b}_1 . d\sigma_1 = 0$) produce no defects, and the crossing dislocation must have a Burgers vector with component perpendicular to the glide plane of the moving dislocation. For two perpendicularly crossing screws $e = 1$; this defines the scale of the efficiency factor. It corresponds to the production of a close packed row of defects. For arbitrary orientations the spacing of the defects is $1/e$ lattice parameters.

The possibility must not be ruled out that the jog formed in the moving dislocation will, on further movement of the latter, displace itself so as to reduce the defect production. No defects are produced at all by the jog when it moves purely by glide, that is parallel to the Burgers vector of the moving dislocation. The character of the latter determines in how far the jog can actually perform such a favourable motion. A jog in a pure screw dislocation has to move along the dislocation axis. In view of the limit set to the possible dislocation velocity, this seems impossible. No accurate computation has been made as to the actual motion of a jog. It seems plausible however to deduce that the efficiency as given in (1.17) will be less in practice, due to the sidewise motion of the jog. To take this into account, another factor ($\mathbf{b}_1 . d\sigma_1$) could perhaps be added to the efficiency formula.

1.1.4. **Formation of dislocations**

In order to explain the phenomenon of plastic flow as being effected by the motion of dislocations on their glide planes, one has to assume that in undeformed crystals dislocations are already present in appreciable numbers. Dislocations not being thermodynamically stable lattice defects, there must be some mechanism or another by which they come into existence during the growth of the crystal.

Up till now, only hypotheses exist to the nature of the mechanisms responsible for dislocation formation. As pointed out by Frank [14]), crystal growth from slightly supersaturated vapour is greatly aided by the presence of screw dislocations. These dislocations produce a step on the surface of the crystal at which new atoms are preferentially absorbed, and which does not disappear on further growth, as normal surface irregularities do. By the aid of dislocation steps the rate of growth can easily be enhanced by a factor of 100 (spiral growth [15])). In the growing crystal the dislocation growths with it. Therefore vapour grown crystals will presumably contain dislocations, as those nuclei already containing them will grow much faster than those without dislocations. An analogous mechanism probably holds for growth from diluted solutions. The existence of dislocations in the original nuclei presents another problem. Recent experiments by Hollomon [16]) show that they are probably formed in small numbers when two nuclei encounter each other accidentally and stresses are set up. These can be relieved by the formation of dislocations in the very small and thin nuclei.

However, metal crystals do presumably contain more dislocations then can be understood in this way; various experiments [17]) yield dislocation densities of 10^6 - 10^8 cm^{-2} in carefully prepared metal crystals. (In other solids these densities may be much less, e.g. it is stated that very carefully prepared germanium crystals would only contain as few as 10^2 - 10^4 dislocations per cm^2 *). We shall not go into the explanation of these differences here.) Approximately the same densities are found in sublimized and melt-grown crystals. A possible hypothesis as to the formation of so many dislocations in metal crystals grown from the melt, has been advanced by Teghtsoonian and Chalmers [19]), on the basis of experimental evidence of so called *striations* in tin crystals grown from a seeded melt. The theory has been further developed by Frank [20]), but as yet only qualitatively. It is based on the assumption that the vacancies present in large numbers in thermal equilibrium in the high temperature zone near the solid-liquid interface will, as the temperature falls, condense progressively into flat disks perpendicular to the interface. When the temperature drops further, these disks collapse and elongated dislocation loops more or less parallel to the growth direction are formed, that grow on as the solidification proceeds. Excess vacancies that remain in the cooler parts of the material, having escaped the elimination process described above, will presumably collapse in their turn into smaller and more arbitrarily oriented dislocation loops, by reason of the lesser diffusivity. By the action of the thermal stresses

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*) These numbers are based on countings of etch pits by Vogel, Pfann and their collaborators at the Bell Laboratories. It seems, however, that the observed numbers depend greatly on the method of attack: Ellis [18]) finds dislocation densities in Ge of 10^7 to 10^8 cm^{-2}.

these loops rearrange themselves and form a dislocation network, the presence of which has already been discussed. By several methods it has been demonstrated that the probable maze width of this network should ly in between 10^{-3} and 10^{-4} cm (see e.g. section 1.1.6.2). The corresponding limiting density of 10^6 to 10^8 cm^{-2} is presumably intimately connected with the unavoidable presence of small traces of impurities in even the purest metals — zone-refined metals possibly excepted; not much is known about the dislocation density in these metals at the moment —. Basing ourselves on the available evidence, we shall accept the presence of a dislocation network of the dimensions mentioned in well-annealed metal crystals. Its existence seems fairly well established.

The stability conditions for such a network have been studied by Thompson [22]), Frank [23]) and others. In face centered cubic metals a stable arrangement of the dislocations seems to be such that each time three dislocations meet at so called nodes, and hexagonal cells are formed. At each node the vector sum of the Burgers vectors of the three dislocations is equal to zero, as required by the theory. Cells of this type have indeed been observed by Hedges and Mitchell [24]) in single crystals of silver bromide.

Such a spatial network is relatively immobile under the action of a stress. That is to say, a given network element acted upon by a suitable shear stress tending to make it glide, cannot move in its glide plane as when its end points were free, but is anchored at the nodes that form its end points. It will however bend out, somewhat like an elastic wire. Frank and Read [25]) have shown that if the shear stress becomes large enough, such an anchored dislocation element can act as a *source* of an indefinite number of dislocation loops. The source starts to work if the shear stress component along the Burgers vector becomes equal to

$$\tau_1 = \frac{aGb}{l}, \tag{1.18}$$

where a is a numerical factor depending on the elastic constants of the material and slightly on the type of the dislocation, it is of order unity; l is the length of the network element. Figure 8 shows the mechanism of a so-called Frank-Read source in detail.

Fisher [26]) pointed out that a dislocation element ending on the surface of the crystal and on a node in the interior could already act as a source at one-half of the stress needed for a double-ended source. Hart [27]) discussed the case of Frank-Read sources not anchored by other dislocations but by foreign solute atoms, and derived the result that such sources could also be activated by stresses considerably lower than that given by formula (1.18).

Suzuki [28]) and Bilby [29]) studied the action of Frank-Read sources anchored at nodes in connection with the special properties of the crystalline structure in closed-packed metals, and pointed out that there are in principle various kinds of sources possible. Whereas that originally proposed by Frank and Read emits its loops all in the same atomic plane, their work shows that sources that emit loops on successive atomic planes are much more probable.

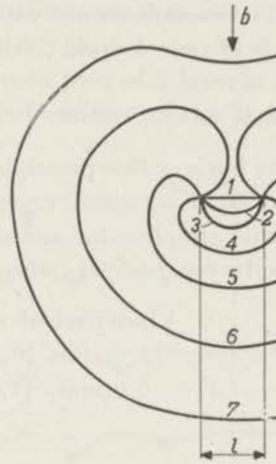

Fig. 8. Frank-Read source. A dislocation element 1 of length l and Burgers vector **b** is anchored at two points. When a shear stress is applied along **b**, the dislocation bends out and takes the forms 1, 2, 3 ..... At a certain stress the critical half-circle-form 3 has been reached. A further slight increase of the stress causes a spontaneous expansion 4, ... 6. In the latter situation the two near lying screw parts eliminate each other, and the closed loop 7 is formed together with the original piece of dislocation 1.

Whatever the detailed mechanism may be, the existence of dislocation sources of some kind or another seems to be clearly established. One inherent difficulty of the dislocation theory of plastic flow is herewith overcome: not only can the dislocations move easily but they are easily formed, too, under the influence of the deforming stresses themselves.

The number of loops emitted by a source will in practice always be limited by secundary phenomena, such as the action of the stresses set up by the loops themselves, the interaction of the sources and the effect of the formation of jogs and other lattice defects as mentioned in the foregoing section. We shall return to this point below. In general, the observed surface displacements in the so-called slip lines of between 10 and 2000 atomic distances on one slip plane, can in principle be easily understood from the action of dislocation sources.

1.1.5. Dislocations in special crystal structures

In a given crystal lattice there is an infinity of possible Burgers vectors, viz. any lattice vector. However, not all the corresponding dislocations are stable. The energy of a dislocation is proportional to the square of its Burgers vector (this follows from a consideration of the stresses and strains around the dislocation), when small terms arising from crystal anisotropy and type of the dislocation are neglected. Therefore, only those dislocations are stable that cannot split up into two dislocations with Burgers vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ (of which the vectorsum is of course equal to that of the original dislocation, $\mathbf{b}$), so that

$$b^2 > b_1^2 + b_2^2. \tag{1.19}$$

Frank and Nicholas 30) have, on the basis of this principle, worked out the possible Burgersvectors for several often occurring crystal structures. As our present interest lies primarily with simple cubic and close-packed cubic crystals, we give here only their results for these structures.

Simple cubic lattice	Close-packed cubic lattice
I: 6 vectors [1,0,0] etc, $b^2 = 1$	I: 12 vectors $[0,\frac{1}{2},\frac{1}{2}]$ etc, $b^2 = \frac{1}{2}$
II: 12 vectors [1,1,0] etc, $b^2 = 2$	II: 6 vectors [1,0,0] etc, $b^2 = 1$
III: 8 vectors [1,1,1] etc, $b^2 = 3$	

All further combinations of primitive vectors are unstable. Even the stability of type II in the simple cubic lattice against dissociation into pairs of type I, of type III in this structure into two dislocations of type I and II, or into three of type I, or of type II in the close-packed lattice into a pair of type I is a matter of doubt. The sum of the squares of the Burgers vectors is invariant against these dissociations, so other factors may play a deciding role.

Dislocations with the Burgers vectors discussed here are all perfect dislocations. The Burgers vectors are lattice vectors, thus the displacements of the atoms occurring when a dislocation passes through the lattice are such that the lattice is transformed into itself. The definition of a dislocation, as given in section 1.1.1 is, however, of a wider scope; the Burgers vector need not be a lattice vector. In the latter case one is concerned with an imperfect dislocation. In the theory of plastic flow only such imperfect dislocations play a role that transform the crystal lattice into a structure that is directly related to it, viz. into a translation twin. A simple cubic lattice has no translation twins that can be constructed in this way, and therefore no imperfect dislocations can exist in this structure.

The close-packed cubic structure (face-centred cubic structure) can be regarded as built of close-packed layers of atoms in }111{ planes. The projections of these layers along the [111] axis occupy three different sets of positions, and the layers can be labelled *a*, *b*, *c*. In the perfect lattice the layers follow upon each other in the sequence *a*, *b*, *c*, *a*, *b*, *c*, *a*, - - - - - - -. Now suppose in this sequence layer *a* is removed and the gap is closed by bringing the neighbouring *c* and *b* layers into contact by a displacement normal to (111). Then the sequence is - - - - *a*, *b*, *c*, *b*, *c*, *a*, *b*, *c*, *a*, - - - - - - , and a translation twin is formed, of the kind called intrinsic twin [31]). Another way of forming a translation twin, a so-called extrinsic twin, is to insert a plane of atoms, say *b*, between *c* and *a* in the sequence. Then the sequence reads: *a*, *b*, *c*, *b*, *a*, *b*, *c*, - - - - -.

If in a crystal only part of a layer is removed or added, then one must have imperfect dislocations at the boundaries (figs 9 and 10). Several

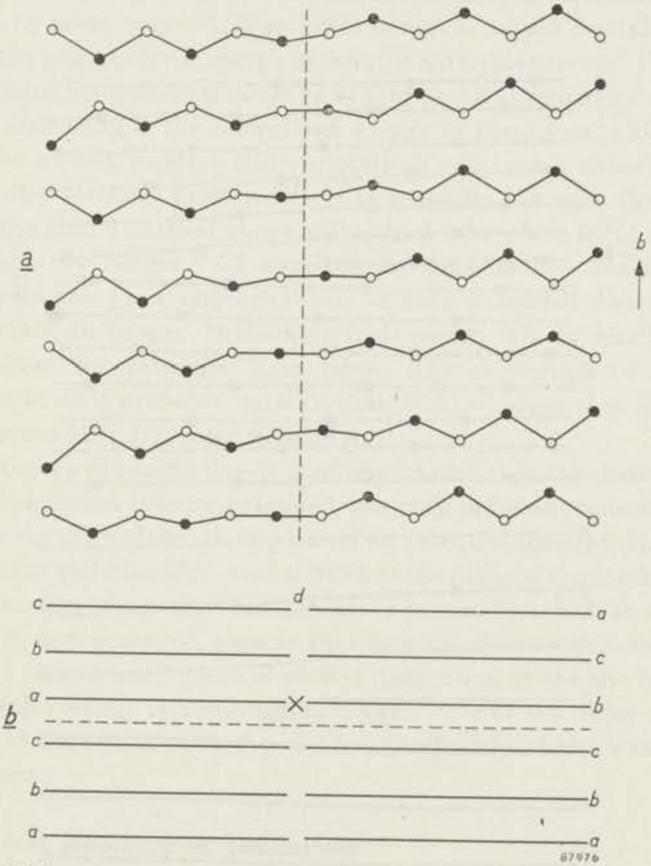

Fig. 9. (a) Half dislocation of screw type in the f.c.c. structure according to Heidenreich and Shockley. The dislocation line *d* runs along the direction of the Burgers vector, that is along [112]. The dislocation is viewed perpendicular to its (111) glide plane; atoms in the plane of drawing are denoted by open circles, atoms one layer above it by dots.
(b) On both sides of the dislocation the stacking is different; if that on the left hand side is normal (*abcabc*. . . .), that on the right hand side of the dislocation has become (*abcbca*. . . .) and a stacking fault is produced.

types of imperfect dislocations can be distinguished, according to the type of twin and to the boundary considered. The geometry of the possible imperfect dislocations is rather complex, we refer for further particulars to the paper of Frank and Nicholas [30]). Special types of imperfect dislocations have been discovered before a general theory existed, such as the so-called half-dislocations of Heidenreich and Shockley [32]), illustrated in fig. 9, and the sessile dislocation of Frank [7]), illustrated in fig. 10. Half-dislocations have a Burgers vector of the type $[\frac{1}{6}, \frac{1}{6}, -\frac{1}{3}]$, which represents a displacement from a lattice point to the nearest twin position in the (111) plane. Frank's sessile dislocation is characterized by a Burgers vector of the type $[-\frac{1}{3}, -\frac{1}{3}, -\frac{1}{3}]$ normal to a (111) plane, and is directly associated with the formation of an intrinsic twin. It is called sessile, as any glide

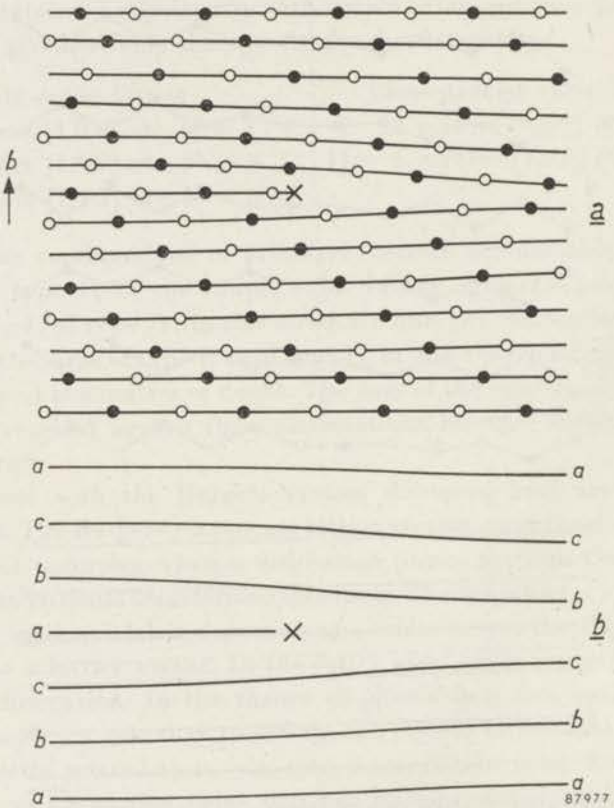

Fig. 10. (a) Frank sessile dislocation in the f.c.c. structure. The plane of drawing is $(10\bar{1})$, open and filled circles denote atoms in different elevations. The dislocation runs along $[10\bar{1}]$ normal to the plane of the figure, and its Burgers vector **b** is along [111]. (After W. T. Read [1]).) (b) This dislocation can also be imagined to have been formed by the partial removal of a lattice plane *a*.

motion of such a dislocation according to the definition of section 1.1.3 is impossible.

The existence of imperfect dislocations implies that stable perfect dislocations in some orientations can become unstable since they can dissociate into two imperfect dislocations. In such a dissociation an area of translation twin is generated between the two imperfect dislocations that is called a *stacking fault* (the term thus being used in a rather narrow sense). The combination of two imperfect dislocations and the associated stacking fault between them is denoted as an *extended dislocation*. An extended dislocation can e.g. be built up out of two half-dislocations, dissociation products of a perfect dislocation of the type I in face-centred cubic lattices. Dissociation of perfect dislocations into extended dislocations is possible in many ways[30]). Whether it occurs in actual crystals is determined by the gain of elastic energy associated with this process. The energy of an extended dislocation is made up of four parts: the energies of the two imperfect dislocations, the interaction energy of these two, which can be shown to be usually positive (the dislocations repel each other) and the energy of the stacking fault itself. It is generally assumed that a dissociation of the kind described above will indeed take place in f.c.c. metals. Computations by Seeger[33 34]) have shown considerable distinctions to exist between the form andebehaviour of such extended dislocations in various metals. In copper thstacking fault energy is very small, whereas in aluminium for instance it is large. The separation of the half-dislocations in Al is probably smaller than 7 Å, whereas that in Cu, Au, Ag etc. is much larger, greater then 20 Å.

For the theory of plastic flow it is of importance that the dissociation of a perfect dislocation into an extended one may influence considerably its mobility in the glide plane. Both parts of an extended dislocation, like that of Heidenreich and Shockley, are confined to the plane of the stacking fault, and the formation of jogs therefore becomes a process for which an additional activation energy is needed, namely that to bring the two half-dislocations together, to form a small piece of perfect dislocation at the site of the jog. This activation energy is according to Seeger[33, 34]) of the order of 0·5 eV in the case of Cu, and of the order of a few hundredths of an eV in the case of aluminium.

1.1.6. **Physical properties of dislocations**

1.1.6.1. *Influence on electrical resistivity*

One of the most important properties of dislocations, in addition to their effect on the mechanical strength of materials, is their influence on the electrical resistivity. Dislocations are perturbations of the perfect lattice and therefore act as scatterers for the conduction electrons. Confining ourselves to metals for which the description of the conduction electrons by an effective mass can be regarded as a reasonable approximation (such as Cu for example), the scattering matrix element of a dislocation can be computed in the following way [35, 36]). The region of the lattice surrounding the dislocation is in a state of strain. Therefore the energy spectrum of the conduction electrons, which in a perfect cubic lattice is given by:

$$E(\mathbf{k}) = E_0 + \frac{\hbar^2 k^2}{2m_1}, \tag{1.20}$$

must be supplemented by a number of terms depending on the strain tensor. In (1.20) **k** is the wave vector of an electron, $\hbar$ is Planck's constant divided by 2π and m_1 is the effective mass of the electrons. The influence of the strains on the (originally) periodic lattice potential can in first instance be expressed as a potential, viz. a deformation potential. This deformation potential depends primarily on the dilatation of the lattice.

Consider a metal crystal where the ions are perfectly screened, thus where the electron density will closely follow the ion density. In an energy band of standard form, the width of the filled portion of the conduction band is given by:

$$E_0 = \frac{\hbar^2}{2m_1} (3\pi^2 n)^{2/3},$$

where n stands for the number of conduction electrons per unit volume. When the ionic density varies, so does the electronic density and thus E_0. Owing to the constancy of the Fermi energy, a variation δE_0 is necessarily associated with an opposite variation of the bottom of the conduction band, δE. It is easily seen that

$$\delta E = -\tfrac{2}{3} E_0 \frac{\delta n}{n} = -\tfrac{2}{3} E_0 \Delta, \tag{1.21}$$

where $\delta n/n = \Delta$ is the relative density variation, thus the dilatation of the lattice. Therefore, the conduction electrons can be regarded as moving in an additional electrostatic potential $V = \tfrac{2}{3} E_0/e \cdot \Delta$. This potential is taken as the scattering potential by Landauer [35]) and Dexter [36]). Of course (1.21) only presents a first approximation, where effects of the strain on the effective mass of the electrons or directly on the shape of the band edge have been neglected. These have been considered in detail by Hunter and Nabarro [37]). Furthermore, the screening is never perfect and all variations of the band edge energy are accompanied by small charge shifts to flatten the Fermi surface again. The corrections to (1.21) due to this are only small, however.

As the dilatations around a suitably oriented screw dislocation in a cubic crystal are zero, such a dislocation is expected to scatter but slightly, at least in metals where the electrons are nearly free. The latter assumption is best realized in the alkali metals and Hunter and Nabarro [37]) indeed find that in these metals screw dislocations only produce very small scattering. In the noble metals such as copper, the contribution to the scattering arising from the other causes mentioned is already comparable to that arising from the dilatation associated with an edge dislocation, and screw dislocations produce thus also appreciable scattering.

Once the deformation potential has been computed, the scattering matrix element of a dislocation can be derived and from it the change in the distribution function $f(\mathbf{k})d\mathbf{k}$ caused by the scattering by such a defect. A different way to describe the distortion of the lattice is to take as the scattering potential the difference of the sums of the screened ionic potentials before and after the distortion. This has been done originally by Sondheimer and Mackenzie [38]). Dexter [37]) has shown that the results of both ways of attack differ but slightly in the case of good screening.

We shall assume in the following that Matthiesen's rule applies, that is, that the scattering by the dislocations is independent of the thermal scattering. Experiment has confirmed the approximate correctness of this hypothesis. Under the influence of an electric field the equilibrium shape of the distribution function is then governed by the "Boltzmann equation"

$$\frac{df}{dt} = \left(\frac{\partial f}{\partial t}\right)_{lattice} + \left(\frac{\partial f}{\partial t}\right)_{field} + \left(\frac{\partial f}{\partial t}\right)_{disl} = 0\,.$$

$\left(\frac{\partial f}{\partial t}\right)_{lattice}$ can be derived from the thermal resistivity when it is assumed that the thermal fluctuations can be described by a single relaxation time τ; the term $\left(\frac{\partial f}{\partial t}\right)_{field}$ also yields no difficulties. Only the third term needs to be considered here.

It is easily seen that a straight dislocation line cannot induce a change in the component of $\mathbf{k}$ parallel to it. Thus such a dislocation does not produce a resistivity change in the direction of its axis. A dislocation with not pure screw character produces non-symmetric strains; the resistivity tensor thus depends on the dislocation orientation. In a lattice with cubic symmetry the resistivity tensor of a straight dislocation has only three components. The component along its axis being furthermore zero, there are only two components to consider, ϱ_1 in the glide plane perpendicular to the dislocation line and ϱ_2 perpendicular to the glide plane. The result of the calculations by Hunter and Nabarro [38]) are the following:

For parallel straight edge dislocations of densitity N, with Burgers vector **b**:

$$\varrho_{1e} = \frac{\pi^2}{80}\frac{N\hbar b^2}{k_f e^2}(\alpha + \beta f), \tag{1.22}$$

$$\varrho_{2e} = \frac{3\pi^2}{80}\frac{N\hbar b^2}{k_f e^2}(\alpha + \beta f). \tag{1.23}$$

For a set of straight screw dislocations of density N, with Burgers vector **b**:

$$\varrho_s = \varrho_{1s} = \varrho_{2s} = \frac{3\pi^2}{80}\frac{N\hbar b^2}{k_f e^2} f. \tag{1.24}$$

Here k_f is the magnitude of the wave vector of the conduction electrons at the Fermi level and e is the electronic charge. As is well known, k_f depends on the number n of conduction electrons per unit volume according to

$$k_f = (3\pi^2 n)^{1/3}; \tag{1.25}$$

α and β are constants of order unity which depend only on the value of Poisson's ratio, and f is a factor in which the dependence of the scattering on the exact form of the periodic lattice potential is expressed. f is equal to zero for perfectly free electrons; it is of order unity in the case of the noble metals.

