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The Differential Geometry of Elementary Point and Line Defects in Bravais Crystals

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Since line defects (dislocations) and point defects (vacancies, self-interstitials, point stacking faults) in Bravais crystals can mutually convert, only theories which comprise these two sorts of defects can be closed in the sense of general field theory. Since the pioneering work of Kondo and of Bilby, Bullough, and Smith it is clear that differential geometry is the appropriate mathematical tool to formulate a field theory of defects in ordered structures. This is done here on the example of the Bravais crystal, where the above-mentioned defects are the only elementary point and line defects. It is shown that point defects can be described by a step-counting procedure which makes it possible to include also point stacking faults as elementary point defects. The results comprise two equations with the appropriate interpretation of the mathematical symbols. The point defects are step-counting defects and are essentially described by a metric tensor $\mathbf{g}$, which supplements the torsion $\boldsymbol{\Sigma}$ responsible for the dislocations. The proposed theory is meant to form a framework for defect phenomena, in a similar way that Maxwell's theory is a framework for the electromagnetic world.

1. INTRODUCTION

Not long after the crystallinity of large classes of solid matter was proved by means of x-ray diffraction, the decisive role played by crystal (or lattice) *defects* was discovered. Ordered structures other than solid crystals, e.g., liquid crystals, spin structures, and polymers in certain states, were investigated as well and again the defects were found to be of extreme importance. This suggests looking at these defects as a very general phenomenon within condensed matter physics and trying to develop a general theory for it. The first steps in this direction were done by Kondo (1952) and Bilby *et al.* (1955), who used the mathematical language of differential geometry to show that the utmost important crystal defect *dislocation* can be understood as the discrete version of the notion of torsion

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of a space, introduced by Cartan in the early 1920s. To understand the term "discrete," note that, contrary to the spaces considered in differential geometry, a crystal is not a continuum, not even if the lattice constant, say a, is considered very small compared with any other length of interest. In fact, a crystal is not defined as a three-dimensional collection of dense-lying material points (to which we also refer as atoms), but the distribution of particles in a crystal is such that at each material point three independent crystallographic directions are defined along which lattice steps can be counted, and so distances between lattice points can be defined. If then one wishes to retain the specific properties of crystals (as compared, e.g., to amorphous structures), but nevertheless utilize the advantages of a continuum or field language, one can use the concept of the *continuized crystal* (Kröner, 1986). This concept is based on a limiting process, in which the lattice parameter (or in some cases several lattice parameters) suffer a limiting process $a \to 0$, however under conservation of the above-mentioned crystal characteristics, namely existence of crystallographic directions and countability of lattice steps. Of course, this makes sense only if also the contents of mass and of defects are conserved in the limiting process.

This limiting process is possible for dislocations, but not for disclinations, since these defects are specified by a finite angle (symmetry angle of the crystal) which must not be divided into smaller angles in the limiting process. This means that a crystal with disclinations cannot be continuized in Euclidean, or, more generally, in flat space (space without curvature). Therefore, disclinations in solid (not in liquid!) crystals are sources of curvature (in the sense of differential geometry) within the otherwise flat crystal, or they are themselves nothing else than such curvatures. It is then suggestive to speak of flat crystals and of curved crystals, a language used, e.g., by Kléman (1981). In this terminology the only elementary (i.e., not composed) line defect in flat crystals is the dislocation. If all dislocations (and point defects, see below) are taken out, then there remains what can be called the Euclidean crystal.

As an illustration of a two-dimensional curved crystal, cut away from a plane primitive cubic crystal a wedge of 90° and, under conservation of the lattice spacings, move the so-generated edges together. In this way a two-dimensional cone-shaped surface is obtained which can be considered as a perfect crystal in a certain two-dimensional Riemannian space. In this case the curvature is singular.

Obviously, curved crystals are possible only if the curvature is, in some sense, compatible with the considered crystal structure—e.g., the angle in the foregoing example should be 90° and not 70° or 80°. One may imagine defects in a curved crystal. However, the curvature itself is not a defect in this picture. A curved crystal situation with *continuous* curvature can be

created, for instance, by nonuniform heating up of a crystal. This work is restricted to the investigation of flat crystals.

As a differential geometrical description, the mentioned theory of dislocations resembles the theory of the universe, in particular the general theory of relativity. This suggests looking at a crystal with defects in a similar way as physicists look at our universe, namely as a space filled with certain objects, which we call elementary particles in the universe and elementary defects in the crystal. Here the term "elementary" is used as the opposite of "composed." There are reasons to believe that the number of types of elementary particles in the universe is finite