The resistivity of an edge dislocation perpendicular to its glide plane is thus three times that in the glide direction; the ratio between the resistivities caused by an edge and a screw dislocation respectively is completely governed by the magnitude of f. Numerical values for copper (dislocations of type I with Burgers vector along [110]) have been given by Hunter and Nabarro:

$$\left.\begin{array}{ll} \text{Resistivity in glide direction of one edge dislocation per cm}^2 & \\ & \varrho_{1e} = 0{\cdot}44.10^{-14}\ \mu\Omega\text{cm}, \\ \text{,,} \quad \text{perpendicular to glide plane of dislocation} & \\ & \varrho_{2e} = 1{\cdot}32.10^{-14}\ \mu\Omega\text{cm}, \\ \text{,,} \quad \text{of screw dislocation} & \varrho_s = 0{\cdot}26.10^{-14}\ \mu\Omega\text{cm}. \end{array}\right\} \tag{1.26}$$

The resistivity produced by an edge dislocation in an arbitrary direction can be computed according to the tensor rule (fig. 11). Let r be the direction along which the resistivity is to be computed. Then

$$\varrho_e(r) = \varrho_{1e}\cos^2(xr) + \varrho_{2e}\cos^2(yr). \tag{1.27}$$

Introduction of the polar angles φ and Θ with respect to the dislocation axis yields:

$$\varrho_e(\varphi,\Theta) = \sin^2\Theta\,(\varrho_{1e}\cos^2\varphi + \varrho_{2e}\sin^2\varphi). \tag{1.28}$$

The resistivity produced by a screw dislocation in an arbitrary direction follows from (1.28) by replacing ϱ_{1e} and ϱ_{2e} both by ϱ_s, thus

$$\varrho_s(\Theta) = \varrho_s \sin^2 \Theta . \tag{1.29}$$

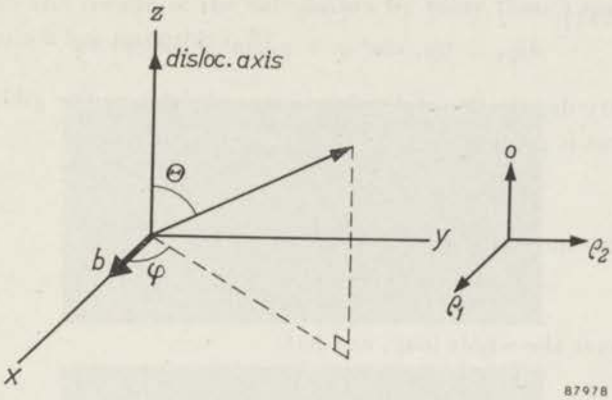

Fig. 11. On the derivation of the angular dependence of the dislocation resistivity.

A random arrangement of N edge and screw dislocations per cm² in copper gives rise to a resistivity of

$$\tfrac{1}{6}(\varrho_{1e} + \varrho_{2e} + 2\varrho_s) = 0{\cdot}38.10^{-14}\, N\, \mu\Omega\text{cm}.$$

A circular loop of dislocation of radius unity and with coplanar Burgers vector has an anisotropic resistivity that can be computed as follows (fig. 12). A line element ds can be regarded as the superposition of a short piece of edge dislocation with Burgers vector $b \cos \varphi$ directed normal to ds, and a

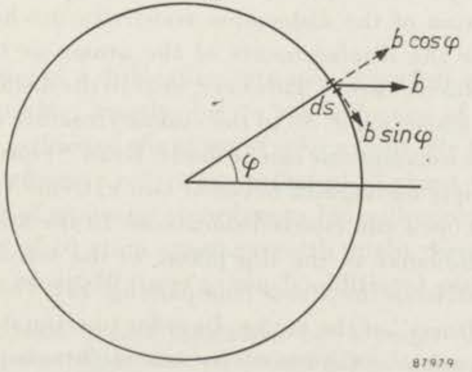

Fig. 12. On the derivation of the resistivity of a dislocation loop.

piece of screw dislocation of Burgers vector $b \sin \varphi$ directed along ds. The resistivity dϱ_{g1} in the glide direction (that of **b**) of this element of dislocation is according to (1.28) and (1.29) and noting that the resistances depend quadratically on the lengths of the effective Burgers vectors (formulae (1.22) to (1.24)):

$$\mathrm{d}\varrho_{g1} = (\varrho_{1e} \cos^4 \varphi + \varrho_s \sin^2 \varphi \cos^2 \varphi)\, \mathrm{d}\varphi\,. \tag{1.30}$$

The resistivity dϱ_{g2} in the glide plane perpendicular to the glide direction of the element is given by:

$$\mathrm{d}\varrho_{g2} = (\varrho_{1e} \sin^2 \varphi \cos^2 \varphi + \varrho_s \sin^4 \varphi)\, \mathrm{d}\varphi\,. \tag{1.31}$$

The resistivity normal to the glide plane is found to be:

$$\mathrm{d}\varrho_n = (\varrho_{2e} \cos^2 \varphi + \varrho_s \sin^2 \varphi)\, \mathrm{d}\varphi\,. \tag{1.32}$$

Averaging over the whole loop, one has:

$$\begin{aligned} \varrho_{g1} &= \tfrac{3}{4}\varrho_{1e} + \tfrac{1}{4}\varrho_s\,, \\ \varrho_{g2} &= \tfrac{1}{4}\varrho_{1e} + \tfrac{3}{4}\varrho_s\,, \\ \varrho_n &= \tfrac{1}{2}\varrho_{2e} + \tfrac{1}{2}\varrho_s\,. \end{aligned} \tag{1.33}$$

In the case of copper one finds for the resistivity caused by the presence of one loop of radius R per cm^3 of the metal:

$$\begin{aligned} \varrho_{g1} &= 0{\cdot}40.10^{-14}\, R\ \mu\Omega\mathrm{cm}, \\ \varrho_{g2} &= 0{\cdot}31.10^{-14}\, R\ \mu\Omega\mathrm{cm}, \\ \varrho_n &= 0{\cdot}79.10^{-14}\, R\ \mu\Omega\mathrm{cm}. \end{aligned} \tag{1.34}$$

There remains thus an anisotropy of the resistivity of about 2 : 1 for the resistivity *perpendicular to* the glide plane with respect to that *in* the glide plane. The anisotropy in the glide plane itself has practically disappeared.

In the computation of the dislocation resistivity use has been made of the expressions for the displacements of the atoms as they follow from ordinary linear elasticity theory. However, near to the dislocation lines these expressions are no longer valid. As to the atomic structure in the dislocation core, only tentative assumptions can be made. Read [39]) has pointed out that one could in principle distinguish between two extreme types of edge dislocations, so called open and closed dislocations. In the first case the lattice is extended perpendicular to the slip plane, in the second case it is not, but voids appear between the atoms (compare fig. 13). The actual state will depend on the "softness" of the atoms. In order to estimate the influence of the core of a dislocation on the resistivity, one might compare a dislocation with a row of vacancies. According to computations of Jongenburger [40]), one row of length 1 cm per cm^3 would contribute in the mean $1{\cdot}5.10^{-14}$ $\mu\Omega$cm to the resistivity; this is about 4 times as much as an average dislocation. Evidently this comparison is a gross overestimate of the importance of the core; thus we can put with safety that the influence of the core cannot alter the results of the calculation by more than a factor 4, and is probably much less important. *)

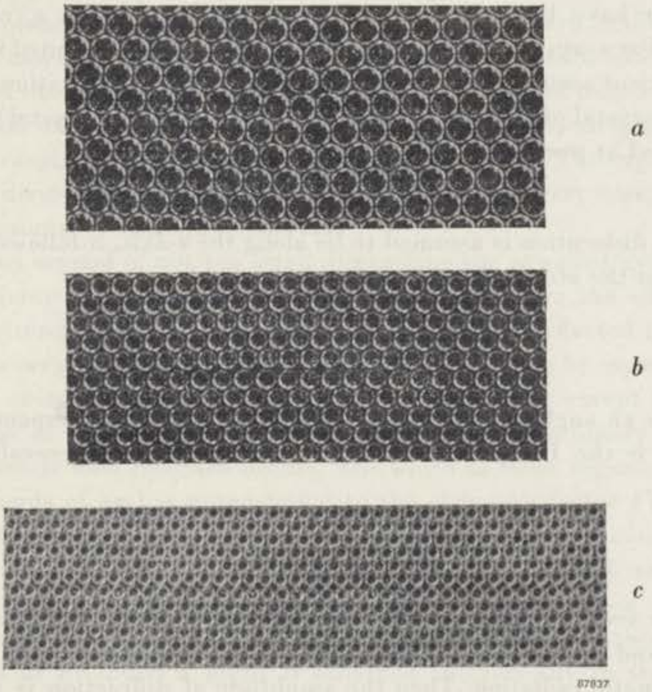

Fig. 13. (*a*) Closed dislocation (soft atoms), (*c*) open dislocation (hard atoms), (*b*) intermediate case. The atomic interaction in copper corresponds to a bubble size between (*b*) and (*c*). From photographs of the bubble model by W. L. Bragg and J. F. Nye, Proc. roy. Soc. **A 190**, 474, 1947.

The dissociation of a dislocation into two imperfect ones gives rise to an increase of scattering, mostly due to the influence of the stacking fault. Klemens [41]) has estimated the effect of such a fault. He finds that the stacking fault has an effective reflection coefficient of about $^1/_2$, that is the same as that of a plane of vacancies according to Jongenburger's computations [40]). A stacking fault of 10 atom spacings width might therefore be responsible for not less than about 40 times as much additional resistivity as a perfect

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*) Note added in proof. Recent calculations by A. Seeger (unpublished) gave the result that the effect of the core on the resistivity is about the same as that of the extended strain field, thus confirming Jongenburger's estimate.

dislocation. In Chapters 3, 4, and 5 various experimental evidence is discussed that actually the effective scattering cross-section of dislocations is larger by this order of magnitude than that obtained by Hunter and Nabarro.

1.1.6.2. *X-ray scattering by dislocations*

The X-ray scattering of a single dislocation can in principle be determined from the theoretical expressions for the displacements associated with it. The latter have been derived by several authors [2,3]) for a continuous medium. For a crystal the atomic displacements can be computed from them with sufficient accuracy. Consider e.g. a straight screw dislocation along the axis of a crystal of cylindrical cross-section. In a perfect crystal the atoms are situated at positions

$$\mathbf{r}_j = j_1\mathbf{a} + j_2\mathbf{b} + j_3\mathbf{c}\,. \tag{1.35}$$

When the dislocation is assumed to lie along the *c*-axis, it follows from the theory that the atoms are now situated at

$$\mathbf{r}'_j = \mathbf{r}_j + \frac{n\psi}{2\pi}\,\mathbf{c}\,, \tag{1.36}$$

where ψ is an angle measured from some fixed direction perpendicular to $\mathbf{c}$, and $n\mathbf{c}$ is the Burgers vector of the dislocation (n is generally unity).

Let

$$\mathbf{S} = \frac{\mathbf{s} - \mathbf{s}_0}{\lambda}$$

denote the vector difference between the normals to the wavefronts of the incident and the reflected beams divided by the wavelength λ of the monochromatic radiation. Then the amplitude of diffraction is given by:

$$G = \Phi \sum_{j_1, j_2, j_3} \exp\,(2\pi i\,\mathbf{S}\,.\,\mathbf{r}'_j)\,, \tag{1.37}$$

where Φ depends on the nature of the crystal. In a perfect crystal where the positions of the lattice points are given by (1.35) ($\mathbf{r}' = \mathbf{r}$), the sum only differs appreciably from zero when

$$\mathbf{S.a} = h\,,$$

$$\mathbf{S.b} = k\,,$$

$$\mathbf{S.c} = l\,,$$

and h, k, l, are integers. In the dislocated crystal only the last condition $\mathbf{S.c} = l$ retains its validity, owing to the independence of ψ on j_3 in (1.36). That is, any spreading of the regions of strong diffraction in reciprocal space is perpendicular to the dislocation axis [42]); an obvious result if one remembers the infinite repetition of the crystal pattern in the axial direction. The summation of formula (1.37) over j_1 and j_2 cannot be performed exactly. By replacing it by an integration over the cross-section of the cylinder, it is found that the amplitude of reflection is no longer large in the points of integral h, k, l, but on loops lying in integral l-planes with these points as centres and with radii that increase about linearly with l. Only for $l = 0$ the diffraction pattern remains unaffected by the presence of the dislocation. In all other planes the intensity of diffraction is exactly zero in the points of integral h and k. Frank [43]) has pointed out that these results follow from the facts that the screw dislocation displaces no atoms out of planes *through* the dislocation axis, and displaces atoms out of planes *intersecting* this axis by amounts ranging continually and uniformly from 0 to nc. The expressions that can be derived [42]) for the integrated intensities are very complicated and have presumably little practical use.

In a perfect crystal of not too small dimensions the so-called dynamical theory of X-ray diffraction should hold. In this theory, the effects of multiple scattering and interference among the waves reflected from all planes in the crystal are taken into account. The result can be expressed as follows: the crystal is completely transparent for X-rays except in very small regions of reflection angle, corresponding to the ordinary Bragg-reflections, where *total reflection* occurs. The width of these regions (of the order of seconds of arc) is proportional to the structure factor $F(h, k, l)$ that depends on the positions of the atoms and on the reflection considered. The integrated intensity of the diffracted radiation is in each reflection region proportional to F (due to the fact that total reflection occurs).

In practice it is found that the integrated intensities are rather better proportional to F^2. Such a result is obtained theoretically in the much simpler kinematical theory of diffraction. In this theory multiple scattering is neglected, and the intensity of the incident radiation is assumed to be constant throughout the material. Then no total reflection, but a smoothed-out intensity profile occurs for each reflection.

It is generally assumed that the dynamical theory does not apply in most crystals because of local deviations of the crystal perfection, that destroy the very sensitive phase relations necessary for the considerations of the dynamical theory to hold. When for instance the distance between two successive lattice planes deviates locally from the "perfect" value by a relative amount that corresponds to a variation of reflection angle of more than the very narrow width of the reflection, the dynamical theory breaks down. The at first sight rather amazing applicability of the kinematical theory is thus explained by the natural imperfectness of most crystals. However, in most natural or carefully prepared synthetic crystals traces of the effects of multiple scattering and interference remain. They appear most conspiciously in the strong reflections. The latter are broad (in the dynamical theory width and intensity are proportional) and small distortions of the crystal do in general therefore not completely destroy the interference conditions. For weak reflections however, the effect of multiple scattering can usually be completely neglected. The result is that, starting from the kinematical theory, the weak reflections are usually observed with about the "correct" integrated intensity, whereas the strong reflections are affected by backscattering, and are observed too weak. This is called *primary extinction*, it is the more apparent if the crystal is more perfect.

In order that the dynamical theory should partially break down, the local distortions of the crystal should be at least so near to each other that nowhere perfect regions occur, large enough for the considerations of this theory to apply in full. Darwin [44]) has therefore proposed that in natural crystals the structure is perfect only over regions of dimensions of the order of 10^{-4} cm or less. Each crystal should be regarded as built up out of perfect blocks of this dimension, that differ slightly from each other in orientation (*mosaic structure*). Bragg [45]) has pointed out that in such a structure, although the primary extinction is limited, another cause of extinction occurs, the so-called *secondary extinction*. This is due to the fact that the intensity incident on a particular mosaic block will not be equal to the intensity incident on the surface of the crystal (as originally assumed in the kinematical theory); the upper blocks differing but slightly from it in orientation may reflect part of the intensity responsible for reflection, and similarly the outgoing reflected beam may be partly reflected backwards on its way out by mosaic blocks of about the same setting. Even if no primary extinction where present (blocks not exactly perfect), this secondary extinction would appear. Hall and Williamson [46]) have shown that by a careful study of the integrated intensity of the various lines it is possible to separate the effects of primary and secondary extinction. They found that in cold-worked as well as in annealed metals only secondary extinction appears. They could further determine the apparent particle size of the corresponding mosaic structure from the width of the lines: it is of the order of 10^{-4} cm in most annealed metals.

It has been proposed that the hypothetical mosaic structure should be identified with the presence of a network of dislocations. From Wilsons considerations discussed above, it is possible to derive, be it in an approximate way, the secondary extinction associated with the presence of a given density of parallel dislocations. The effect of the dislocations is that the lines become in first instance broadened, thus the same as that of mosaic blocks of a certain average size. This "apparent particle size" associated with the presence of dislocations is about equal to the average distance between them. An observed mean particle size of 10^{-4} cm thus corresponds to a density of parallel dislocations of 10^8 cm^{-2}. The identification of the mosaic structure with the presence of a dislocation network seems therefore well warranted, although a determination of the characteristics of this network from X-ray data is not yet possible. Also the observation of Hall and Williamson that no primary extinction occurs, can now be explained: the "blocks" in between the dislocations are not exactly perfect, due to the long-range strains of the dislocations. Therefore the very sensitive phase relations necessary for primary extinction are not obeyed and consequently only secondary extinction occurs.

The results of these and many other investigations [47,48]) are then that presumably in well-annealed metals a network of dislocations is present with a mean maze-width of about 10^{-4} cm. Assuming the dislocations to be randomly distributed as to the possible crystallographic orientations of line and Burgers vector, this corresponds to a density of 10^8 dislocations per cm^2, in accordance with the assumptions made in section 1.1.4. However, the "randomness" of the dislocation distribution may be far from realized (Seeger [12])); and thus this number might easily be wrong by a factor 10.

The presence of stacking faults also influences the diffraction image. The effect has been studied theoretically by Paterson [49]): stacking faults on one parallel set of $\}111\{$ planes in an f.c.c. lattice result in broadening and displacement of those lines for which the sum of the indices $h + k + l = 3n \pm 1$, where n is an integer or zero. The displacement is towards larger Bragg-angles when the $+$ sign applies and to smaller angles when the $-$ sign applies. The other lines remain sharp. It is possible to distinguish the stacking fault broadening from that due to other causes by performing a Fourier analysis of the line shapes, as has been proposed by Warren and Averbach [50]). No reliable observational data have as yet been published.

1.2. Vacancies and interstitial atoms in metal crystals

Vacancies and interstitial atoms, in the following together to be called point-defects, are presumably present in large numbers in materials deformed plastically at a temperature low enough to prevent diffusion. Their presence, as has been explained in section 1.1.3.2, is caused by the motion of dislocations that necessarily contain jogs. These defects have an appreciable effect on the physical properties of the materials: moreover, they influence the mechanical properties, although in a lesser degree. It is therefore relevant to study the point-defects here somewhat in detail. We shall confine ourselves to the physical properties of point-defects in face-centered cubic metals.

1.2.1. Energy and free energy of point-defects in metals

Whereas the energy necessary to form a dislocation is practically completely an elastic energy, and can be estimated once the displacements around the dislocations are known (in Cu for example a dislocation of mixed character represents an energy of about 6 eV per atomic plane [51]), see also section 1.1.2), the energy of formation of a vacancy is largely an electronic energy. This is partly due to the fact that the elastic strains around a vacancy are so small that for all practical purposes they can be neglected, and also due to the important charge disturbance caused by the removal of a positively charged metal ion from the lattice. The same holds true for an interstitial, although then the elastic strains are not entirely negligible. The energy of formation of vacancies in monovalent metals has been calculated by Huntington and Seitz [52]) and very recently by Fumi [53]). As the results of the latter author seem the most reliable, we shall discuss them here. Fumi considered the energy change of the electron gas in a metal sphere when a positively charged ion is removed from the centre and its charge distributed over the surface. The electrons were considered to be perfectly free. In order to compute the perturbed wavefunctions in the Born approximation, it is not necessary to know the exact shape of repulsive potential around the vacancy, if a rule first proposed by Friedel [54]) is used. This rule relates the phase shifts of the perturbed wavefunctions of the electrons to the effective charge due to the vacancy, that is $-e$ in monovalent metals. The change in electronic energy can then be directly related to their Fermi energy E_F ($= 7{\cdot}2$ eV in Cu); Fumi finds $\Delta E_{el} = \frac{2}{3} E_F$. From this must be subtracted the contribution to the energy made by the positive charge smeared out on the surface, viz. $2/5\ E_F$. There remains then $4/15\ E_F$ as the electronic energy needed to form a vacancy. In a better approximation for the s-wave functions the Born approximation is replaced by the exact computation of the phase-shifts, and the total electronic energy is found to be somewhat smaller, viz. $\approx 1/6\ E_F$. In the noble metals there is another contribution to the energy of a vacancy that arises from the closed-shell ion-ion repulsion. According to earlier calculations by Huntington [52]) and Huntington and Seitz [51]), this energy amounts to about $-0{\cdot}3$ eV in copper and gold.

Thus it is found that the energies of formation of a vacancy in the noble metals have the following theoretical values:

	U_F
Cu	0·87 eV
Ag	0·62 eV
Au	0·62 eV .

From an analysis of the calculation [55]) it seems plausible that these values have an uncertainty of about 0·1 eV.

No exact calculations exist for the case of an interstitial in the noble metals. Even the structure of such a defect is not accurately known. As Lomer and Cottrell [56]) have pointed out, it is possible that interstitial atoms have a one-dimensionally extended structure, presumably along [111]-directions, of several atoms length. Such a structure has been termed *crowdion* by Paneth [57]). It is due to the relatively large strains that are caused by an interstitial atom (displacements of nearest neighbours of 20% are present in the Cu lattice [58])), which can be relieved by the extension into a crowdion. One might suppose that the electrostatic contribution to the energy of formation of an interstitial or crowdion is again of the order of 1 eV in Cu. That due to the elastic strains may easily amount to about 4 eV. We shall therefore take $E_F = 5$ eV as a plausible value for the energy of formation of an interstitial in copper, silver or gold. An estimate of this order is in agreement with experimental determinations to which we return in following sections *).

Introduction of vacancies and interstitials produces a large increase of the configurational entropy of the crystal [59]). In an ideal crystal that contains N atoms, the introduction of n vacancies (that is, the removal of n atoms) can be realized in

$$m = \frac{N!}{(N-n)!\,n!}$$

ways. The increase in entropy resulting from this is

$$S = k \log m \approx kn \left\{ \log \frac{N}{n} + 1 \right\},$$

which is proportional to the volume of the crystal, as must be. Thus per additional vacancy the entropy increases with the amount

$$\Delta S_{conf} = k \log \frac{N}{n} = -k \log p_{vac}, \tag{1.38}$$

where p_{vac} stands for the vacancy concentration.

An increase of the entropy of the same order is associated with the introduction of an interstitial atom. Apart from these contributions to the configurational entropy, there exists a contribution arising from the change of the vibrational frequencies of the atoms near the point-defect. In an Einstein solid (frequency ν_E) the vibrational entropy between room temperature and the melting point ($kT \gg h\nu_E$ for the monovalent metals) is given by:

$$S_{vibr} \approx 3\,Nk \log \frac{kT}{h\nu_E}.$$

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*) Note added in proof: A. Seeger has estimated the effect of the relaxation of the electron gas around the interstitial. He arrives at the much lower value of 2 eV for the total energy of formation (unpublished).

Assuming that only the nearest neighbours (12 in an f.c.c. lattice) change their vibrational frequency by an amount $\Delta\nu$, the change in vibrational entropy associated with the removal of one atom amounts to

$$\Delta S^{(vac)}_{vibr} = -3\,k \log \frac{kT}{h\nu_E} - 36\,k\,\frac{\Delta\nu}{\nu_E}. \tag{1.39}$$

In the case of a vacancy $\Delta\nu$ is negative and presumably $|\Delta\nu| \ll \nu_E$; as $a = \log \dfrac{kT}{h\nu_E}$ is of order unity in the temperature region between room temperature and the melting point,

$$\left|\Delta S^{(vac)}_{vibr}\right| \approx \left|\left(36\,\frac{|\Delta\nu|}{\nu_E} - 3\,a\right)k\right| \approx k.$$

Seeger [34]) derives $\Delta S^{vac}_{vibr} = 3{\cdot}4\ k$ in copper, from an analysis of recovery experiments of the electrical resistivity. As we shall see below, the equilibrium vacancy concentration in copper is generally so small (e.g. 10^{-15} at room temperature) that the contribution of the vibrational entropy is relatively insignificant. Only near the melting point, where p_{vac} approaches 10^{-3}, the configurational entropy becomes of some significance.

For an interstitial atom the change of the vibrational frequency is presumably much greater and positive, it may easily amount to $\dfrac{\Delta\nu}{\nu_E} \approx 0{\cdot}1$. Furthermore, not only nearest neighbours change their frequency, also next nearest neighbours do so appreciably and the total change in vibrational entropy may become of the order

$$\Delta S^{(int)}_{vibr} \approx -30\,k. \tag{1.40}$$

This large value of $\Delta S^{(int)}_{vibr}$ is comparable to the configurational entropy for all practically encountered interstitial concentrations. In the alkali-metals, where moreover the energy of formation of these defects is very small, the vibrational entropy plays therefore an important role in determining the equilibrium concentrations. This is not so in Cu, Ag and Au, as the equilibrium concentrations of interstitials are there always immeasurably small. These are obtained by minimizing the change of free energy of the crystal due to the introduction of the defects. One has:

$$n = \alpha\, N\, \mathrm{e}^{-U_{vac}/kT} \text{ for vacancies}, \tag{1.41}$$

$$n = \beta\, N\, \mathrm{e}^{-U_{int}/kT} \text{ for interstitials}, \tag{1.42}$$

where U_{vac} and U_{int} stand for the energies of formation, and $\alpha = \exp\{\Delta S^{(vac)}_{vibr}/k\}$ is a factor slightly larger than unity, $\beta = \exp\{\Delta S^{(int)}_{vibr}/k\}$ a factor of order 0·1 to 0·01. Due to the large value of U_{int}, even at the melting point the thermal equilibrium concentration in the noble metals of interstitials is completely negligible. (In the alkali metals this is not so.) Vacancies, however, can occur in appreciable concentrations at reasonably high temperatures. For copper one finds for the atomic concentration p_{vac}, if $a = 1$:

T	300° K	600° K	900° K	1200° K	1356° K
p_{vac}	10^{-15}	3×10^{-8}	10^{-5}	$1{\cdot}7 \times 10^{-4}$	$4{\cdot}5 \times 10^{-4}$

At the melting point the concentration of vacancies is thus of the order of 0·1%.

1.2.2. **Diffusion of point-defects**

The diffusion of point-defects is governed by a diffusion constant D which depends on the temperature in the usual way:

$$D = D_0 \, e^{-Q/kT}, \tag{1.43}$$

where Q is the activation energy for diffusion. D_0 is in good approximation given by an expression of the form

$$D_0 = \nu_0 \, a^2 \, e^{\Delta S_D/k}, \tag{1.44}$$

where ν_0 is the mean frequency of vibration of the atoms ($\approx 10^{13}$ sec^{-1}), a is the lattice constant and ΔS_D the change in entropy associated with the elementary vacancy or interstitial diffusion process, that is, the change of entropy in moving an atom from a lattice site to the potential barrier separating it from the neighbouring vacancy, or in moving an interstitial over the neighbouring potential barriers [51, 52, 60, 61]). The reason for the occurrence of an entropy of activation is that in studying the energy of a diffusing atom at the saddle point separating two equilibrium sites, one should actually consider the free energy, as this maxium potential depends on temperature through the elastic constants and the density, and the diffusion can be regarded as an isothermal process. The value of ΔS_D can be derived from the temperature variation of the latter quantities; it follows from LeClaire's [61]) computations that for vacancies in copper $\Delta S_D/k \approx 6$, i.e. for vacancies, D_0 is of order unity. The estimate is rough, however, so in practice D_0 may vary between 0·1 and 10 cm^2/sec, in agreement with experimental determinations [62]). For interstitials ΔS_D is probably about 5 times as great, and D_0 thus about 100 times as large as for vacancies.

By far the most important quantity in (1.43) is Q. A few theoretical attempts, based on much the same ideas as those used in the computation of the formation energy, have been made to calculate the activation energy for migration of vacancies and interstitials. Huntington and Seitz [51]) and Huntington [52]) obtained approximately 1 eV for Q_{vac} in copper; Huntington [60]) found the diffusion energy of interstitials to be very small: $Q_{int} \approx 0{\cdot}25$ eV or even less. Seeger has recalculated the height of the potential barrier for interstitial diffusion in the noble metals, and finds the much larger value 0·6 eV for Q_{int} (to be published shortly). Fumi [53]) also derived more or less approximate values of Q for vacancy diffusion, he found $Q_{vac} = 1{\cdot}2$ eV in copper.

The determination of the value of Q_{vac} is directly connected to that of the energy of formation. This is so in theory as well as in experiment, as most determinations relate to the coefficient of self-diffusion in metals, that is assumed to follow a vacancy mechanism. The self-diffusion coefficient is the product of the fractional concentration of vacancies as given by (1.41) and the diffusion coefficient of these vacancies as given by (1.43). In the final expression for the self-diffusion coefficient an activation energy thus appears which is equal to the sum of U_{vac} and Q_{vac}:

$$Q_{self} = U_{vac} + Q_{vac}\,. \tag{1.45}$$

As seen above, it follows from theory that in copper both are of the order 1 eV. Indeed the activation energy for self-diffusion in Cu is found to be 2·03 eV [63]). The same conclusion holds true for all noble metals; even numerically very much the same values apply.

Le Claire [61]) has studied the kinetics of the self-diffusion process more in detail and has derived the values $Q_{vac} = 1{\cdot}24$ eV and thus $U_{vac} = 0{\cdot}79$ eV in copper, in fair agreement with Fumi's computed value of U_{vac}, although this computation follows completely different lines.

As will become clear in the following, a precise knowledge of U_{vac} and Q_{vac} is of the utmost importance for the interpretation of the recovery phenomena displayed by deformed metals and thus for a precise understanding of the mechanism of plastic deformation. As shown above, theoretical arguments point rather unambiguously to the conclusion that in the noble metals copper and gold the energy of formation of vacancies is appreciably smaller than the energy of migration. The most probable values are, for copper: $U_{vac} = 0{\cdot}85 \pm 0{\cdot}05$ eV, $Q_{vac} = 1{\cdot}2 \pm 0{\cdot}05$ eV; for gold: $U_{vac} = 0{\cdot}8 \pm 0{\cdot}1$ eV, $Q_{vac} = 1{\cdot}3 \pm 0{\cdot}1$ eV. The theory is not sufficiently accurate for these values to be regarded as final.

The case of interstitials is still less satisfactory. Except for the recovery experiments to be discussed in Chapter 5, no effects directly related to the formation or migration of interstitials in the noble metals can be studied experimentally. We are therefore obliged to use the very rough theoretical values quoted above, viz. both in copper and gold: $U_{int} = 5$ eV, $Q_{int} =$ 0·25-0·6 eV.

1.2.3. **Experimental determination of activation energies of formation and migration of vacancies in the noble metals**

The available evidence to the values of Q_{vac} and U_{vac} in the noble metals has been reviewed by Jongenburger [64]). There exist in principle three classes of experiment, called in the following respectively high-temperature, low-temperature and recovery experiments. To the latter category, that yields results that are most difficult to interpret, we shall return in chapter 5. In the high-temperature experiments the deviations at high temperatures from the theoretical temperature dependence of a physical quantity are studied and interpreted as being caused by the presence of appreciable numbers of vacancies in thermal equilibrium at these temperatures. From a study of the electrical resistivity Meechan and Eggleston [65]) found for copper $U_{vac} = 0{\cdot}90 \pm 0{\cdot}05$ eV. Jongenburger [64]) analyzed data in literature on the temperature coefficient of thermal expansion of copper and gold, and derived from them values of U_{vac} in copper between 0·7 and 0·9 eV, in gold between 0·6 and 0·8 eV. These are all in excellent agreement with the theoretical data quoted above. Whereas the recovery experiments also yield results that can be interpreted in accordance herewith, the experiments of the low-temperature category yield quite different results. In these experiments a metal wire is quenched very rapidly from a high temperature, and its electrical resistance at a very low temperature is compared with that of an unquenched wire. The (positive) difference is attributed to quenched-in vacancies, and the dependence of this difference on the quenching temperature yields again a value for U_{vac}. Kauffman and Koehler [66]) quenched thin gold wires in a helium blast and found $U_{vac} = 1{\cdot}28$ eV, a value very much larger than that expected theoretically. Jongenburger [64]) has reanalyzed the published data of Kauffman and Koehler and found the slightly smaller value of 1·1 eV for U_{vac} in gold, which is, however, still very large. Lazarev and Ovcharenko [67]) performed essentially the same experiment, but used lower quenching temperatures and lower quenching rates. They found 0·7 eV for U_{vac} in gold, in disagreement with Kauffman and Koehler. They also recovered the quenched wires, and observed a migration energy of the defects of only 0·5 eV!

Still more discrepancies arise when one compares the absolute densities of vacancies e.g. extrapolated to the melting point as they follow from these results. Then it appears that the high temperature results yield absolute densities that are in good agreement with the theory, whereas the low-temperature experiments yield densities that are too low by at least a factor of 20. It seems to the author that the quenching experiments do not yield reliable results, as the underlying assumption that practically all defects are frozen in during the quench, is probably incorrect. Even when cooling in a helium blast ($\mathrm{d}T/\mathrm{d}t = -10^4$ °C/sec), the vacancies still carry out 10^7 jumps. Diffusion of vacancies, resulting in the possible formation of *vacancy pairs*, which in their turn can move very rapidly to dislocations, must then surely be taken into account (compare also Bartlett and Dienes [68])).

Preliminary experimental evidence on these phenomena has been published by Maddin and Cottrell [69]), who observed a rise in the critical shear stress of Al single crystals after quenching from a high temperature, and by Levy and Metzger [70]), who noted a decrease in internal friction under the same conditions. These effects must be interpreted as caused by a condensation of quenched-in vacancies or pairs at dislocations, which process already starts at an appreciable rate during the quench. We shall not discuss the theory of the quenching-in of vacancies more in detail here; the mathematical difficulties that arise are rather forbidding, and a discussion would lead us too far astray *).

1.2.4. Electrical resistivity caused by vacancies and interstitials in metals

Two factors contribute to the scattering matrix-element of a point-defect: one takes into account the elastic strains of the lattice in the neighbourhood of the defect, and another describes the influence of the removal or addition of an extra positive charge. Dexter [71]) made an estimation of the relative importance of the first factor and found it to be negligible in f.c.c. metals for both vacancies and interstitials. This conclusion is doubtless correct for the case of vacancies that produce only very small short range strains; for an interstitial, however, the strains are much larger. A recent estimate by Jongenburger [72]), based on a (necessarily crude) comparison between the deviations of the atoms from their equilibrium places caused by the presence of an interstitial and those caused by thermal vibrations, yields a rather appreciable value for the influence of the strains; interpreted in terms of resistivity, the strain around an interstitial in copper contributes as much, possibly even 2 or 3 times as much as the (screened) extra positive charge associated with it. Applying the same argument to estimate the resistivity of a dislocation, he finds a value that compares very well with that derived on a firmer theoretical basis. The same holds true for quite

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*) In a recent study by Friedel (to be published shortly) the possibility of the formation of "dislocation tunnels" by absorbed vacancies is advanced. This process, when occurring during quenching, could be responsible for a very rapid decrease of the vacancy concentration.

another case, viz. the resistivity caused by solute carbon atoms in α-iron.

In Dexter's treatment, the summation over the displacement of the neighbouring atoms is replaced by an integration. It is suggested that this explains the difference between the results of Jongenburger and Dexter. The individual perturbations of the lattice potential by the displaced atoms are smeared out in Dexter's computation, and their influence on the electronic scattering is lowered by about a factor of 10. Moreover, for the atomic displacements Dexter uses too small values; according to the most recent computations by Huntington [58]), the values used by Dexter must be multiplied by at least a factor two, resulting in an increase of the scattering matrix element by a factor 4. This, together with the factor 10 dealt with before, is enough to invalidate Dexter's estimate and to make that of Jongenburger fairly plausible.

Blatt [73]) recently rediscussed this question and arrives at the opposite conclusion, viz. that the influence of the strains around an interstitial in copper on the resistivity can be neglected. Neither his arguments, however, can be regarded as conclusive, as he himself is aware. In view of these facts, we accept in the following Jongenburger's result as being the most probable one.

The influence of the extra positive or negative charge has been treated by Jongenburger [72, 74]), by Abeles (for vacancies only) [75]), and by Blatt (for interstitials only) [73]). They take account of the redistribution of the electrons by using a screened Hartree potential, and normalize this in such a way that certain phase relations derived by Friedel [76]) are obeyed. These relations are so stringent that the exact form of the scattering potential becomes unimportant [77]), and Jongenburger [74]) has shown that the use of a simple square well potential, suitably adapted, works equally well. All investigators agree that, for vacancies and for interstitials, the influence of the extra charge is about the same, viz. 1·3-1·4 $\mu\Omega$cm per atomic percent of defects in copper and gold. Recent (unpublished) calculations by Seeger result in the slightly larger value 1·67 $\mu\Omega$cm in Cu. For the total resistivity caused by point-defects in copper we shall adopt here the results of Jongenburger's computations:

Resistivity increase caused by one vacancy per cm^3: $1{\cdot}53.10^{-21}$ $\mu\Omega$cm;
Resistivity increase caused by one interstitial per cm^3: $5{\cdot}7.10^{-21}$ $\mu\Omega$cm.
The latter value is built up of $1{\cdot}5.10^{-21}$ $\mu\Omega$cm due to the charge and $4{\cdot}2.10^{-21}$ $\mu\Omega$cm due to the strains.

The experimental evidence as to the resistivity caused by point-defects has been reviewed by Blatt [73]). The most direct results can be derived from measurements of the release on heating of the stored energy in low-temperature irradiated metals and of the simultaneous decrease of the electrical resistivity. Overhauser [78]) thus found (accepting Jongenburger's value for the vacancy resistance) for the resistivity of interstitials about 10^{-20} $\mu\Omega\mathrm{cm}/\mathrm{cm}^{-3}$, if it was further assumed that the energy of formation of a vacancy-interstitial pair is 5 eV, another uncertain value. If this latter value were actually smaller (as is probable), the resistivity caused by interstitials should be smaller too. The results seem to indicate, however, that the influence of the strains can certainly *not* be neglected. Exact determinations of the resistivities caused by vacancies and interstitials have not yet been carried out. For vacancies the theory can, however, be regarded as rather accurate; for interstitials this is not the case.

1.3. Summary of the results of chapter 1.

In the following table I the most important numerical data discussed in this chapter have been compiled. All numerical values refer to pure copper and are to be considered as most plausible estimates. For gold about the same numerical values apply.

The data referring to vacancy pairs are based on the considerations of Bartlett and Dienes [68]) and on very recent calculations by Seeger (unpublished). The energy of association of two vacancies was calculated by the latter author to be 0·3 eV, the energy of migration was estimated by the former investigators to be about $^1/_2$ of that of a single vacancy. The resistivity produced by a vacancy pair does not differ appreciably of that of two single vacancies [79]).

TABLE I

Physical properties of lattice defects in copper.

Defect	Energy of defect	Migration energy	Electrical resistivity
Dislocation edge Dislocation screw	≈ 8 eV per atomic plane ≈ 5 per atomic plane	≈ 2 eV (climb) —	$0{\cdot}4 - 3.10^{-10}\, N \mu\Omega\mathrm{cm}$
Vacancies	0·85	1·2	$1{\cdot}53.10^{-21}\, n_v\ \mu\Omega\mathrm{cm}$
Interstitials	≈ 5	0·25 ?	$5{\cdot}7.10^{-21}\, n_i\ \mu\Omega\mathrm{cm}$
Vacancy pairs	$\approx 1{\cdot}5$	$\approx 0{\cdot}6$	$\approx 3.10^{-21}\, n_p\ \mu\Omega\mathrm{cm}$

2. PLASTIC DEFORMATION OF METALS

2.1. Action of dislocation sources

The facts and theories compiled in chapter 1 lead us to the following schematic outline of the atomic mechanism of plastic deformation in simple f.c.c. metals, of which copper may be taken as an example [80, 81, 82, 83]). The treatment applies only at very low temperatures, where no thermal activation takes place.

Consider a metal crystal containing a network of dislocations. In well-annealed metals the density d_0 of dislocations is probably $10^6 - 10^8$ cm^{-2} (section 1.1.6.2). Supposing that the elements are homogeneously distributed in the lattice and that in each node three elements meet, the mean length of the elements is $\bar{l} = 10^{-3}$ to 10^{-4} cm, and their total number amounts to $N = 10^9 - 10^{12}$ cm^{-3}. Most of these dislocations have presumably Burgers vectors of the type $[0,\frac{1}{2},\frac{1}{2}]$ (section 1.1.5), of which 12 possible orientations can occur. Given a stress component along one [110] axis, only 1/6 of the network elements can therefore in principle act as sources (Frank-Read sources of a more general kind). Most of the dislocations are presumably split up into partial dislocations; however, this does not affect in an appreciable way their activity as sources. One may thus assume that one tenth or less of the network elements can act in principle as sources under a given shear stress, that is $N_e \leqslant 10^{11}$ per cm^3. Consider a network-element of length l with Burgers vector parallel to the shear stress τ. When τ reaches the critical value (1.18):

$$\tau_1 = aGb/l, \tag{2.1}$$

the source starts to work. Let the number of emitted loops be n, and the mean area covered by them be A. Each loop has crossed in the mean d_0A dislocation elements and has formed d_0A jogs. Suppose that each loop has a circular shape (fig. 14). The jogs in the loops have each run a certain distance (we assume that every jog retains its place in the loop, compare section 1.1.3.2). According to formula (1.17), the efficiency with which the jogs have formed vacancies or interstitials depends on the orientation of the Burgers vectors $\mathbf{b}'$ of the crossing dislocations with respect to the glide plane and on the azimuth of the site of the jog in the expanding loop (fig. 14).

Consider an element of the loop (radius R) with azimuth between φ and $\varphi + \mathrm{d}\varphi$. The efficiency with which this element forms point-defects is according to (1.17) given by

$$e_\varphi = \sin\,\varphi \cdot \overline{(\mathbf{b}'.\mathbf{v})}^{\,\mathbf{b}'} \tag{2.2}$$

where the bar means averaging over all possible orientations of $\mathbf{b}'$ and $\mathbf{v}$ denotes the unit vector perpendicular to the plane of the loop. When we assume that the Burgers vectors $\mathbf{b}'$ are indeed all oriented according to [110] directions,

$$\overline{(\mathbf{b}'\mathbf{v})}^{\,\mathbf{b}'} = \tfrac{1}{3}\sqrt{3}$$

and thus

$$e_\varphi = \tfrac{1}{3}\sqrt{3}\,\sin\varphi\,. \tag{2.3}$$

The loop of radius R contains $\pi R^2 d_0$ jogs, the element in question has therefore $^1/_2 R^2 d_0 \mathrm{d}\varphi$ jogs and on expansion of the radius to $R + \mathrm{d}R$ (leaving out second order terms), the number of point-defects formed is

$$\mathrm{d}f \approx 4\int\limits_0^{\pi/2} \mathrm{d}\varphi \,.\, \tfrac{1}{2} R^2 d_0 \frac{\mathrm{d}R}{b}\, e_\varphi = \tfrac{2}{3}\sqrt{3}\,\frac{R^2 d_0}{b}\,\mathrm{d}R\,. \tag{2.4}$$

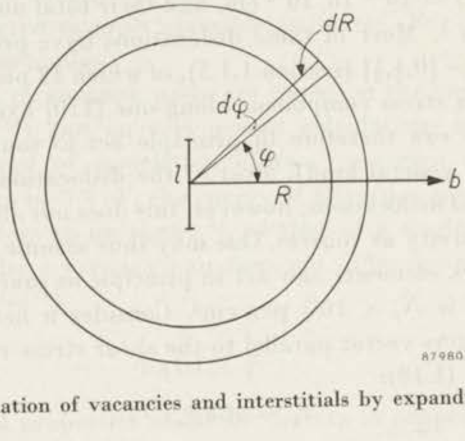

Fig. 14. On the formation of vacancies and interstitials by expanding dislocation loops.

A loop that has reached an ultimate area A has thus formed

$$f(A) = \tfrac{2}{9}\sqrt{3}\,\frac{d_0}{\pi^{3/2} b}\,A^{3/2} \tag{2.5}$$

point-defects. This holds for circular loops; in general, owing to the larger drag excerted by the defect formation on the screw parts, the loop will assume an elliptical shape. However, as pointed out by Mott [84]), the axial ratio will probably ultimately reach a constant value, say $^1/_2$, and formula (2.5) can be written approximately as:

$$f(A) \approx 0{\cdot}04\,\frac{d_0}{b}\,A^{3/2}. \tag{2.6}$$

The energy stored in the metal due to this expansion is given by the sum of three terms:

$$E = E_1 + E_2 + E_3. \tag{2.7}$$

(1) The energy of formation of the total length of dislocation of the loop. Calling the mean energy of a dislocation per atomic plane crossing its axis $\overline{U}_d$ (about 6 eV, section 1.1.2), we have:

$$E_1 \approx 4 \, \frac{A^{1/2}}{b} \, \overline{U}_d \tag{2.8}$$

(the numerical factors in this and the following formulae depend on the shape of the loop).

(2) The energy of formation of the total number of jogs. Denoting the mean energy of a jog by $\overline{U}_j$ (of the order of $\overline{U}_d$, as a jog is an element of dislocation of length b), we have:

$$E_2 = A d_0 \overline{U}_j \, . \tag{2.9}$$

(3) The energy of formation of the defects. Denoting the mean energy of formation of a defect by $\overline{U}_f$, then we have

$$E_3 = 0{\cdot}04 \, \frac{d_0}{b} \, A^{3/2} \, \overline{U}_f \, . \tag{2.10}$$

U_f is 0·85 eV for a vacancy and between 2 and 5 eV for an interstitial (table I). Presumably interstitials are formed in lesser amounts then vacancies, due to their high energy, and we shall therefore take as a weighted mean $\overline{U}_f = 1$ eV.

The energy supplied by the applied stress is simply

$$E_\tau = \tau A b \, , \tag{2.11}$$

where τ stands for the local shear stress component parallel to **b** in the vicinity of the loop.

With the expansion of dislocation loops is associated a dissipation of energy in the form of vibrations of the lattice, resulting from the atomic motion coupled with the propagation of a dislocation [2]). To take account of this we put the available energy for defect production equal to λE_τ, where λ is a numerical factor smaller than unity: λ denotes the fraction of the strain energy that is used for defect formation. Its magnitude depends very sensitively on the velocity of the dislocations; λ is presumably of order unity.

The energy balance thus reads:

$$\lambda \tau A b = 4 \, \frac{\overline{U}_d}{b} \, A^{1/2} + d_0 \overline{U}_j A + 0{\cdot}04 \, \frac{d_0}{b} \, \overline{U}_f A^{3/2} . \tag{2.12}$$

The mean source length is 10^{-4} cm, thus A is larger than 10^{-8} cm^2. In that case it is easily found by inserting the numerical values quoted above, that the second term at the right hand side of (2.12) is completely negligible compared to the first and third terms; this means that the formation of jogs only cannot enhinder the expansion of dislocation loops at all. Solving (2.12) for A, therewith leaving out this second term, the result is:

$$A = \left\{ \frac{\lambda b^2 \tau}{0{\cdot}08\, d_0 \overline{U}_f} \left(1 + \sqrt{1 - \frac{0{\cdot}64\, d_0 \overline{U}_f \overline{U}_d}{\lambda^2 b^4 \tau^2}} \right) \right\}^2 . \tag{2.13}$$

Of course the formula is only valid when the root occurring in it is real, thus when

$$\tau \geqslant \sqrt{0{\cdot}64\, d_0 \overline{U}_f \overline{U}_d / \lambda^2 b^4}\,. \tag{2.14}$$

An imaginary root simply means that the source has not been activated at all. This gives rise to the following conclusion: by reason of the necessary formation of point-defects there exists, apart from the fundamental condition (2.1) for the activation of a source, still another condition, viz. (2.14). The latter becomes of importance when:

$$\alpha G b / l < \sqrt{0{\cdot}64\, d_0 \overline{U}_f \overline{U}_d / \lambda^2 b^4}\,. \tag{2.15}$$

Putting $\overline{U}_d \approx G b^3$ (compare (1.3a)), (2.15) goes over into

$$l > \lambda l_0 = \lambda \sqrt{\alpha^2 G b^3 / 0{\cdot}64\, d_0 \overline{U}_f}\,. \tag{2.16}$$

This means that for sources of length $l > \lambda l_0$ ordinary activation at the critical shear strength $\tau_1 = \alpha G b / l$ will not take place, the formation of point-defects preventing this. Only at appreciably higher stresses can the critical circular shape of the source dislocation be reached, and even then probably no source action will occur, that is, the segment will expand but none or only a few new segments will be formed subsequently. l_0 stands thus for an upper limit to the length of the sources that can be activated. For copper l_0 is about 4×10^{-4} cm.

The emitted loops produce a back-stress at the site of the source. The component of this stress that opposes the local activating shear stress is given by

$$\tau_b = \gamma \frac{n G b}{A^{1/2}}, \tag{2.17}$$

where γ is a numerical factor of order 0·1, depending on the value of Poisson's ratio and on the shape of the loops. For A in (2.17) one must read the mean area covered by the loops; in view of the uncertainties inherent to the theory one may simply assign the same value of A to all loops. Even if the loops run with a velocity of only 0·01 or 0·001 of that of sound, the time for a loop to attain its final area is of the order of 10^{-7} to 10^{-8} sec. In this time the local shear stress has (under normal experimental conditions) not changed appreciably and we may insert in (2.17) the momentary value of A following from (2.13). We then find:

$$\tau_b = \frac{0{\cdot}08\, \gamma G d_0 \overline{U}_f}{b} \frac{n}{\tau} \frac{1}{f(\tau)}, \tag{2.18}$$

where

$$f(\tau) = \lambda \left\{ 1 + \sqrt{1 - 0{\cdot}64\, d_0 \overline{U_f}\, \overline{U_d} / \lambda^2 b^4 \tau^2} \right\}.$$

The source will be activated again when the shear stress at the site of the source, $\tau - \tau_b$, attains anew the value τ_1, thus when:

$$\tau - \frac{0{\cdot}08\, \gamma G d_0 \overline{U_f}}{b} \frac{n}{\tau} \frac{1}{f(\tau)} = \frac{\alpha G b}{l}. \tag{2.19}$$

According to a hypothesis of Fisher, Hart and Pry 85, 86), a source, once activated, can continue emitting dislocation loops until the resultant stress at the source has dropped to a value as low as τ_1/p, where p is about 3. This dynamic generation of loops will occur when the dislocations move with approximately the velocity of sound in the material, so that their kinetic energy becomes comparable to the potential energy of the source. In the case that this presumption is not realized (static generation), the loops are emitted one at a time. Then in formula (2.19) n takes as a value successively all positive whole numbers, whereas, should the hypothesis of dynamic generation hold, n jumps in amounts appreciably larger than unity. Solving the discontinuous equation (2.19) for n, one gets thus a function displaying a large number of small jumps, or a function characterized by a smaller number of larger jumps. However, as will be shown below, in practice the total number of loops emitted already attains very quickly rather large values, of the order of 100, and we may safely replace the discontinuous solution by a continuous one in the former case. As the number of loops emitted per burst in the dynamic case is of the order of 10, also in this case this replacement is allowed. One finds, using (2.1) and the definition of l_0 (2.16):

$$n = \frac{8}{\gamma} f(\tau) \frac{l_0^2}{l^2} \left\{ \left(\frac{\tau}{\tau_1} \right)^2 - \frac{\tau}{\tau_1} \right\}. \tag{2.20}$$

2.2. Formation of defects by plastic strain

2.2.1. Single glide

Suppose there are N_e sources per cm^3 working under the influence of a local stress τ.
These contribute to the total strain the amount:

$$\varepsilon = N_e\, n\, b A. \tag{2.21}$$

The total number of defects formed by these sources is according to (2.6)

$$F = N_e\, n \times 0{\cdot}04 \frac{d_0}{b} A^{3/2}, \tag{2.22}$$

whereas the total length of dislocation formed is:

$$D = N_e n \times 4A^{1/2}. \tag{2.23}$$

The dependence on τ is governed by the expressions (2.13) and (2.20) and by an unknown relation, if it exists, between N_e and τ. Presumably, N_e will increase with the stress as successively shorter sources will be activated. The function $N_e(\tau)$ depends on the distribution of stress in the material and on the distribution of source lengths. As both are completely unknown, we shall take N_e simply constant. As most of the strain is contributed to by sources that have been activated from the beginning and the activation of new sources will probably be strongly hindered by the action of the stress fields of the sources already activated, the error made in this approximation will not be too serious.

The quantity τ describes the *local* stress in the immediate vicinity of the source. It is related in an intricate way to the *applied* stress; explicit determination of τ would require knowledge of the work-hardening characteristics of the material. We assume that on the average τ scatters not very much from source to source and can therefore be eliminated from (2.21), (2.22) and (2.23). When τ/τ_1 is at least so much larger than unity that it can be considered negligible compared to $(\tau/\tau_1)^2$ in (2.20), and when we take $f(\tau) = 1$, as is indeed practically true, this elimination yields:

$$F = 0{\cdot}06 \sqrt[4]{\frac{\gamma \lambda G d_0^3}{b^6 \overline{U_f} N_e}}\, \varepsilon^{5/4}; \tag{2.24}$$

$$D = 2{\cdot}4 \sqrt[4]{\frac{d_0 \overline{U_f} N_e}{\gamma \lambda G b^6}}\, \varepsilon^{3/4}. \tag{2.25}$$

These formulae no longer depend on l. A further advantageous property of these expressions is that they contain the parameters γ, λ, $\overline{U_f}$ and N_e under the fourth power root sign; the uncertainties in the values of these parameters do therefore affect the accuracy of the result but slightly.

Taking $\gamma = 0{\cdot}1$, $\lambda = 1$, $G = 4.10^{11}$ dyn/cm², $b = 2{\cdot}5.10^{-8}$ cm and $\overline{U_f} = 1{\cdot}2.10^{-12}$ erg, values pertaining to copper as well as to silver and gold, one finds:

$$F = 7.10^{15}\, d_0^{3/4}\, N_e^{-1/4}\, \varepsilon^{5/4}\ \mathrm{cm}^{-3}; \tag{2.24a}$$

$$D = 1{\cdot}4.10^{6}\, d_0^{1/4}\, N_e^{1/4}\, \varepsilon^{3/4}\ \mathrm{cm}^{-2}. \tag{2.25a}$$

2.2.2. **Multiple glide**

The formulae (2.24) and (2.25) have been derived under the assumption that d_0, the density of intersecting dislocations, does not change during the slip process. This assumption is realized in the case of single glide; in multiple glide, however, the "forest" of dislocations crossed by a given loop thickens continually. This effect can be taken into account schematically as follows.

Suppose there are g active slip systems. The total number of activated sources being again N_e, the density of sources on a given glide plane, belonging to slip system i, is then

$$\Delta_i = \frac{N_e}{g} s \tag{2.26}$$

sources per cm^2, where s is the mean spacing between successive glide planes. Suppose all dislocation zones are circular, with the same radius R on all slip systems. Consider an activated source surrounded by its loops on an intersecting glideplane belonging to system j. The length of the intersection of this zone with a given glide plane of system i be L; then the average number of zones on the latter glide plane that intersect the first zone is (fig. 15):

$$N_i = \Delta_i \,(2RL + \pi R^2)\,. \tag{2.27}$$

N_i is of course a number much smaller than unity. A given dislocation zone on system j intersects in the mean R/s glide planes of system i. The average length L amounts to $4R/\pi$, thus the total number of sources on system i intersected by a given source on system j is:

$$N_a = \left(\frac{8}{\pi} + \pi\right) \frac{\Delta_i}{s} R^3 .$$

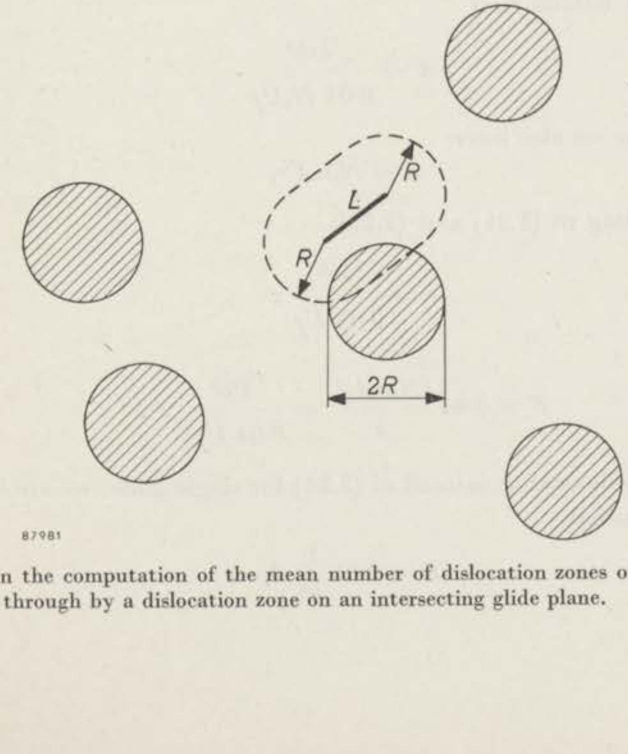

Fig. 15. On the computation of the mean number of dislocation zones on a given glide plane, cut through by a dislocation zone on an intersecting glide plane.

As there are $g-1$ intersecting glide systems, we find for N_a, using (2.26):

$$N_a = \frac{g-1}{g}\left(\frac{8}{\pi} + \pi\right) N_e\, R^3 \approx N_e\, A^{3/2}. \qquad (2.28)$$

Suppose that each source has emitted n loops. Then in addition to the density of originally present crossing dislocations d_0, the effective density $N_e n A^{1/2}$ of newly formed dislocations must be counted. That is, instead of d_0 one should write in the case of multiple glide:

$$d = d_0 + N_e n A^{1/2}. \qquad (2.29)$$

Equation (2.12) describing the energy balance of an expanding source now becomes:

$$\lambda\tau A b = \frac{4\overline{U}_d}{b}\, A^{1/2} + 0{\cdot}04\, \frac{d_0}{b}\, \overline{U}_f A^{3/2} + 0{\cdot}04\, \frac{N_e \overline{U}_f}{b}\, nA^2; \qquad (2.30)$$

and when $N_e n A^{1/2} \geqslant d_0$ the state of affairs is completely changed. We shall consider here only the limiting case that

$$N_e\, n A^{1/2} \gg d_0. \qquad (2.31)$$

In this case the first term on the right hand side of (2.30) can also be neglected and we have

$$\lambda\tau A b \approx 0{\cdot}04\, \frac{N_e \overline{U}_f}{b}\, nA^2,$$

from which it follows that

$$nA = \frac{\lambda\tau b^2}{0{\cdot}04\, N_e \overline{U}_f}. \qquad (2.32)$$

As in this case we also have:

$$d \approx N_e n A^{1/2},$$

we get according to (2.21) and (2.22):

$$\varepsilon = \frac{\lambda b^3}{0{\cdot}04\, \overline{U}_f}\, \tau \qquad (2.33)$$

and

$$F = 0{\cdot}04\, \frac{(N_e n A)^2}{b} = \frac{\lambda^2 b^3}{0{\cdot}04\, \overline{U}_f^{\,2}}\, \tau^2. \qquad (2.34)$$

From this it follows that instead of (2.24) for single glide, we are left with the simple relation

$$F = 0{\cdot}04\, \frac{1}{b^3}\, \varepsilon^2, \qquad (2.35)$$

in the case of multiple glide. Numerically one has for the noble metals:

$$F \approx 2{\cdot}5 . 10^{21}\, \varepsilon^2 . \qquad (2.35a)$$

In this theory the interaction of dislocations other than that of a purely geometrical nature has been neglected. In multiple glide the change of elastic interaction energy with the distance between dislocations may appreciably influence the energy balance. Equation (2.35) must therefore be considered with care.

3. ELECTRICAL RESISTIVITY OF PLASTICALLY STRAINED METALS

3.1. **Introduction**

The theory discussed in chapter 2 has primarily been developed to study the defect concentrations in plastically deformed metals; it is not suited to describe e.g. the work-hardening of a metal. The defect concentrations can also be studied experimentally, viz. by measuring physical quantities that depend on them. One of the quantities most suited for this is the electrical resistivity. This increases appreciably by plastic strain, due to the scattering of the conduction electrons by the defects introduced during the deformation. In this chapter we shall discuss the available experimental data on the subject of the electrical resistivity of deformed metals, and compare them to the theory.

The relative change of resistivity on deformation of a metal is very sensitive to purity and temperature. For obvious reasons it is advisable, in order to obtain an insight into the fundamentals of the effect, to study very pure metals and to measure their resistance at very low temperatures. Also to avoid unwanted effects due to diffusion phenomena the temperature of deformation should be very low. Only a small part of the literature that exists on the subject [87, 88]) conforms to these restrictions, and even there really systematic observations are rather scarce. The metals studied most accurately are the noble metals Cu, Ag and Au. These metals are easily deformable at low temperatures and also easy to obtain in a pure state (impurity content less than 0·01%). We have therefore also chosen these metals, especially copper and silver, as the subject of out investigations. It should be mentioned here, however, that a study of other metals, e.g. of those with different crystal structure such as iron and the alkalis, is badly needed.

3.2. **Resistivity measurements on noble metals deformed at very low temperatures**

3.2.1. **Extension and torsion experiments**

The first systematic observations of the resistivity changes of deformed metals were carried out in Delft by Druyvesteyn and his collaborators Molenaar and Aarts [89]). They measured resistivity and stress as a function of plastic strain on wires of polycrystalline copper, silver and gold (and aluminium) stretched at the temperature of liquid nitrogen. These experiments have been repeated by Manintveld [90]). The present author showed [89]) that the observed resistivity-strain relations could all be represented remarkably accurately by the relation:

$$\Delta\varrho/\varrho = c(\Delta l/l)^{3/2}, \qquad (3.1)$$

in which $\Delta l/l$ stands for the elongation, $\Delta\varrho/\varrho$ for the relative increase of resistivity. The coefficient c, of order unity, varies a little between the various experiments.

In order to check the validity of this relation, the other available data on polycrystalline copper deformed at a low temperature were analyzed. The results are given in fig. 16. It was found that an exact 3/2-exponent has not been observed by other authors, although the deviations are but slight.

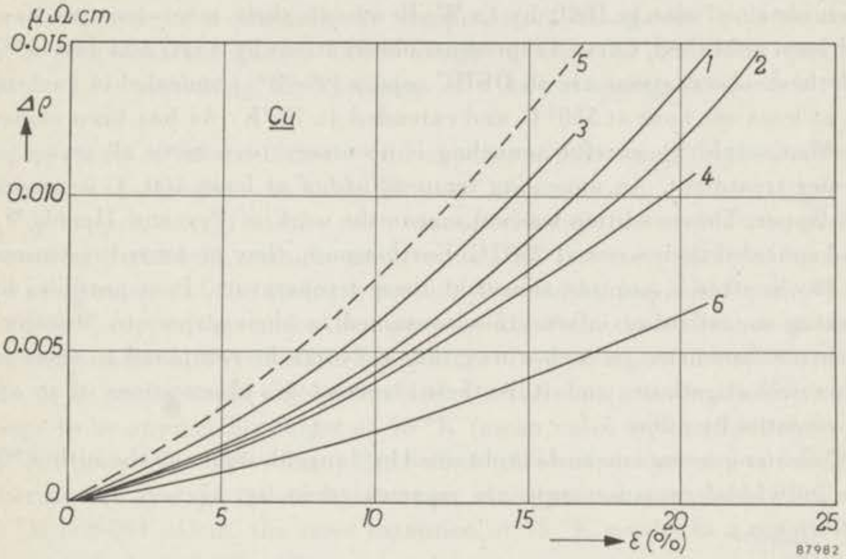

Fig. 16. Observed resistivity-strain relations of extended polycrystalline copper wires. Plotted is the absolute amount of additional resistivity against the mean shear strain according to (3.3), measured at 78 °K or less. (1) Observations by Molenaar and Aarts; (2) by Druyvesteyn and Manintveld; (3) by Berghout; (4) by Aarts and Jarvis; (5) by Pry and Hennig (extrapolated); (6) by Jongenburger and the author (mean of 9 series of measurement, see fig. 17).

The results of all experiments can be described by the more general formula:

$$\Delta\varrho = a\varepsilon^{p} \tag{3.2}$$

where ε is the mean shear strain that can be defined as

$$\varepsilon_e = 2{\cdot}24\ \Delta l/l \tag{3.3}$$

in fine-grained polycrystalline wires that are stretched [91]), and approximately as

$$\varepsilon_t = \frac{3}{2}\,\Theta\,\frac{r}{l} \tag{3.4}$$

in wires that are twisted. Here Θ is the angle of twist and r and l are radius and length of the wire. Expressing $\Delta\varrho$ in μΩcm, the coefficient a lies between 0·04 to 0·16 μΩcm, and p varies between 1·3 and 1·5.

The observations used to construct fig. 16 are as follows. They all refer to copper, the other metals have been studied far less and no reliable comparison is possible. The curves denoted 1 and 2 represent measurements of Molenaar and Aarts 89), and of Druyvesteyn and Manintveld 90) respectively, and are described in detail in Manintveld's thesis 92). Curve 3 has been obtained also in Delft by C. W. Berghout; these measurements have not been published. Curve 4 represents observations by Aarts and Jarvis 93). All these observations are on OFHC copper (99·98%) annealed in vacuum for at least one hour at 550° C, and extended at 78 °K. As has been shown by Manintveld 92), careful annealing is necessary to remove all traces of former treatment. An annealing temperature of at least 400 °C is needed for copper. This condition was not met in the work of Pry and Hennig 94), who annealed their wires at 250° C. Furthermore, they measured resistance at 78 °K after 5 minutes anneal at room temperature. It is possible, by making use of other information contained in their paper, to "correct" their measurements in such a way that they can be compared to those of other investigations, and it is these "corrected" observations that are represented by curve 5.

Curve 6 represents mean data obtained by Jongenburger and the author 95); the individual measurements are represented in fig. 17.

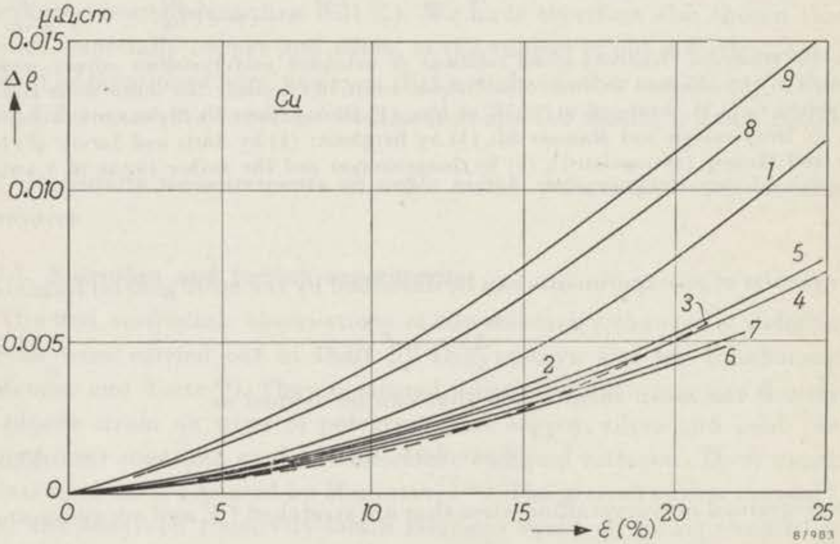

Fig. 17. Resistivity-strain relation of polycrystalline copper wires extended at the temperature of liquid nitrogen or hydrogen. The figures near the curves correspond to the specimen numbers of table II.

Polycrystalline copper (of two grades of purity) and silver wires were annealed for one hour at 650 °C in vacuum and deformed at 78 °K (liquid N_2) or 20 °K (liquid H_2). The apparatus consists of a small tensile machine driven by a synchronous motor and provided with a torsion head, in order that both twisting and extension experiments can be carried out. The specimen, in the form of a 0·5 mm wire, is immersed in liquid hydrogen or nitrogen, together with a comparison wire. Copper potential leads were soldered to the wire at a sufficient distance from the clamps and resistances are compared in a Diesselhorst compensator. Elongation is measured by a simple strain gauge, and a rough measure of the stress can be obtained by measuring the extension of a helical spring mounted in the loading rod.

The values of the coefficients and exponents pertaining to the various observations are given in table II.

For copper, except in one case, viz. specimen 3, the exponents all lie between 1·3 and 1·55, with the mean value 1·45. The exception (not used in the computation of the mean) is probably caused by impurities present in the OFHC copper that make their presence known in the resistance at very low temperatures. A systematic dependence of p on temperature of deformation or on purity could not be detected. On the contrary, the coefficient a seems to be appreciably larger at 78 °K (mean value 0·08 μΩcm) than at 20 °K (mean value 0·05 μΩcm). This effect can also be expressed as follows: whereas the average resistivity increase of copper wire extended 10% at 20 °K is 0·004 μΩcm, the same extension at 78 °K results in a resistivity increase of about 0·007 μΩcm.

As to silver, too few experiments have been performed to reach more than one conclusion, that p seems to be appreciably less than in copper, viz. about 1·2. The one twisting experiment carried out so far yields essentially the same result (when strains are compared according to (3.3) and (3.4)).

Those observations of other authors that have been published in a sufficiently extensive form can also be analyzed in the way described, although unknown differences in the experimental conditions, purity, pre-treatment etc. make the comparison considerably less accurate. Table III lists the relevant data.

The conclusion can be drawn that the other authors have obtained results that do not fundamentally deviate from our own. The scatter between the various data in table III, especially in a, is too large to allow further inference to be drawn.

3.2.2. **Combined deformation methods**

As we have seen in table II, the dependence of the additional resistivity on plastic strain is roughly the same in extension and in twisting experiments.

TABLE II

Observed constants in power-law expressions (3.2) of copper and silver

Wire No.	Metal and temperature of deformation	a (μΩcm)	p
1	OFHC Cu, 78° K	0·073	1·52
2	ibid.	0·056	1·45
3	OFHC Cu, 20° K	0·073	1·7
4	99·998% Cu, 20 °K	0·048	1·40
5	ibid.	0·051	1·47
6	ibid.	0·052	1·55
7	ibid.	0·048	1·50
8	99·998% Cu, 78 °K	0·100	1·41
9	ibid.	0·091	1·32
	mean value Cu	0·065	1·45
10	99·99% Ag, 20° K	0·052	1·25
11	99·99% Ag, 78° K	0·055	1·15
12	99·99% Ag, 20° K (torsion)	0·040	1·21
	mean value Ag	0·052	1·20

TABLE III

Constants a and p of powerlaw (3.2) by other authors

Author	Metal and temperature of deformation	a (μΩcm)	p
Manintveld 92)	OFHC Cu, 78 °K	0·138	1·51
Berghout, unpubl.	ibid.	0·16	1·43
Molenaar-Aarts 89)	ibid.?	0·09	1·3
Aarts-Jarvis 93)	ibid.	0·1	1·4
Manintveld 92)	99.98% Ag, 78 °K	0·140	1·53
Aarts-Jarvis 93)	99.99% Ag, 78 °K	0·1	1·4
Manintveld 92)	99.98% Au? 78 °K	0·129	1·52
Aarts-Jarvis 93)	99.99% Au 78 °K	0·07	1·4

This is what might have been expected in polycrystalline metals. As the spatial distribution and the type of dislocation produced will presumably differ between the two methods of straining (but not the total number), it was thought that particular effects might possibly be observed when the two ways of deformation were applied one after the other. The results obtained are presented in fig. 18. The curve in this diagram refers to a polycrystalline 99·99% Ag wire first twisted (at 20 °K) to a "mean torsional strain" (equation (3.4)) of 21% (part *OA*), then twisted in the opposite sense by 7% (*AB*); afterwards stretched by an amount corresponding to 31% strain (*BC*), then twisted again in the original sense by 14% (*CD*) and ultimately stretched to fracture (*DE*). After each change of deformation a slight stand-still of the resistivity increase was observed. This is probably due to the influence of the elastic part of the deformation and to the dead range of the torsion head, and not to some kind of "Bauschinger" effect. In the further parts of the curve nothing peculiar was observed; twisting and stretching produced about equal changes of resistivity, although a power law could not be fitted to the later parts of the curve.

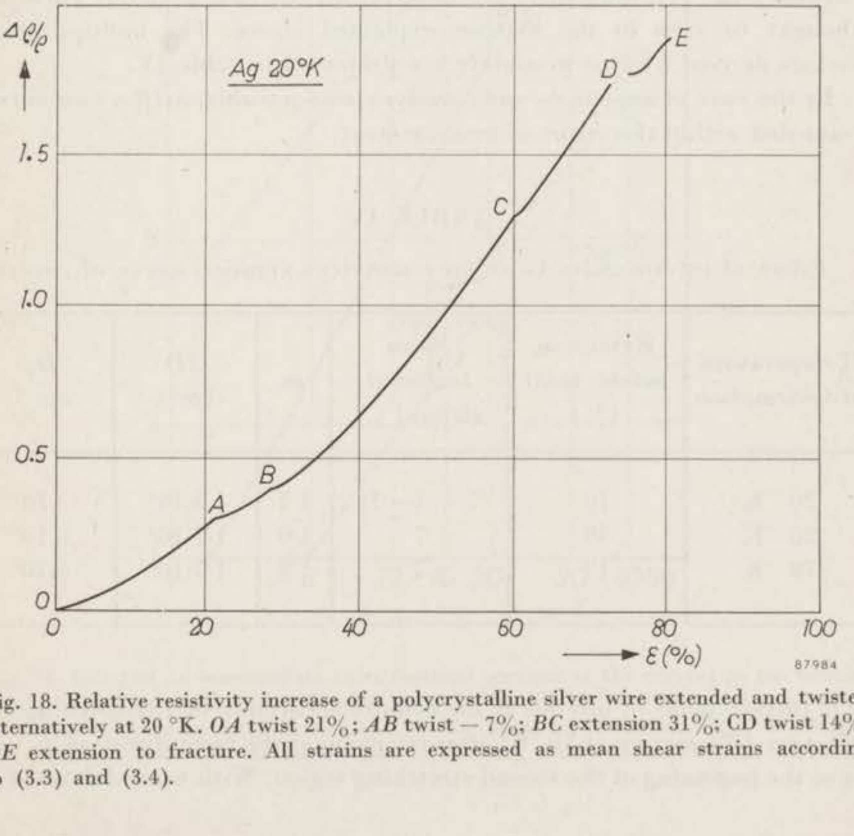

Fig. 18. Relative resistivity increase of a polycrystalline silver wire extended and twisted alternatively at 20 °K. *OA* twist 21%; *AB* twist — 7%; *BC* extension 31%; CD twist 14%; *DE* extension to fracture. All strains are expressed as mean shear strains according to (3.3) and (3.4).

A more detailed study of the effect of combined deformations was undertaken [95]), bearing the following idea in mind. An intermediate twist given during a stretching treatment produces naturally dislocations with orientations different from those of the dislocations formed during the stretching itself. On further stretching the latter dislocations have to cut through the newly formed "torsion" dislocations, in addition to through those already present before the twist. The efficiency of formation of point-defects will therefore be increased by a "multiplication factor" that is some function of the ratio between the density of intersecting dislocations after the twist and before it:

$$m = f\left(\frac{D_1 + \Delta D}{D_1}\right), \tag{3.5}$$

where D_1 is the density before the twist and ΔD stands for the effective density of the "torsion" dislocations.

The experimental evidence is presented in fig. 19. When the second part of the (logarithmically plotted) elongation curve is compared to the extrapolated first part, with the effect of the twist simply added to it, (thin curves in fig. 19), differences are observed in the case of silver. These are thought to arise in the manner explained above. The multiplication-factors derived by this procedure are presented in table IV.

In the case of copper no such analysis was possible, as the two curves coincided within the errors of measurement.

TABLE IV

Effect of intermediate twist on resistivity-extension curve of silver

Temperature of deformation	Extension before twist (%)	Mean torsional strain (%)	m	ΔD cm^{-2}	D_1 cm^{-2}
20 °K	19	7 + (– 7)	1·2	$\sim$3.10^8	10^9
20 °K	38	7	1·0	1·7.10^8	$\geqslant$ 10^{10}
78 °K	19	7	1·2	1·7.10^8	6.10^8

A further point of interest is the definite occurrence of a "Bauschinger"-effect on deformation at 78 °K, after reversion of the twist direction as well as in the beginning of the second stretching region. With wires deformed at

20 °K the effect is so small that it cannot be separated from the unavoidable effects of the machine (compare the discussion of fig. 18). At the temperature of liquid nitrogen, however, an appreciable *drop* in the resistivity occurs on changing the method or direction of deformation.

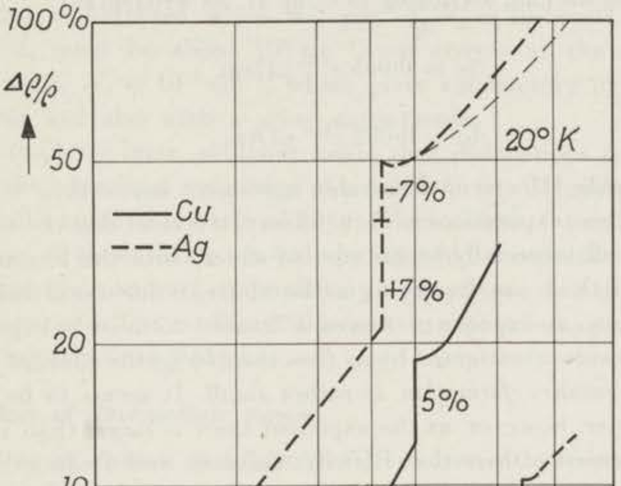

Fig. 19. Effect of an intermediate twist (vertical portions of the curves) on the relative resistivity-extension relation of Cu and Ag at 20 °K and 78 °K. Strains are again mean shear strains according to (3.3) and (3.4). The thin curves are extrapolations of the primary extension parts, based on the assumption of additivity of the effects of torsion and extension.

3.3. Interpretation of the observations

3.3.1. Resistivity-strain relation

The observed values of a and p (tables II and III) in the empirical relation (3.2) can be directly compared to the theoretical formulae (2.24a), (2.25a) and (2.35a), bearing in mind that the resistivity increase on straining is caused by the formation of lattice defects. The averaged results of the observations can, according to table II, be written as:

For copper:

$$\Delta\varrho = 0{\cdot}065\ \varepsilon^{1{\cdot}45}\ \mu\Omega\text{cm} \tag{3.6}$$

and for silver:

$$\Delta\varrho = 0{\cdot}052\ \varepsilon^{1{\cdot}20}\ \mu\Omega\text{cm}\,. \tag{3.7}$$

The data of table III are in reasonable agreement herewith.

Comparing these expressions with the theory, it is clear that the exponents agree rather well (especially in the case of silver) with the assumption of "easy glide". In that case, depending on the relative influences of dislocations and point-defects, an exponent between 0·75 and 1·25 must be expected. In the range of strains investigated by us (less than 40%) the effect of multiple glide on the *vacancy formation* is rather small. It seems to be notably present in copper, however, as the exponent there is larger than 1·25.

It may be remarked here that Blewitt, Coltman and Redman [96]) have strained copper single crystals by more than 100% and found a quadratic dependence of resistivity on strain, as is expected in multiple glide. The absolute amount of resistance increase was much smaller than that predicted by equation (2.35a), however. Polycrystalline wires cannot be stretched by more than about 40%, so that no check has been possible in this respect.

Assuming for the moment that the exponents do agree, we can compare the coefficients with the theoretical expectations. According to the simple theory outlined in chapter 2, vacancies and interstitials should occur in about equal numbers. However, the energy of formation of interstitials being much larger than that of vacancies, it is very probable that the geometry of the jog motion is changed in such a way as to reduce as far as possible the formation of interstitials. Therefore, most point-defects formed will be vacancies (a similar argument was used to estimate the energy of formation of point-defects in chapter 2). To translate densities of point-defects into resistivities, we thus take as a yardstick a value in between those relating to vacancies and interstitials, but closer to the former, viz. 3.10^{-21} $\mu\Omega\text{cm}/\text{cm}^3$ (compare table 1). As to dislocations, as explained in section (1.1.6.1) the mean resistivity caused by these defects must be described by a factor $\alpha \times 10^{-14}$ $\mu\Omega\text{cm}/\text{cm}^2$, where theory predicts that $\alpha \approx 1$, but various experiments (see below and chapters 4 and 5) indicate α to be of order 10. From formulae (2.24a) and (2.25a) one obtains then for the theoretically expected resistivity increase caused by point-defects and dislocations:

$$\Delta\varrho = 2{\cdot}1.10^{-5}\left(\frac{d_0^3}{N_e}\right)^{1/4}\varepsilon^{5/4} + 1{\cdot}2a.10^{-8}\,(d_0N_e)^{1/4}\,\varepsilon^{3/4}\ \mu\Omega\text{cm}. \tag{3.8}$$

Comparing with (3.6) and (3.7) numerical agreement (at least to order of magnitude) is obtained when we put $d_0^3/N_e \approx 10^{14}\,\text{cm}^{-3}$. Remembering that d_0 must be about $10^8\ \text{cm}^{-2}$, one arrives at the set of values $d_0 \approx 10^8\ \text{cm}^{-2}$, $N_e \approx 10^{10}\ \text{cm}^{-3}$, which gives satisfactory agreement with experiment and also with a priori expectation.

As we shall see later, evidence exists that dislocations cause about as much of the additional resistivity as point-defects. Assuming both contributions to be equal at a strain of 20% we can estimate a and find $a = 26$.

Of course all these values can only be regarded as estimates, the assumption of easy glide and other simplifying suppositions do not allow a more exact comparison. The combined deformation experiments provide a means for checking these assumptions.

3.3.2. **Effect of intermediate torsion**

According to Paxton and Cottrell [97]) one can estimate the amount of dislocations formed during the twist of a circular wire from the formula:

$$\Delta D = \Theta/bl = \tfrac{3}{2}\,\varepsilon_t/rb. \tag{3.9}$$

From this and the observed multiplication factors in table IV one can estimate the density of dislocations D_1, active as intersecting dislocations *before* the twist, according to formula (3.5). When formula (2.25) is assumed to hold, (3.5) can be written in the more definite form:

$$m = \left(\frac{D_1 + \Delta D}{D_1}\right)^{3/4}. \tag{3.5a}$$

From this one finds the values of D_1 that are entered (together with ΔD) in table IV. D_1 is found to be about $10^9\ \text{cm}^{-2}$ after 20% strain. This can be compared to the total density as given by formula (2.25a), using the values for d_0 and N_e derived above. One finds after 20% strain: $D = 1{\cdot}5 \times 10^{10}$ cm^{-2}, which means that the increase of the dislocation density on the *active* glide systems has indeed been much larger than that on other systems, and that the assumption of single glide is more or less justified, at least in the case of silver deformed less than 20%. This is not true in copper, where the effect of torsion is practically completely additive. It is interesting to compare this difference in behaviour between the two metals with the observed difference in the value of the component p (section 3.2.2). Whereas in silver p is fairly well in accord with theory for single glide as far as the formation of vacancies is concerned, in copper it is obviously too high. One must conclude that the assumption at all allowed of single glide is not in copper. This same conclusion holds, as follows from the data of table IV, for silver extended by 40%.

Summarizing, one can conclude that the observational evidence on the change of resistivity by deformation seems to agree at least semi-quantitatively with the assumption that point-defects and dislocations produced in the way described in chapters 1 and 2, are both responsible for the increase of the resistivity. A second conclusion is that the original density of dislocations in well-annealed copper and silver is about 10^8 cm^{-2}, that about 10^{10} sources per cm^3 are activated during plastic strain, and that in polycrystalline silver deformed less than say 30% the state of deformation with regard to the defect production resembles somewhat that of easy glide as observed in single crystals. In copper this is not so, or in a much lesser degree.

As to the observed temperature dependent phenomena, such as the systematic variation of the coefficient a and the "Bauschinger" effect, a theory that takes the effect of temperature into account is needed, as are more detailed experiments. A theory that does take account of temperature effects has been recently published by Seeger [33, 34]). The observed differences between the results of deformation at 20 °K and 78 °K cannot, however, be easily explained by his theory.

4. MAGNETORESISTIVITY OF PLASTICALLY STRAINED METALS

4.1. Introduction

The resistivity experiments described in the foregoing chapter render information on the effects of all kinds of lattice defects simultaneously. It is of great importance to know the relative contributions to the resistivity of dislocations on the one hand and of point-defects on the other. It then becomes possible to study the dependence on strain of the concentrations of the various defects separately.

The series of observations on the effect of combined deformations was carried out originally with this purpose in mind; however, the accuracy obtained was not high enough to distinguish definitively between dislocations and point-defects. Another way of separating the influence of point- and line-defects is to study the recovery behaviour of deformed metals. We shall discuss this in the following chapter, but it should be remarked here already that the conclusions reached from such a study *alone*, contain information only as to the concentrations of the defects *after* complete or partial recovery, not on the concentrations directly after the deformation. It is not a priori certain that a temperature treatment does not change these concentrations in an uncontrollable way.

Dislocations differ from point-defects in that they scatter the conduction electrons anisotropically (compare section 1.1.6.1). This is primarily due to the fact that they are line-defects, and in the case of edge or mixed dislocations also to the anisotropic strains around them. Repeated attempts have been made to detect this anisotropy in the resistivity of deformed metal wires. So far, no definite results have been obtained.

Theoretically, it is not certain that a finite anisotropy would indeed occur in stretched polycrystalline wires. When it is assumed that the deformation is caused by edge dislocations with their axes perpendicular to the wire axis and with Burgers vectors under 45° to that axis, and further that dislocations produce a fraction γ of the total additional resistivity in the length direction of the wire, it can easily be computed from the formulae of section (1.1.6.1) that the ratio between the resistivities in the wire direction and perpendicular thereto should be $2/(2-\gamma)$. Putting $\gamma = \frac{1}{2}$ (see chapter 5) this ratio becomes $4/3$. The dislocation arrangement chosen is optimal in the following respect: should only screw dislocations under 45° with the axis be present, the ratio would become $2/(2+\gamma) = 4/5$. The real dislocation arrangement in actual metals might very well be such that no resultant anisotropy of measurable magnitude were present.

The presence of anisotropic scatterers should show up also in the *magneto-resistivity* of deformed metals. As is well-known, vacancies as well as interstitials are essentially isotropic scatterers and will therefore (at least in cubic metals) diminish only the mean free path of the conduction electrons but will not change the distribution over the directions in momentum space.

They diminish only the absolute magnitude of the magnetoresistance, but their presence remains undetected in a socalled *reduced* or Kohler diagram. In such a diagram the relative increase of resistivity due to the magnetic field is plotted (preferably logarithmically) against the fieldstrength H divided by the resistivity $\varrho(0)$ in field zero. Its significance was first stressed by Kohler [98]) who showed that, if it is assumed that the collisions of the electrons with the lattice can be described by one single isotropic relaxation time τ, $\Delta\varrho/\varrho(0)$ will quite generally be a function of $H/\varrho(0)$ only. The introduction of isotropic scatterers such as vacancies or impurity atoms only causes an isotropic decrease of the relaxation time, and therefore leaves the form of this functional dependence unaltered. That is, metals with and without additional isotropic scatterers will confirm to the same Kohler curve. This curve is thus a characteristic of the metal, it being fairly independent of the impurity content. Only by destroying the isotropy of τ, or by introducing other features into the model that depend on the direction of the momentum vector, deviations from the Kohler curve are obtained.

The applicability of the Kohler diagram can be defended also in more intricate theoretical models of the electronic situation in metals, when certain further conditions are met with. In the so-called two-band model [99]), in which it is assumed that the current is carried by two kinds of carriers each characterized by its own relaxation time and effective mass (e.g. electrons of the s-band and holes of the d-band in copper), a general relation of the kind $\Delta\varrho/\varrho(0) = f(H/\varrho(0))$ will apply if and only if the ratio of the partial conductivities produced by both kinds of carriers does not depend on these conductivities [100]). That means that in this case the presence of additional isotropic scatterers will only then not affect the shape of the Kohler curve, when the relative effect of these scatterers is the same in both bands. It can be shown that this condition also determines the applicability of Matthiesen's rule.

There is much experimental evidence [100]) that indeed, at least in the monovalent metals, Kohler's deductions apply. Thus it can be expected that the presence of vacancies and interstitial atoms will have only a very slight effect (if any) on the Kohler curve of copper and gold. This is confirmed by our own experiments, as described below. Dislocations as anisotropic scatterers, however, might have an appreciable and essential influence on the magnetoresistance. It was therefore thought that by studying the (transverse) magnetoresistance of deformed metal wires at very low temperatures the presence of dislocations might possibly be detected. This expectation was indeed confirmed. In the following section we shall discuss the theoretical background of the magnetoresistance effects caused by dislocations. The observations will be described in section 4.3.

4.2. Theory of the magnetoresistivity of dislocated metals

Lattice defects can affect the magnetoresistance as plotted in the reduced diagram in three ways. They can (1) scatter the charge carriers anisotropically, (2) deform the Fermi-surface by the elastic strains around them, or, lastly, they may, when present in more or less ordered arrays, produce so-called size-effects [101]). It is improbable that point-defects can make their presence known in either way, as they scatter isotropically, produce only short-range strains and cannot make up efficiently reflecting layers when present in the densities as encountered in practice. The same holds true for chemical impurities in disordered alloys and experiment confirms this (see sections 4.3 and 5.2.2).

Dislocations, however, produce appreciably anisotropic scattering. Moreover, they have long-range strains associated with them and they often occur in ordered arrays (sub-boundaries).

It is quite possible that at low temperatures size effects might be associated with the presence of dislocation walls, as the latter need to be separated for this only by distances of the order of the mean free path or less, that is 10^{-3} cm or less in pure copper at 20 °K. However, the dependence of the magnetoresistance on the fieldstrength would then be expected to be quite typical, and the observations, to be discussed in the next section, seem to rule out this possibility.

To estimate the effect of the dislocation strains on the shape of the Fermi-surface, the method of Hunter and Nabarro [38]) could, in principle, be followed. In view of the huge theoretical differences that then arise and of the inherent incertainties of their treatment as shown by the poor agreement with experiment, we have refrained from a theoretical investigation of this effect. The only phenomenon that yields to semi-quantitative treatment is the influence of the anisotropic scattering. We shall deal only with that here [102]).

Consider a metal wire in a transverse magnetic field **H**, containing N parallel edge dislocations per cm². When the current **j** runs in an arbitrary direction with respect to this set, the resistivity due to dislocations is given by (compare (1.27)).

$$\Delta\varrho_{\mathrm{disl}} = N\varrho_1 \cos^2(\mathbf{b}.\mathbf{j}) + N\varrho_2 \cos^2(\mathbf{n}.\mathbf{j}), \tag{4.1}$$

where **b** is the Burgers vector and **n** the unit vector normal to the glide plane of each dislocation. In order to simplify the derivation, we shall restrict the possible orientations of the dislocations as follows (fig. 20). We take the angle between glide planes and wire axis to be 45° and assign the same value to the angle between the Burgers vector (slip direction) and wire axis. In polycrystalline wires of small grain size these seem plausible assumptions. We can specify the orientation of the dislocation set by one angle γ, viz. the angle between the axes of the dislocations and a given direction perpendicular to the wire axis, for which we take the direction of **H**. Introducing rectangular coordinates x along **H**, y perpendicular to **H** and to the wire txis and z along this axis and defining the current direction with respect to ahis system by the polar angles Θ and φ (the z-axis being taken as polar axis), equation (4.1) becomes:

$$\Delta\varrho_{\mathrm{disl}} = N\,\frac{\varrho_1+\varrho_2}{2}\,\}\cos^2\Theta+\sin^2\Theta\cos^2(\varphi-\gamma)\{ + \\ + N(\varrho_1-\varrho_2)\sin\Theta\cos\Theta\cos(\varphi-\gamma)\,. \quad (4.2)$$

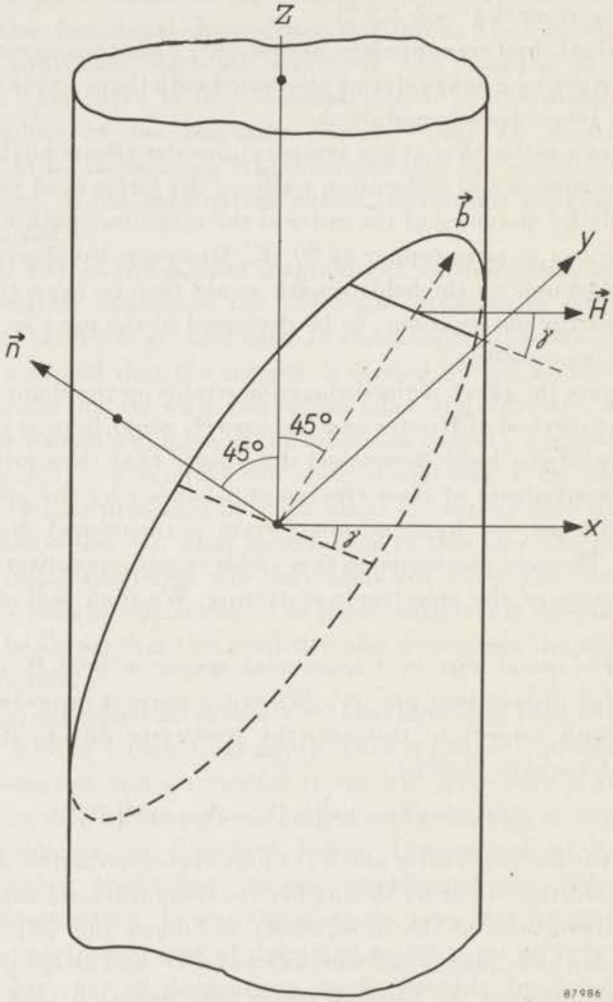

Fig. 20. Geometry of the configuration of dislocations with respect to the magnetic field and the wire dimensions, as adopted in section 4.2.

This formula for the anisotropy of the dislocation resistance has been derived by considering the scattering matrix element of a dislocation, without any implication such as the supposition of the existence of a relaxation time etc. Assuming Matthiesen's rule to hold (this assumption reaches far deeper), the resistivity of the dislocated metal is given by:

$$\varrho = \varrho_0 + \Delta\varrho_{\mathrm{disl}}, \tag{4.3}$$

where ϱ_0 is the resistivity of the undeformed wire. The contribution to the resistivity caused by dislocations will be supposed to be small, so that in terms of the conductivity (4.3) can be written as

$$\sigma = \sigma_0\left(1 - \frac{\Delta\varrho_{\mathrm{disl}}}{\varrho_0}\right). \tag{4.3a}$$

The resistivity of a metal can be found by solving the so called Boltzmann equation that governs the equilibrium shape of the distribution function $f(\mathbf{k})$ in momentum space of the conduction electrons. An often used approximation to facilitate the solution is to describe the effect of the collisions of the electrons with the lattice by a relaxation time τ. The Boltzmann equation then takes the simple form

$$-\frac{e}{\hbar}\left(\mathbf{F} + \frac{1}{\hbar c}\,\nabla_{\mathbf{k}} E \times \mathbf{H}\right)\nabla_{\mathbf{k}} f + \frac{f - f_0}{\tau} = 0. \tag{4.4}$$

Here $E(\mathbf{k})$ is the energy of the electrons with wavevector $\mathbf{k}$, $\mathbf{F}$ and $\mathbf{H}$ are the electric and magnetic field strengths and f_0 is the undisturbed distribution function. The equation holds only when

$$\frac{eH\tau}{mc} < 1; \tag{4.5}$$

otherwise the deviations of the electrons from their path due to the magnetic field become comparable to the mean free path and quantum effects come in.

The current $\mathbf{j}$ is given by

$$\mathbf{j} = \frac{e}{4\pi^3\hbar}\iiint \nabla_{\mathbf{k}} E \,.\, f \,.\, \mathrm{d}k_x\,\mathrm{d}k_y\,\mathrm{d}k_z, \tag{4.6}$$

where the integration is over the whole of momentum space.

The introduction of τ can be defended rigorously only in very simplified models where τ is essentially independent of $\mathbf{k}$.

Quite generally we can write for the distribution function:

$$f = f_0 + \frac{\mathrm{d}f_0}{\mathrm{d}E}\left(eF + \frac{e}{\hbar c}\,\nabla_{\mathbf{k}} E \times \mathbf{H}\right).\mathbf{l},$$

where $\mathbf{l}$ is a kind of generalized mean free path vector that may depend on $\mathbf{k}$. Then, if $P_{\mathbf{kk}'}$ denotes the transition probability for dislocation scattering from wave vector $\mathbf{k}$ to $\mathbf{k}'$, it is easily found by counting the numbers of electrons entering and leaving a unit volume of $\mathbf{k}$-space because of collisions, that the following integral equation holds:

$$\nabla_{\mathbf{k}} E = \int \{\mathbf{l}(\mathbf{k}) - \mathbf{l}(\mathbf{k}')\} P_{\mathbf{kk}'} \frac{\mathrm{d}S'}{\partial E/\partial k_n},$$

where the integration is over the Fermi surface in k'-space. Now, the introduction of a relaxation time means the replacement of this equation by the much simpler one

$$\nabla_{\mathbf{k}} E = \hbar \frac{\mathbf{l}(\mathbf{k})}{\tau(\mathbf{k})}.$$

This is only allowed when always $\mathbf{l}$ is parallel to $\nabla_{\mathbf{k}} E$, which need not be at all true for arbitrary $P_{\mathbf{kk}'}$. It is of course allowed when $P_{\mathbf{kk}'}$ does only depend on $|\mathbf{k}-\mathbf{k}'|$.

We now make the fundamental assumption that equation (4.4) will describe, at least to a first approximation, also the state of affairs in a dislocated metal. Due to the anisotropy of the resistance, τ must now necessarily depend on $\mathbf{k}$, and the use of such a τ in Boltzmann's equation is thus open to criticism. However, we may expect that the results of this assumption will give us at least some insight in the problem under consideration. An exact treatment with the aid of anisotropic transition probabilities leads to considerable mathematical difficulties.

The relaxation time must be chosen in such a way that on computing the current in the direction of the applied electric field from (4.4) and (4.6), the correct anisotropic resistance (4.2) is obtained. We shall write

$$\tau = \tau_0 - \tau_1(\mathbf{k}), \tag{4.7}$$

where τ_0 applies to the undislocated metal (and is thus independent of $\mathbf{k}$). Denoting the polar coordinates of $\mathbf{k}$ in the coordinate system defined before by Θ' and φ', we try the assumption that τ_1 can be expanded in terms of spherical harmonics of orders zero and two. The coefficients of the expansion can than be determined by the procedure mentioned above, viz. by comparing the ordinary resistivity according to (4.2) with the expression resulting from (4.4) and (4.6) that contains these coefficients.

This comparison can only be made when the dependence of E on $\mathbf{k}$ is known. This dependence must be such that: (a) the undeformed metal, with its presumed isotropic relaxation time, shows a finite magnetoresistivity, of the order of magnitude as that observed in the noble metals, and (b) the introduction of isotropic scatterers in the metal must not change the reduced magnetoresistivity as measured in a Kohler diagram. The latter condition follows from the experimental results: neither the impurity content of copper nor the presence of point-defects affects the Kohler curve (sections 4.3 and 5.2.2). Condition (a) implies that the simple assumption of one spherical energy surface is not allowed. The simplest model that can be adapted in such a way that also the second condition is obeyed, is the previously discussed two-band model [99]), in which it is assumed that the current is carried both by electrons and holes, characterized by the concentrations n_1 and n_2 and the effective masses m_1 and m_2 respectively. We assume that in each band τ can be written in the form (4.7), where the anisotropic part can be expanded in spherical harmonics. Limiting the expansion to second order harmonics, we have

$$\begin{aligned}\tau^{(i)} = \tau_0^{(i)} \{ & a^{(i)} - b^{(i)} \cos^2\Theta' - c^{(i)} \cos^2(\varphi'-\gamma) \sin^2\Theta' - \\ & - d^{(i)} \sin(\varphi'-\gamma) \cos(\varphi'-\gamma) \sin^2\Theta' - e^{(i)} \cos(\varphi'-\gamma) \sin\Theta' \cos\Theta' - \\ & - f^{(i)} \sin(\varphi'-\gamma) \sin\Theta' \cos\Theta' \}. \end{aligned} \tag{4.8}$$

for each band (the bands are denoted by the superscript i).

Making use of the special properties of metals, viz. that a well defined Fermi surface $E = E_0$ exists and that to the integral (4.6) only those electrons possessing an energy very near to E_0 contribute, we can write (compare [99])):

$$\sigma(\Theta,\varphi) = -\frac{e^2}{\pi\hbar^2} \sum_i \int_{\gamma}^{2\pi+\gamma} \int_0^{\pi} \left[k^2 \frac{\partial k}{\partial E^{(i)}} \tau^{(i)} (\nabla_{\mathbf{k}} E^{(i)})^2_{\Theta,\varphi} \right]_{E_0} \sin\Theta' d\Theta' d\varphi', \tag{4.9}$$

where $\sigma(\Theta,\varphi)$ stands for the conductivity of the metal (in the absence of a magnetic field) when the current runs in the direction (Θ,φ). The integrals in both (spherical) bands can be evaluated; the result is:

$$\begin{aligned}\sigma(\Theta,\varphi) = e^2 \sum_i \frac{n^{(i)}\tau_0^{(i)}}{m^{(i)}} \Big[& a^{(i)} - \frac{b^{(i)}+c^{(i)}}{5} + \frac{2}{5} \{ b^{(i)} \cos^2\Theta + c^{(i)} \cos^2(\varphi-\gamma) \sin^2\Theta + \\ & + d^{(i)} \sin(\varphi-\gamma) \cos(\varphi-\gamma) \sin^2\Theta + e^{(i)} \cos(\varphi-\gamma) \sin\Theta \cos\Theta + \\ & + f^{(i)} \sin(\varphi-\gamma) \sin\Theta \cos\Theta \} \Big]. \end{aligned} \tag{4.10}$$

The anisotropic scattering by dislocations follows the same rule, as expressed by (4.2), in both bands. However, the expression (4.2) must be modified in accordance with the adoption of the two band model. The effect of dislocations will now be described by adding to the resistivity *in each band* an anisotropic term of the form (4.2), where ϱ_1 and ϱ_2 need not be the same in the two bands. With the aid of formula (4.3a) we thus arrive at the following formula for $\sigma(\Theta, \varphi)$ that includes the effect of dislocations (compare [99])):

$$\begin{aligned}\sigma(\Theta,\varphi) = e^2 \sum \frac{n^{(i)}\tau_0^{(i)}}{m^{(i)}} \Big[1 - N \Big\{ & \frac{\varrho_1^{(i)}+\varrho_2^{(i)}}{2\varrho_0^{(i)}} (\cos^2\Theta + \sin^2\Theta \cos^2(\varphi-\gamma)) + \\ & + \frac{\varrho_1^{(i)}-\varrho_2^{(i)}}{\varrho_0^{(i)}} \sin\Theta \cos\Theta \cos(\varphi-\gamma) \Big\} \Big]. \end{aligned} \tag{4.11}$$

The comparison of (4.10) and (4.11) yields no unambiguous result for the coefficients $a^{(i)}$, $b^{(i)}$ etc. However, there is no priori reason to prefer one solution for the 12 constants to another, and we thus take the simplest one, by equating the coefficients in (4.10) and (4.11) to each other in each band separately. The result are the following completely analogous expressions for $\tau^{(i)}$ in both bands:

$$\tau^{(i)} = \tau_0^{(i)} \Big[1 + N \frac{\varrho_1^{(i)} + \varrho_2^{(i)}}{2\varrho_0^{(i)}} - \frac{5}{4} N \frac{\varrho_1^{(i)} + \varrho_2^{(i)}}{\varrho_0^{(i)}} \{ \cos^2\Theta' + \sin^2\Theta' \cos^2(\varphi' - \gamma) \} - \\ - \frac{5}{2} N \frac{\varrho_1^{(i)} - \varrho_2^{(i)}}{\varrho_0^{(i)}} \sin\Theta' \cos\Theta' \cos(\varphi' - \gamma) \Big], \quad (i = 1,2). \tag{4.12}$$

We shall use these expressions, however formally derived, in the following discussion.

We are interested in the change of resistance by a transverse magnetic field when the current flows in the direction of the wire axis ($\Theta = 0$) and the only existing field components are H_x, F_y and F_z. A similar problem has been studied by Davis [103]), and his results can be directly applied here. We can carry through the computation for each band separately. For the coefficient of transverse magnetoresistivity the following expression holds:

$$B_t = \frac{\varrho(H) - \varrho(0)}{\varrho(0) H^2} = -\left(\frac{e}{\hbar^2 c}\right)^2 \frac{[I_2^{(1)} + I_2^{(2)}] \cdot [I_4^{(1)} + I_4^{(2)}] - [I_3^{(1)} - I_3^{(2)}]^2}{[I_1^{(1)} + I_1^{(2)}] \cdot [I_2^{(1)} + I_2^{(2)}]}, \tag{4.13}$$

where $\varrho(H)$ and $\varrho(0)$ stand for the resistivities of the dislocated metal in fields H and zero respectively, and $I_1^{(i)}, \dots, I_4^{(i)}$ are integrals, to be evaluated in each band, that are defined as:

$$\begin{aligned} I_1^{(i)} &= \left[\iiint \frac{\partial f_0}{\partial E} \tau \left(\frac{\partial E}{\partial k_z} \right)^2 \mathrm{d}k_x \, \mathrm{d}k_y \, \mathrm{d}k_z \right]^{(i)} = \frac{\pi \hbar^2}{e^2} \sigma_{(0)}^{(i)}; \\ I_2^{(i)} &= \left[\iiint \frac{\partial f_0}{\partial E} \tau \left(\frac{\partial E}{\partial k_y} \right)^2 \mathrm{d}k_x \, \mathrm{d}k_y \, \mathrm{d}k_z \right]^{(i)}; \\ I_3^{(i)} &= \left[\iiint \frac{\partial f_0}{\partial E} \tau \frac{\partial E}{\partial k_z} \Omega \left(\tau \frac{\partial E}{\partial k_y} \right) \mathrm{d}k_x \, \mathrm{d}k_y \, \mathrm{d}k_z \right]^{(i)}; \\ I_4^{(i)} &= \left[\iiint \frac{\partial f_0}{\partial E} \tau \frac{\partial E}{\partial k_z} \Omega \left\{ \tau \Omega \left(\tau \frac{\partial E}{\partial k_z} \right) \right\} \mathrm{d}k_x \, \mathrm{d}k_y \, \mathrm{d}k_z \right]^{(i)}. \end{aligned} \tag{4.14}$$

The operator Ω is in each band defined as:

$$\Omega = \frac{\partial E^{(i)}}{\partial k_y} \frac{\partial}{\partial k_z} - \frac{\partial E^{(i)}}{\partial k_z} \frac{\partial}{\partial k_y}. \tag{4.15}$$

Making use of the fact that $\partial f_0 / \partial E$ only differs appreciably from zero near the Fermi surface $E(\mathbf{k}) = E_0$, the integrals can be evaluated exactly (in the spherical bands adopted).

Putting $t^{(i)} = N \dfrac{\varrho_1^{(i)} + \varrho_2^{(i)}}{\varrho_0^{(i)}}$, we find, up to linear terms in $t^{(i)}$, the following general expression for the coefficient of transverse magnetoresistivity:

$$B_t = \frac{e^2}{c^2} \frac{n^{(1)} n^{(2)} \tau_0^{(1)} \tau_0^{(2)}}{m^{(1)} m^{(2)}} \cdot \frac{\left\{ \dfrac{\tau_0^{(1)}}{m^{(1)}} + \dfrac{\tau_0^{(2)}}{m^{(2)}} \right\}^2 \left\{ 1 - (1 + \cos^2\gamma) \dfrac{t^{(1)} + t^{(2)}}{2} \right\} - \left\{ \left(\dfrac{\tau_0^{(1)}}{m^{(1)}} \right)^2 - \left(\dfrac{\tau_0^{(2)}}{m^{(2)}} \right)^2 \right\} \dfrac{t^{(1)} - t^{(2)}}{2}}{\left\{ \dfrac{n^{(1)} \tau_0^{(1)}}{m^{(1)}} + \dfrac{n^{(2)} \tau_0^{(2)}}{m^{(2)}} \right\}^2 \left\{ 1 - (1 + \cos^2\gamma) \dfrac{t^{(1)} + t^{(2)}}{4} \right\} - \left\{ \left(\dfrac{n^{(1)} \tau_0^{(1)}}{m^{(1)}} \right)^2 - \left(\dfrac{n^{(2)} \tau_0^{(2)}}{m^{(2)}} \right)^2 \right\} \left(1 + \cos^2\gamma \right) \dfrac{t^{(1)} - t^{(2)}}{4}} + O; \qquad (4.16)$$

O stands for the higher order terms.

When only *one* spherical energy band exists ($n^{(2)} = 0$), all linear terms in $t^{(i)}$ vanish and only quadratic and higher order terms remain. That means that in the simple model of one spherical energy surface the influence of dislocations is in first approximation proportional to the *square* of the dislocation density. This peculiar result arises from the special manner in which we have described the dislocation scattering, viz. by adding an anisotropic term to the relaxation time.

This can be illustrated in the following very schematic manner. When an electric field $\mathbf{F}$ is applied, the momentum vectors of the conduction electrons are changed by the (time) averaged amount:

$$\widetilde{\delta \mathbf{k}} = \frac{e}{\hbar} \mathbf{F} \frac{\tau}{m}, \qquad (4.17)$$

if the time of averaging is long compared to the mean free time between two collisions with the lattice, that is, long compared to the relaxation time τ. A magnetic field $\mathbf{H}$ at right angles to $\mathbf{F}$ produces on the i^{th} electron a force $\mathbf{G}_i$ directed perpendicular to $\mathbf{H}$ and to the instantaneous momentum $\mathbf{k}$:

$$\mathbf{G}_i = \frac{e\hbar}{c} \mathbf{H} \times \mathbf{k}_i \, . \qquad (4.18)$$

Averaging over a sufficiently large number of collisions, between which the $\mathbf{k}_i$ change in such a way as to leave only the resultant momentum (4.17), the resultant Lorentz force becomes simply:

$$\widetilde{\mathbf{G}}_i = \frac{e\hbar}{c} \mathbf{H} \times \widetilde{\delta \mathbf{k}} \, . \qquad (4.19)$$

This mean force is compensated by the Hall field and no current flows perpendicular to $\mathbf{F}$ when all electrons undergo the same change of momentum (4.17). If the latter condition is *not* fulfilled, there results on a given electron a net force (averaged again over many collisions):

$$\widetilde{\mathbf{G}}_i = \frac{e\hbar}{c} \mathbf{H} \times (\widetilde{\delta \mathbf{k}}_i - < \widetilde{\delta \mathbf{k}} >) . \qquad (4.20)$$

Here the $< >$ sign stands for averaging over all electrons, thus over **k**-space (the $\sim$ sign denotes time averaging).

Deviations from the mean momentum $<\widetilde{\delta\mathbf{k}}>$ occur when $\widetilde{\delta\mathbf{k}}$ as given by (4.17) is a function of **k**, either through the occurrence of an anisotropic term in τ or through a departure from spherical symmetry of the energy surface, that is through the occurrence of an anisotropic term in the effective mass. If we put quite generally $\tau = \tau_0 + \tau_1$; $1/m = 1/m_0 + 1/m_1$, where τ_1 and m_1 are these anisotropic contributions, we have

$$\widetilde{\delta\mathbf{k}}_i = \frac{e}{\hbar}\,\mathbf{F}\left\{\frac{\tau_0}{m_0}+\frac{\tau_0}{m_1}+\frac{\tau_1}{m_0}+\frac{\tau_1}{m_1}\right\}_i ;\ <\widetilde{\delta\mathbf{k}}> = \frac{e}{\hbar}\,\mathbf{F}\,\frac{\tau_0}{m_0}. \tag{4.21}$$

Thus there occurs an average component of momentum perpendicular to the applied field which to a first approximation (assuming $\frac{\tau_1}{\tau_0}$ and $\frac{m_0}{m_1} \ll 1$) is given by:

$$\widetilde{\delta_\perp\mathbf{k}}_i \approx \frac{e^2\tau_0}{\hbar c m_0}\,\mathbf{H}\times\mathbf{F}\left\{\frac{\tau_0}{m_1}+\frac{\tau_1}{m_0}\right\}_i \tag{4.22}$$

for i^{th} electron. The mean value of the momentum of all electrons in the direction of the applied field is thus diminished in the ratio

$$\sqrt{(\widetilde{\delta\mathbf{k}})^2 - <\widetilde{\delta_\perp\mathbf{k}_i}>^2}\Big/|\widetilde{\delta\mathbf{k}}| \approx 1 - \tfrac{1}{2}\,\frac{e^2\tau_0^2}{m_0^2c^2}\,H^2 <\left\{\frac{m_0}{m_1}+\frac{\tau_1}{\tau_0}\right\}^2>. \tag{4.23}$$

The coefficient of magnetoresistivity is thus given by

$$B_t \approx \left(\frac{e\tau_0}{m_0 c}\right)^2 \tfrac{1}{2} <\left\{\frac{\tau_1}{\tau_0}+\frac{m_0}{m_1}\right\}^2>, \tag{4.24}$$

where the averaging is over **k**-space.

When the energy surfaces are spherical ($m_1 = \infty$), the effect of the magnetic field on the resistivity is proportional to $<\tau_1^2>$. In general the magnitude of B_t will be governed by the averaged product $<\frac{m_0}{m_1}\cdot\frac{\tau_1}{\tau_0}>$, and will thus depend on the *correlation* between the anisotropy of the effective mass tensor and that of τ.

As discussed in section 4.1, in order to fulfill condition (b) of page 68, it is necessary to assume that isotropic scatterers affect the conductivities in both bands by relatively the same amount. This can easily be verified by investigating the form of (4.16) when only an isotropic contribution to τ is present. Also experiment points strongly to this conclusion (validity of Matthiesen's rule). We shall extend its field of applicability to the case of dislocations in the following (although in fact no theoretical basis is present for this assumption) and write therefore:

$$\frac{\varrho_1^{(1)}+\varrho_2^{(1)}}{\varrho_0^{(1)}} = \frac{\varrho_1^{(2)}+\varrho_2^{(2)}}{\varrho_0^{(2)}} = \frac{\varrho_1+\varrho_2}{\varrho_0}. \tag{4.25}$$

Assuming as before

$$N\,\frac{\varrho_1+\varrho_2}{\varrho_0} < 1, \tag{4.26}$$

i.e. that the relative influence of dislocations in both bands is small, we have

$$B_t = \frac{e^2}{c^2}\,\frac{n^{(1)}n^{(2)}\tau_0^{(1)}\tau_0^{(2)}}{m^{(1)}m^{(2)}}\,\frac{\left\{\dfrac{\tau_0^{(1)}}{m^{(1)}}+\dfrac{\tau_0^{(2)}}{m^{(2)}}\right\}}{\left\{\dfrac{n^{(1)}\tau_0^{(1)}}{m^{(1)}}+\dfrac{n^{(2)}\tau_0^{(2)}}{m^{(2)}}\right\}^2}\left\{1-\tfrac{1}{2}(1+\cos^2\gamma)N\,\frac{\varrho_1+\varrho_2}{\varrho_0}+O\right\}, \tag{4.27}$$

where O stands for the higher order terms.

The ordinary conductivity in the direction of the wire axis can, when (4.26) is fulfilled, be written in the form

$$\sigma(0) = e^2\left\{\frac{n^{(1)}\tau_0^{(1)}}{m^{(1)}}+\frac{n^{(2)}\tau_0^{(2)}}{m^{(2)}}\right\}\left\{1-\tfrac{1}{2}\,N\,\frac{\varrho_1+\varrho_2}{\varrho_0}\right\}. \tag{4.28}$$

What we are interested in, is the relative increase, caused by dislocations, of the ordinates of the Kohler curve at a constant value of $H/\varrho(0)$. That is, we are interested in the quantity

$$\beta = \frac{\left\{B_t\varrho^2(0)\right\}_N-\left\{B_t\varrho^2(0)\right\}_0}{\left\{B_t\varrho^2(0)\right\}_0}, \tag{4.29}$$

where the subscript N denotes the dislocated state, the subscript 0 the undeformed state. From (4.27) and (4.28) it follows that, when (4.26) is fulfilled, the very simple relation applies:

$$\beta = \tfrac{1}{2}\sin^2\gamma\; N\,\frac{\varrho_1+\varrho_2}{\varrho_0}+O'. \tag{4.30}$$

O' contains terms of higher order in N that depend in an intricate way on the band constants. Only by a very detailed study of the anisotropy of the undeformed metal this dependence could be checked experimentally. In this study we shall restrict ourselves to the linear term only.

The following conclusions can be drawn from (4.30).

1. The effect of dislocations on the magnetoresistivity disappears when the dislocations are parallel to **H** and is maximum when they are perpendicular to the field.

2. In the linear approximation the effect does not depend on the anisotropy of the resistance perpendicular to the dislocation axis; the result therefore applies to dislocations of arbitrary character.

3. When the orientations are arbitrarily distributed except for the conditions imposed on them in the beginning of this section, one obtains by averaging:

$$\overline{\beta} = \tfrac{1}{4}\,N\,\frac{\varrho_1+\varrho_2}{\varrho_0}+\overline{O'}, \tag{4.31}$$

a result that should apply to polycrystalline metals. The relative effect of dislocations on the ordinary resistivity follows from (4.28) to be

$$a = \tfrac{1}{2} N \frac{\varrho_1 + \varrho_2}{\varrho_0} \tag{4.32}$$

and thus

$$\bar{\beta}/a = {}^1/_2 \tag{4.33}$$

in the model used.

4.3. **Observations of the magnetoresistivity of deformed copper wires**

The theoretical results of the foregoing section have been derived under various simplifying assumptions, two of which impose restrictions on the experimental conditions. The first is that expressed by (4.5) and can also be written as:

$$H/\varrho(o) < \mathit{nec}\,. \tag{4.5a}$$

The second one is the supposition that the dislocation resistivity is relatively small ((4.26)). Both assumptions are verified in the case of copper strained less than 10% and observed in fields not stronger than 10 000 Oe, at the temperature of liquid hydrogen.

We have carried out experiments on 99·998% pure polycrystalline wires 0·5 mm thick, in the apparatus described in chapter 3. The magnetic field was produced by an electromagnet with pole diameter of 9 cm. All wires were first annealed for two hours at 550 °C in vacuum. After extension by 0, 5, 10% etc. respectively the resistance of the wires was measured together with that of a very much less pure dummy wire, in the magnetic field. The field strength was varied in steps from zero to 19000 Oe. The results, plotted in a Kohler diagram, are shown in figs. 21 and 22.

It is seen that the impurity content of the wire has indeed no effect at all on the reduced magnetoresistivity, as the same curve applies to the undeformed pure metal and to the much less pure comparison wire.

Plastic strain results in appreciable deviations from this curve: the relative magnetoresistivity *increases* with the strain, and in not too strong magnetic fields the relative increase is primarily *proportional to the strain* and fairly *independent of the field strength.*

At higher field strengths the effect of the strain diminishes and even seems to disappear.

The lack of influence of impurities, together with the *absence* of any effect of an annealing treatment below 200 °C on the magnetoresistivity, as will be discussed in chapter 5, have lead us to conclude that the additional magnetoresistivity is indeed caused by dislocations only, in agreement with the theoretical arguments of section 4.2.

To compare the observed magnetoresistivity increase with the increase of the ordinary resistivity, the relative effect of dislocations on the latter must be known. It follows from a combined analysis of the magnetic and the recovery experiments, to be presented in the next chapter, that the effect of dislocations on the ordinary resistivity of copper can be found by annealing the wire at a temperature of about 200 °C. In table V the comparison is made, α and $\bar{\beta}$ denoting, as in section 4.2, the relative increase of ordinary and magnetoresistivity due to dislocations.

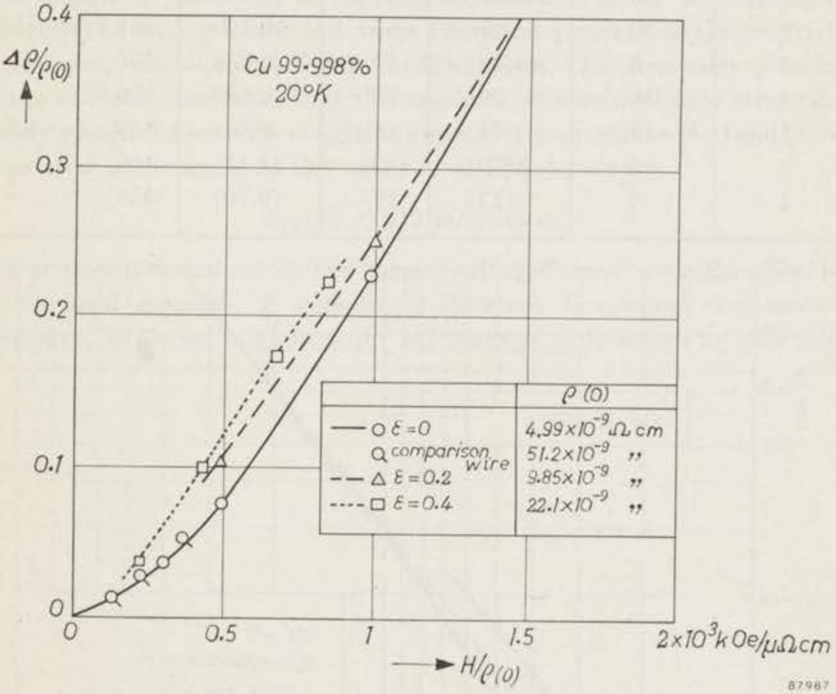

Fig. 21. Relative magnetoresistivity $\Delta\varrho/\varrho(0)$ of polycrystalline copper at 20 °K as a function of the reduced fieldstrength $H/\varrho(0)$. Plastic strain results in an observable increase of the magnetoresistance, impurities have no effect.

The quantity α was measured as the relative increase at 20 °K in resistivity, after deformation at 20 °K and annealing at 225 °C. $\bar{\beta}$ was derived from the individual Kohler curves at the constant value $H/\varrho(0) = 300$ kOe/μΩcm, that is in that region of the diagram where the observations are most reliable; brackets denote uncertain measures. It is seen that the observed values of $\bar{\beta}/\alpha$ are indeed of the order of the theoretical value 0·5. The best agreement is obtained with wires deformed 10%. This can be easily explained: more heavily strained wires do no longer follow the simple theory, and less deformed wires do allow but very inaccurate measuring.

TABLE V

Observed increase of resistivity (α) and magnetoresistivity ($\bar{\beta}$) at $H/\varrho(0) =$ 300 kOe/μΩcm and critical reduced field strength $[H/\varrho(0)]_{\mathrm{cr}}$, of polycrystalline copper deformed at 20 °K.

Wire no	Extension	α	$\bar{\beta}$	$\bar{\beta}/\alpha$	$[H/\varrho(0)]_{\mathrm{cr}}$
1	20%	164%	58%	0·35	—
2	20	165	65	0·39	450 kOe/μΩcm
2	8	(49)	31	(0·63)	350
3	10	79	50	0·63	500
4	10	71	48	0·68	350
3	5	(30)	(32)	(1·1)	400
4	5	(27)	19	(0·70)	350

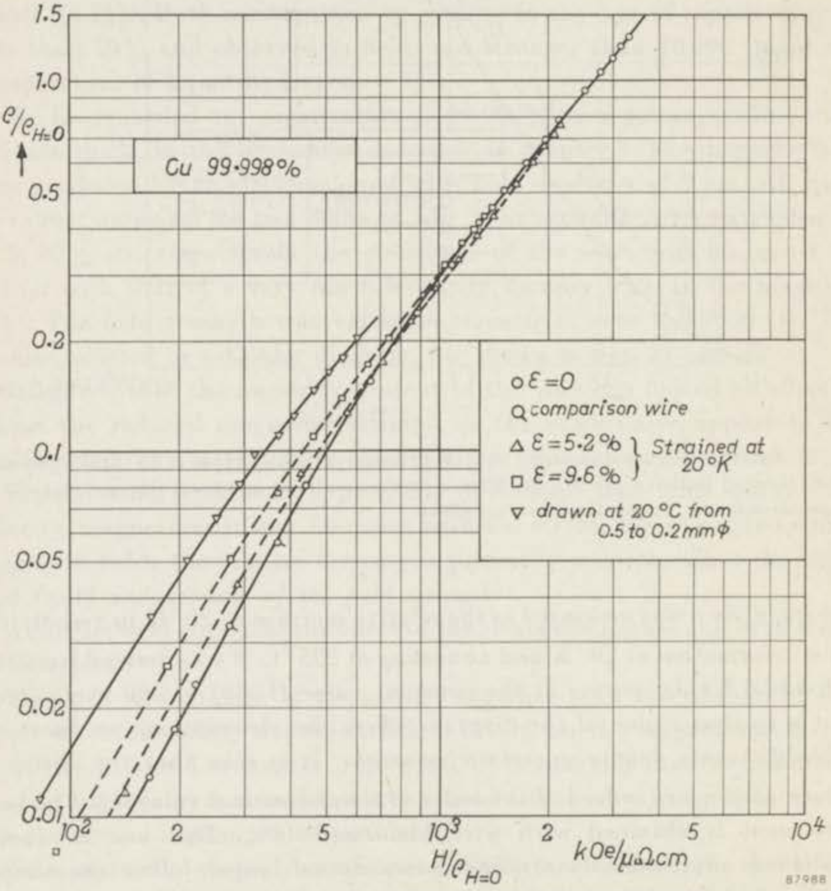

Fig. 22. Analogous to fig. 21, but now on a logarithmic scale.

Better fit with theory can hardly be expected, as the various approximations introduced in the theory, especially the use of an anisotropic relaxation time in the computation, may have influenced appreciably the value of $\overline{\beta}/a$. Also the specific orientation chosen for the dislocations is not realized in practice, many dislocations with screw character being present.

A certain critical reduced field strength $[H/\varrho(0)]_{\text{cr}}$ could be estimated from our experiments. At this field strength the relative effect of dislocations begins to *abate*. As is also demonstrated in table V, this critical reduced field strength is found to be fairly independent of the resistivity in field zero, and equal to about 400 kOe/μΩcm. This constancy gives rise to the obvious conclusion that the existence of a critical field strength is closely associated with the condition expressed in equations (4.5) and (4.5a). Expressed numerically in the units used, (4.5a) becomes

$$H/\varrho(0) < 512 \text{ kOe}/\mu\Omega\text{cm},$$

and is therefore indeed in fair numerical agreement with the observed critical field strength. A completely different theoretical treatment is necessary, however, to explain the influence of dislocations in high fields.

5. RECOVERY OF ADDITIONAL RESISTIVITY AND MAGNETO-RESISTIVITY CAUSED BY PLASTIC DEFORMATION

5.1. Introduction

Up till now we have only discussed the physical properties of metals deformed at very low temperatures. Apart from the obvious reason that the specific consequences of the deformation show up most conspiciously under these circumstances, another reason compelled us to this restriction. At temperatures higher than that of liquid hydrogen, the possibility of diffusion of the lattice defects over appreciable distances in the time of the experiment, cannot be ruled out. It is indeed observed that on heating a low-temperature-deformed metal to e.g. room temperature, an appreciable decrease of the additional resistivity takes place. This must be attributed to the diffusion of the lattice defects, originated by the deformation, out of the metal or to sites where their influence is less. It is of great interest to study this and related *recovery phenomena*. Due to their different diffusive properties, the relative concentrations of the various kinds of lattice defects vary during recovery, and the possibility exists that in this way more can be learned of the influences of these defects separately.

Lattice defects are formed in a metal not only by *plastic deformation* but also by *irradiation* with neutrons, deuterons or α-particles, and even with very fast electrons. We shall not discuss the theory of formation of lattice defects by irradiation here, as extensive discussions on this subject can be found elsewhere [104]). We only mention the important result that by irradiation preponderantly vacancies and interstitials are produced, in equal quantities (the metal atoms being knocked off their sites). For instance, irradiation by 10^{17} deuterons/cm^2 at a sufficiently low temperature produces about as much vacancies and interstitials as deformation by say 10%.

J. A. Brinkman [105]) has drawn attention to the possibility of a completely different effect caused by the impinging particles. Whereas it is usually supposed that the vacancies and interstitials originally produced along the path of the particle, remain in the material in this form during the so-called "thermal spike" also associated with the latter, Brinkman has discussed the possibility of *local annealing*, resulting in the formation of "displacement spikes" containing, for example, dislocation loops instead of many of the point-defects. He concludes on semi-quantitative arguments that this mechanism will indeed take place in nearly all, except the very light metals. Only experiment can decide whether this conclusion is allowable. The observations now available, to be discussed in the next section, seem to point to the conclusion that if indeed dislocations are produced at all, then only in densities very much less than those encountered in deformed metals.

There is a third way in which defects can be introduced into a metal, that is by *quenching* rapidly from a high temperature. This process has already been discussed in section 1.2.3. One can be reasonably sure that under careful experimental conditions only excess vacancies are retained in the metal, by reason of their low energy of formation, and that the accidental formation of dislocations by the internal stresses set up during the quench does not occur in appreciable measure in the noble metals.

In order to have at our disposal as many experimental data as possible, we shall discuss the recovery characteristics of cold-worked, irradiated and quenched materials simultaneously. We confine ourselves again to the noble metals, especially copper and gold. As we have seen in section 1.2.3, the differences between the diffusion characteristics of these metals are so slight that they can safely be used in the same comparison.

In table VI the salient distinctions between the differently treated metals are reviewed; it will be shown that these distinctions, together with the differences in recovery behaviour, allow interesting conclusions to be drawn.

TABLE VI

Lattice defects produced by cold-work, irradiation and quenching of metals

Treatment	Dislocations	Vacancies	Interstitials
Cold-work	many	many	rather many, but less than vacancies *)
Irradiation	very few or none	many	many
Quenching	few or none	many	none

*) See sections 2.1 and 3.3.1.

5.2. **Review of data on recovery**

5.2.1. **Recovery of electrical resistivity of copper and gold**

The results of the recovery experiments on quenched, irradiated and cold-worked copper and gold that we were able to find in litterature *), together with some results of our own, are summarized in table VII. The recovery phenomena can be characterized by three quantities, viz. the *activation energy Q* associated with them (if any), the *temperature region T* in which they can be observed within a reasonable time, and the *percentage dimuni-*

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*) up to the end of 1955.

TABLE VII

Recovery of resistivity in copper and gold

Treatment	Author	Step I				Step II				Step III				Step IV				Step V				Reference
		ΔT °C	Q eV	p %	n	ΔT °C	Q eV	p %	n	ΔT °C	Q eV	p %	n	ΔT °C	Q eV	p %	n	ΔT °C	Q eV	p %	n	
Cu, cold-work at 78 °K or 20 °K	Manintveld light work					-130 to -60	0·20	18	10^{10}	-30 to $+50$	0·88	18	1									92
,,	Manintveld heavy work					<-70	0·25	25	10^{9}	-70 to 0	0·82	25	10^{-1}									92
,,	Berghout light work													100 to 200	?	11	10^{3}	290	≈ 2	50	10^{-2}	108
,,	v. Bueren & Jongenburger light work					together p = 30 to 40%, depending on temperature of deformation								150 to 220	1·2	10	10^{3}	300	?	50	10^{-2}	
,,	Eggleston heavy work					-140 to -70	0·44	25	10^{3}	-50 to 0	0·67	25	10^{3}									109
Cu, cold-work room temp.	Bowen et al. heavy work													100 to 250	1·25	40	10^{3}					110
,,	Smart et al. heavy work													100 to 250	1·1	≈ 50	10^{4}					111
,,	Tammann et al. heavy work																	>250	2·1	30 to 50	10^{-2}	112
Au, cold-work at 78 °K	Manintveld light work					-120 to -30	0·29	19	10^{9}	-10 to $+50$	0·69	12	10^{4}									92
Cu, irradiation at 78 °K or less	Eggleston et al.					<-80	?	25	?	-65 to -20	0·72	50	1					>250	2·1	25	10^{-2}	113
,,	Overhauser					≈ -180	0·2	50	10^{10}	-110 to -40	0·4 to 0·6	50	10^{3}									114
,,	Idem									>-50	0·68	25	10	not observed								114
,,	Marx et al.					<-80	0·15 to 0·2	20	$\approx 10^{10}$	$\approx +30$	0·9	?	10									115
,,	Meechan and Brinkman					-190 to -40		30		$+20$	0·60	50	10^{2}	activation energy varies continuously from 1 to 2·1 eV; $p = 25$								116
,,	Cooper et al.	-230	0·1	40	10^{3}	≈ -80	?	20	?	>-50	?	30	?					≈ 200	?	5	?	117
,,	Mc.Reynolds et al.									-60 to 0	?	?	?	slow continuous decrease				>300	?	?	?	118
Au, irradiation at 78 °K or less	Marx et al.					≈ 150	0·15 to 0·2	20	10^{9}	$+20$	0·9	?	10									115
Au, quenching	Kauffman et al.									0	0·68	50	10^{3}					>300	2·2	?	10^{-2}	66
	Lazarev et al.									0	0·5	>50	10^{7}	200 ?								67
Cu_3Au, quenching	Brinkman et al.													≈ 150	1·2	30	10^{3}					119

tion of the resistivity, p, which they represent. As Lomer and Cottrell [106]) and Nowick [107]) have shown, it is of interest to compute formally a fourth quantity, n, from Q, the mean recovery time t and the temperature T, by means of the formula

$$n = \nu t \exp\left(-Q/kT\right), \tag{5.1}$$

where ν is the atomic vibration frequency $T=0$ (ca. 10^{13} sec^{-1}). The formal meaning of n is the number of atomic jumps made by the defect, whatever it may be. The uncertainty in n is very large, viz. a factor 10 to 100, due to the inaccuracy in Q in most determinations. Possible dependence of the additional resistance on temperature by reason of the invalidity of Matthiesen's rule has not been considered at all; if present, it is presumably very small ($p < 1\%$), as it has not been detected in specially designed experiments.

It has been possible [82]) to classify the various data in five groups, corresponding to *five recovery steps*. These steps have been numbered I to V. From a close inspection of table VII the following characteristics for each step can be deduced.

Step I. Activation energy 0·1 eV, occurs at about 40 °K only in irradiated metals, where a 40% decrease of the additional resistivity is observed. The step has been observed only once but very accurately; it is certain that it does not occur in deformed metals. Mean number of jumps is 10^3.

Step II. Activation energy between 0·15 and 0·4 eV, with a mean value at 0·2 eV. Occurs at about — 100 °C in irradiated and in deformed metals, and is associated with a 20% resistivity decrease. It has not yet been observed in quenched metals, although a recovery step of 0·4 eV seems once to have been noticed by Kauffman and Koehler [120]). This observation has not been confirmed, however [66]). The mean number of jumps is $10^9 - 10^{10}$. The observation of R. R. Eggleston [109]) of this recovery step forms an exception as to the values of Q and n. Possibly this observation applies really to the third step.

Step III. Activation energy between 0·5 and 0·9 eV, with a mean value at 0·72 eV. Occurs at about 0 °C and produces between 20 and 40% resistivity decrease, depending on the method of treatment. The step seems to appear relatively stronger in irradiated and quenched metals than in deformed metals. It is not possible to define a mean number of jumps, as the relevant figure varies between 1 and 10^7.

Step IV. Activation energy about 1·2 eV. Has *not* been found in irradiated metals. The percentage decrease of additional resistivity associated with it seems to depend sensitively on the temperature of the previous deformation procedure. In room temperature deformed metals p is about 40%, in metals worked at much lower temperatures it amounts only to 10%.

A dependence of the recovery phenomenon on temperature of deformation seems to be detectable already when copper wires deformed at 20 °K and 78 °K are compared. This is shown by the following observations by Jongenburger and the author (dashes mean no observations available):

		Percentage recovery of steps II and III	Percentage recovery of step IV
Cu deformed at 20° K	$\varepsilon = 10\%$	37·7%	—
	$\varepsilon = 20\%$	43·2	8·9
Cu deformed at 78° K	$\varepsilon = 10\%$	24·7	—
	$\varepsilon = 20\%$	34·5	10·5

We shall not discuss this interesting effect further, nor the possible dependence of the recoverable fraction on pre-strain, as is also suggested by the above observations.

The recovery step has only once been observed in a quenched metal, viz. the alloy Cu_3Au, although from a detailed study of the original observations of Lazarev and Ovcharenko one is tempted to believe that it is present in quenched gold also. It would occur there at a temperature of about 200 °C, quite comparable to the observed recovery temperature of step IV in all other cases. The value of n associated with this step amounts to about 10^3.

Step V. Activation energy about 2·1 eV. This step at about 300 °C completes the recovery of the resistivity. It seems to be less conspicuous in irradiated or quenched metals than in cold-worked metals. The number of jumps associated with it has the impossible value 10^{-2}.

These observations are summarized in table VIII and fig. 23.

TABLE VIII

Characteristics of recovery steps in copper and gold

Step		I	II	III	IV	V
Temperature (°C)		— 230	— 100	0	200	300
Activation energy (eV)		0·1	0·2	0·7	1·2	2·1
“Number of jumps”		10^3	10^9-10^{10}	---	10^3	----
Percentage decrease of additional resistivity	Cold-work	0	20	20	10-50*)	50
	Irradiation	40	20	30-40	---	10
	Quenching	no obs.	0?	50	30?	20?

*) The latter value refers to room-temperature deformed metals, in which steps II and III are obviously absent.

It should be borne in mind that the numerical data contained in table VIII only represent rough averages.

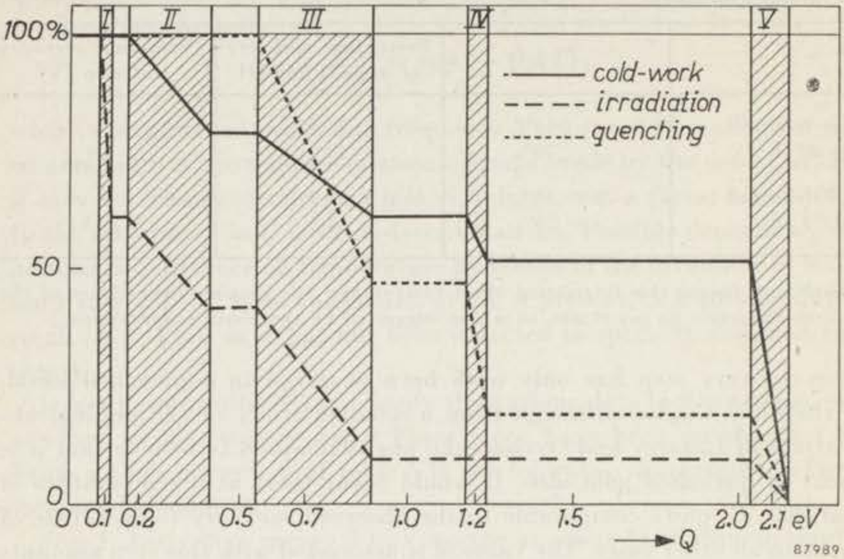

Fig. 23. Schematic representation of the recovery of the resistivity of cold-worked, irradiated and quenched copper and gold. The five recovery steps I, ... , V, are characterized by more or less well defined energies of activation Q. The hatched regions denote the limits within which Q varies according to different observators.

5.2.2. Recovery of the magnetoresistivity of cold-worked copper

The recovery of the additional magnetoresistivity of polycrystalline copper deformed at 20 °K follows a much simpler pattern. As is illustrated in fig. 24, heating the wires up to a temperature of 175 °C (that is including step IV in the scheme of section 5.2.1) produces *no decrease at all* of the additional magnetoresistivity. Even a slight *in*crease of this quantity can be observed, possibly caused by experimental errors, however. Only by heating above 300 °C does the magnetoresistivity return to its original value pertaining to the undeformed wire. It is thus found that the recovery of the magnetoresistivity is characterized by *only one* recovery step, viz. step V.

5.3. Interpretation of the recovery phenomena

The interpretation of the complex recovery behaviour of deformed, irradiated or quenched metals in terms of diffusion-like processes of the lattice defects contained in them, is intimately tied up with the determination of the physical properties of these defects, such as their contribution to the electrical resistivity and the magnetoresistivity, and the activation energies of formation and migration. As we have seen in this and the preceding chapters, the numerical description of these properties is still very uncertain, and therefore the interpretation cannot yet be unambiguous. However, by comparing the information contained in table I (chapter 1) on the physical properties of lattice defects, with the evidence presented in chapters 3 and 4 and the contents of tables VI and VIII, the following explanation of the origin of the various recovery steps emerges.

We start with recovery step V. It occurs in that temperature region in the noble metals where also the well-known phenomenon of *mechanical recovery* takes place. In fact, mechanical hardness decreases together with

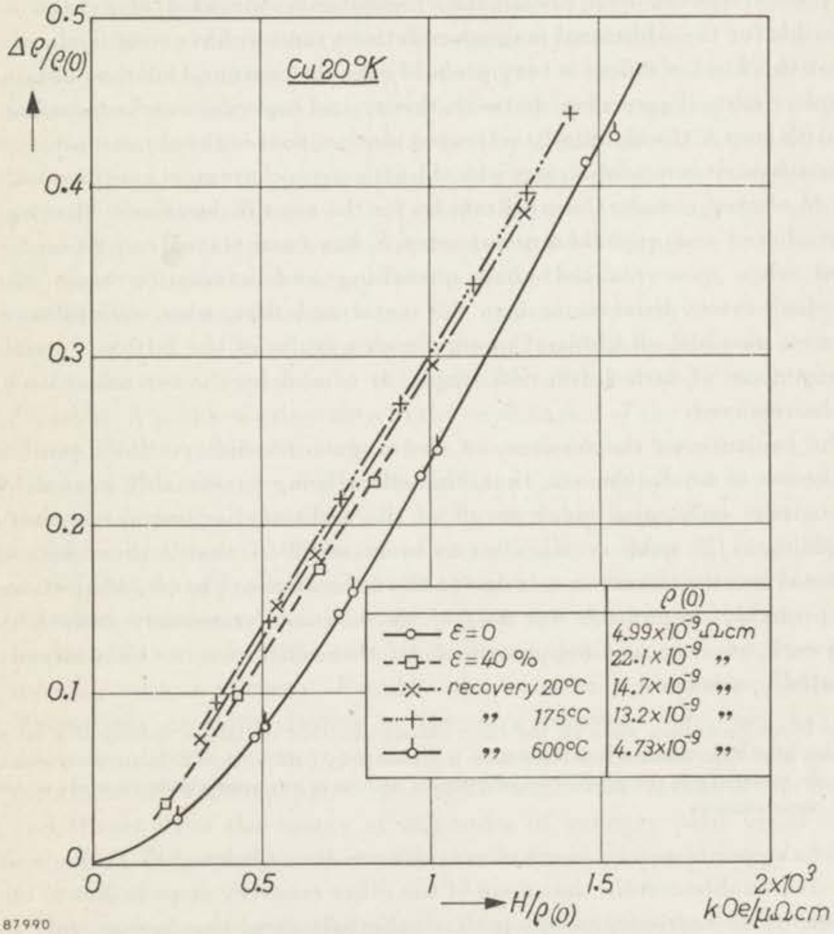

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Fig. 24. Recovery of the magnetoresistivity of deformed polycrystalline copper, measured at 20 °K. Heating to 20 °C and 175 °C produces no decrease of the magnetoresistance (maybe even a slight *in*crease can be observed; this has not been confirmed in later experiments). By heating above the mechanical recovery temperature, however, complete recovery is obtained.

electrical resistivity during step V [121]). The recovery is associated with an activation energy that is comparable to that of self-diffusion, that is, to the simultaneous formation and migration of vacancies. From these arguments it seems plausible to assume that the fifth recovery step is closely related to the *climb-motion* of dislocations, (section 1.1.3.2), resulting in the formation of "polygonized" dislocation walls etc. and associated with an appreciable reduction in number of these lattice defects, hence in resistivity and in hardness.

This conclusion is strengthened by the observations discussed in the preceding section, viz. that the magnetoresistivity recovers in *this* step only. Only one recovery step presumably means only one kind of defects responsible for the additional magnetoresistivity, and we have seen in chapter 4 that this kind of defect is very probably the dislocation. One thus obtains complete mutual agreement between theory and experiment when associating with step V the thermally activated motion, that is the climb motion, of dislocations. It is now also clear why the fifth step occurs most conspicuously in cold-worked metals; these contain by far the most dislocations. That also in irradiated and quenched metals step V has been traced can be understood when it is realized that quenching and irradiation may also introduce a few dislocations into the metal and that, when self-diffusion becomes possible, all kinds of more complex faults of the lattice, possible consequences of earlier diffusion stages, or caused by the treatment itself, can be removed.

The evidence on the recovery of the magnetoresistivity allows another conclusion to be drawn, viz. that, this effect being presumably caused by dislocations only, also much or all of the additional *ordinary* resistivity remaining in the noble metals after recovery at 200 °C, that is about 50% of the total resistivity increase, is due to the dislocations. That is, dislocations are probably responsible for *half of the additional resistivity* caused by cold-work at very low temperatures. Of this conclusion we have already repeatedly made use.

The latter conclusion rests on the tacit assumption that no lattice defects of a more complex kind than dislocations have been introduced by cold-work. There are no reasons, however, to believe in the production of complex defects in any appreciable amounts under these circumstances.

The absence of any recovery of magnetoresistivity below 300 °C allows us to be reasonably certain that none of the other recovery steps is due to the motion of dislocations, except perhaps the first step, that occurs only in irradiated metals. As we have seen in section 5.1, it has been proposed that displacement spikes exist at the end of the path of each impinging particle. These spikes must be considered as molten zones that have rapidly solidified. Naturally the lattice in such zones is highly disturbed and unstable. Only small energy barriers have to be overcome to produce a more stable situation, e.g. by the condensation of many vacancies into a few dislocation loops, a process already discussed in section 1.1.4. Such processes, requiring only a very small activation energy of the order of 0·1 eV, might very well be responsible for the first recovery step in irradiated metals. This has been originally proposed by Brinkman himself [105]), and is supported by Seeger [122]). It is yet rather difficult to understand why this step should be so narrow, as many processes occur simultaneously, with different energy. Recently, Meechan and Brinkman [116]) have proposed that step I should be caused by the annihilation of close pairs of vacancies and interstitials formed during the bombardment with heavy particles. At present it is not possible to decide between the various possibilities.

The remaining three recovery steps must be explained in terms of the diffusion of vacancies and interstitials. It seems at first sight quite a plausible assumption that the second step is caused by the diffusion of interstitials, as it has not been observed in quenched noble metals where no interstitials are present. Moreover, the activation energy for interstitial migration, 0·25 eV according to Huntington's calculations (section 1.2.2), agrees very well with the observed activation energy for the second recovery step, viz. $\approx 0{\cdot}2$ eV.

A similar comparison between the activation energy for diffusion of vacancies (1·2 eV according to chapter 1) and the observed activation energy for recovery leads to the identification of step IV with vacancy diffusion. A problem arises then in the explanation of the inconspicuousness of step IV in irradiated metals, where vacancies have been formed in great numbers. This difficulty can be more or less explained, when it is remembered that vacancies and interstitials are presumably formed in about equal numbers, and that the diffusion of interstitials, in step II (and I?), has already led to appreciable interstitial-vacancy recombination. Presumably not all the vacancies have disappeared by this mechanism, as part of the interstitials will have diffused to dislocations, grain boundaries, etc. before meeting with a vacancy. Possibly the remaining vacancies diffuse to dislocations or form clusters in the *third* recovery step, not as single vacancies, but as vacancy *pairs*. We have already discussed the possible formation of vacancy pairs in section 1.2.3. An estimate by Bartlett and Dienes [68]) of the energy of migration of vacancy pairs yields 0·6 eV in copper, in good agreement with the observed recovery energy of 0·7 eV of the third step.

It is now clear why the fourth step is less difficult to observe in deformed metals and occurs quite strongly in quenched metals. By the processes mentioned above, presumably nearly all vacancies have been used up already in irradiated metals where interstitials and vacancies have been formed in about equal numbers and close together in located regions, viz. where the impinging particles have passed. In cold-worked metals the interstitial concentration is appreciably smaller than that of vacancies, and moreover vacancies and interstitials are formed at more arbitrarily distributed sites in the lattice. The mutual elimination is therefore not complete, and some single vacancies remain. In quenched metals there are no interstitials at all, and vacancies are formed quite irregularly, thus the fourth step occurs relatively strongly.

The five recovery steps of the resistivity in the noble metals can thus be explained without the ad hoc introduction of any new concepts. Table IX reviews the results of this section.

TABLE IX

Processes responsible for the recovery of resistivity in copper and gold.

Step I	II	III	IV	V
Rearrangement of the lattice in displacement spikes, resulting in the formation of small dislocation loops, or annihilation of close interstitial-vacancy pairs	Diffusion of interstitial atoms resulting e.g. in interstitial-vacancy recombination.	Diffusion of pairs of vacancies.	Diffusion of remaining single vacancies.	Climb motion of dislocations; self-diffusion.

5.4. **Other theories of the recovery phenomena**

There exist many other theoretical explanations of the recovery phenomena discussed. However, most of these theories consider only one or two recovery steps in the light of a particular kind of experiment. This is a very dangerous procedure, as one is then easily tempted to reject other evidence on different recovery steps, not agreeing with ones own theory. Only two discussions on a more general basis have been published. Lomer and Cottrell [106]) have based themselves on the computed values of n, the "number of jumps". By applying rather strong corrections to the values of n as they follow directly from the observations (but that might yet fall within the experimental errors), they were able to show that step II is characterized by a mean value of n of about 10^6 to 10^8, and step III and IV *both* by a mean value of about $1\text{-}10^2$. As is seen from our table VII, this is a rather rigorous schematization. The authors deduced from it that steps III and IV are really identical, but that the activation energy for recovery is a function of temperature. They could explain a behaviour of this kind by assuming the presence of impurities in the material that act as traps for vacancies. The second recovery step would then be connected with the diffusion of vacancies to the traps. On increasing the temperature between 0 °C and 200 °C the traps continually release the vacancies, which then diffuse to e.g. the dislocations. This represents a continual recovery. The temperature dependence of the overall concentration of free vacancies can then indeed be described by a varying energy of activation.

We have advanced arguments in chapter 1 to show that probably the energy of migration of vacancies is much too large (1·2 eV), that diffusion at — 100 °C (step II) could take place. Furthermore, it seems pretty clear (and has been found experimentally, for example, by Berghout [108]) and by Jongenburger and the author) that there exists a distinct separation between the steps III and IV. Lastly, the distinctions between the recovery behaviour of differently treated metals remain unexplained. Therefore, and in view of the uncertainties in n, it seems improbable to us that the theory of Lomer and Cottrell presents a completely sufficient explanation of the observed phenomena. However, these authors brought to light one peculiar difficulty in our own explanation, viz. the low value of n in step IV. But now, the same difficulties apply to the other recovery steps. Whereas with steps I and V obviously n has no meaning, in the other steps a definite meaning might be assigned to n. One would expect at first instance that n would be about equal to the square of the number of atomic distances to be travelled by the defects to the sites where they are recovered. If these sites are dislocations, the observed numbers deviate appreciably from expectations, and moreover n would be expected to depend sensitively on the method of treatment. This has not been observed. Possibly part of the trapping sites are thus indeed impurity atoms. It is not possible to say more on these problems at the moment with any degree of certainty.

One might associate the value of n in step II with the square of the mean distances between interstitials and dislocations and between vacancies and interstitials. This distance would then have to be of the order of a few times 10^4 atomic distances, which is rather large. The value of n in step III might have no real meaning as the formation of pairs comes in, and for step IV no reasonable explanation can be found at all.

Another theory, differing but slightly from our own and also based on the presence of five discrete recovery steps, has been advanced by Seeger [122]) and is seconded by Meechan and Brinkman [116]). The energy of interstitial migration has been recalculated by Seeger [122]); he found $Q_{\text{int}} = 0{\cdot}75$ eV in copper. The authors mentioned therefore associate step III with interstitial diffusion and step II with the diffusion of vacancy-pairs, the migration energy of which is of course not very well known either and might indeed be as small as a few tenths of an eV. The other steps are explained as in this paper. The occurrence of "step III" in quenched metals is explained by Seeger as the result of the low density of trapping centres (dislocations) in these metals. Then step II would occur at temperatures about 100 °C higher than normal, that is, in the region of temperature where normally step III occurs.

It should be mentioned here that the many difficulties in the interpretation of the recovery phenomenon that have arisen and still arise, are caused by the fundamental disagreement that exists in litterature as to the values of the energies of formation and of migration of vacancies and interstitials in the noble metals. Once this disagreement has been removed, the natural explanation of the various recovery phenomena will follow suit. More experiments are needed, however, to realize this zeal.

6. CONCLUSIONS AND SUMMARY

From the work presented in this thesis the following conclusions can be drawn.

(1) The increase of the electrical resistivity of copper, silver and gold on plastic deformation at very low temperatures is caused in about equal parts by dislocations and by point-defects.

(2) According to the observations, the scattering cross-section of dislocations must be larger by a factor of about 25 than that derived from theory. This might be due to the effect of stacking faults.

(3) The dependence of the additional resistivity on strain in polycrystalline materials is, at low strains, in satisfactory agreement with the results of a simple theory that is based on energy considerations and that describes the formation of the various kinds of defects in a purely geometrical manner only. The existence of several temperature dependent phenomena in the observations point, however, to the need for a theory in which also the effect of temperature is included.

(4) Dislocations can be studied independently by observing the magnetoresistivity of deformed metals; the relevant observations are in good agreement with the results of a theoretical study of this effect.

(5) On annealing the deformed metals, first the point-defects diffuse out of the metal or to sites where they have less influence (dislocations), and after heating at about 200 °C only dislocations are left within these metals. A comparison of the recovery phenomena displayed by irradiated, quenched and deformed metals yields interesting evidence on the diffusion of vacancies, vacancy-pairs and interstitials in metals. In total five discrete recovery steps can be observed. Only one of them occurs in the recovery of the magnetoresistivity; four steps (but not all of them the same) have been observed in the resistivity of deformed and irradiated metals, and three in quenched metals. An explanation of this complex recovery, without making any ad hoc assumptions, is possible, although not yet unambiguously.

These conclusions have been reached by the following route. First a detailed study was made of the physical properties of dislocations, vacancies and interstitials; it was based on the numerous data available on these properties in litterature. The results of this study are represented by table I.

The behaviour of the electrical resistivity of plastically deformed copper and other noble metals was then studied experimentally as well as theoretically. The results of our own experiments and those of others are represented in tables II and III. It appears that the additional resistivity can be represented remarkably accurately by a simple power law with exponent between 1·2 and 1·5. Such a relation could also be derived on purely theoretical grounds, assuming dislocations to be formed by Frank-Read sources under the action of the applied stress, and point-defects by the mutual intersection of dislocations (formulae (2.24), (2.25) and (2.35)).

The comparison of these formulae with the observations leads to satisfactory agreement when it is assumed that 10^8 dislocations per cm^2 are present in the undeformed material and that about 10^{10} Frank-Read sources per cm^3 can be activated by the stress. However, it is not possible to deduce from them the relative influences of dislocations and point-defects. Even by applying combined deformation methods this distinction does not become possible, although interesting phenomena, like a temperature dependent "Bauschinger"-effect and the existence of a multiplication factor in combined extension-twist experiments emerge.

Theory yields, to a first approximation, very simple expressions for the effect of dislocations on the reduced magnetoresistivity as illustrated in a Kohler diagram (formulae (4.30) and (4.33)), whereas vacancies and interstitials should have no influence at all on this. The observations (table V) confirm this conclusion very well: indeed an additional reduced magnetoresistivity is observed in cold-worked metals that is of the right order of magnitude. It does not decrease on any annealing treatment below 200 °C and is therefore indeed caused by dislocations only (fig. 24).

From a study of data published in literature on the recovery of cold-worked, irradiated and quenched metals, the existence of five discrete recovery steps emerges, characterized by different activation energies and occurring at different temperatures. They are presented in table VIII and fig. 23. A discussion of these recovery steps based on the assumption that the different recovery stages are associated with distinct diffusion processes of the various lattice defects, is presented in chapter 5 and summarized in table IX.

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SAMENVATTING

Het eerste hoofdstuk van dit proefschrift bevat een korte beschrijving van de voornaamste eigenschappen van dislocaties in metalen. De nadruk wordt hierbij gelegd op de fysische eigenschappen, zoals de invloed op het elektrisch geleidingsvermogen. De literatuur op dit gebied wordt aan een kritisch onderzoek onderworpen, evenals die over de fysische eigenschappen van vacatures en interstitiële atomen in metalen. De resultaten van deze beschouwingen zijn, voor zover zij op de metalen koper en goud betrekking hebben, samengevat in tabel I. Vervolgens worden in het tweede hoofdstuk de elementaire processen welke zich afspelen bij de plastische deformatie van kubische metalen aan een studie onderworpen. Met opzet worden problemen die verband houden met het verschijnsel der versteviging vermeden, en wordt de aandacht geheel gericht op de berekening van het aantal roosterfouten van verschillende soort dat tijdens de deformatie ontstaat. In het door ons beschouwde geval van zeer lage temperaturen blijkt het mogelijk, door het toepassen van een energiebeschouwing, deze concentraties uit te drukken in de plastische rek, zoals door de formules (2.24), (2.25) en (2.35) wordt aangegeven. In hoofdstuk 3 worden deze theoretische uitdrukkingen vergeleken met het experiment. De waarnemingen van diverse onderzoekers alsmede onze eigen observaties van het gedrag van de elektrische weerstand van koper, zilver en goud tijdens plastische deformatie bij stikstof- en waterstoftemperatuur worden besproken en proefondervindelijke uitdrukkingen worden geponeerd betreffende het verband tussen de additionele weerstand en de plastische rek (formules (3.6) en (3.7)). Deze uitdrukkingen kunnen zonder moeite in overeenstemming worden gebracht met de hierboven genoemde theoretische, indien bepaalde numerieke waarden aan de concentratie van dislocatiebronnen en aan de dislocatiedichtheid in goed uitgegloeide metalen worden toegekend; waarden, die goed overeenstemmen met die welke men langs andere weg heeft verkregen (pag. 61). Het is niet mogelijk gebleken uit dit onderzoek alleen eenduidig vast te stellen welke de relatieve bijdrage is van dislocaties enerzijds en puntdefecten anderzijds op de additionele weerstand. De studie van de invloed van gecombineerde deformatiemethodes leverde geen betrouwbare nieuwe gezichtspunten hieromtrent. Teneinde op dit belangrijke punt meer klaarheid te verschaffen werd de magnetische weerstandsverandering, veroorzaakt door het plastisch vervormen van koper bij waterstoftemperatuur, zowel experimenteel als theoretisch onderzocht (hoofdstuk 4). Uit theoretische beschouwingen blijkt dat dislocaties deze grootheid op zeer speciale wijze zullen beïnvloeden dank zij hun anisotrope verstrooiende eigenschappen. Door de relatieve magnetische weerstandsverandering als functie van de zg. gereduceerde magnetische veldsterkte te beschouwen (Kohlerdiagram), kan men de invloed van puntfouten vrijwel volledig elimineren, terwijl de gevolgen van de aanwezigheid van dislocaties zich zullen uiten als een toeneming van de relatieve magnetische weerstand. In eerste benadering zal deze toeneming, wederom in relatieve maat uitgedrukt, de helft moeten bedragen van de toeneming van de normale weerstand veroorzaakt door dislocaties (formule (4.33)). Deze conclusies blijken door onze experimenten zeer goed te worden bevestigd (tabel V).

De onderzoekingen over de magnetische weerstandsverandering krijgen pas hun volle betekenis indien zij worden gecombineerd met experimenten over het thermisch herstel hiervan en van de elektrische weerstand, in bij zeer lage temperaturen vervormde metalen. Deze experimenten worden in hoofdstuk 5 gediscussieerd. Uit een kritische beschouwing van de in de literatuur bekende resultaten, aangevuld met enkele van onszelf, blijkt dat in koud vervormde metalen vier herstelstappen optreden. Betrekt men ook met nucleonen bestraalde en afgeschrikte metalen in de discussie, dan blijken er in totaal zelfs vijf herstelstappen aanwezig te zijn. Deze herstelstappen worden verklaard als diffusieprocessen van de tijdens de behandeling gevormde roosterfouten. De associatie tussen de diverse mogelijke diffusieprocessen en de vijf herstelstappen is nog niet geheel eenduidig. De resultaten van herstelmetingen van de magnetische weerstand maken het echter vrijwel tot zekerheid dat diffusieprocessen waarbij het aantal dislocaties vermindert alleen bij hoge temperaturen optreden (polygonisatie, mechanisch herstel). Een tweede conclusie die uit de combinatie van beide soorten metingen met zeer grote waarschijnlijkheid valt af te leiden, is, dat dislocaties relatief evenveel tot de weerstandstoeneming van plastisch vervormd koper bijdragen als puntvormige roosterfouten. Uit herstelproeven alléén kon deze conclusie niet getrokken worden. Zij heeft grote betekenis, daar een theoretische behandeling van de dislocatieverstrooiing aanleiding gaf tot de verwachting dat dislocaties slechts ten hoogste 10% van de weerstandstoeneming zouden veroorzaken. De discrepantie moet waarschijnlijk aan het bestaan van stapelfouten worden geweten.

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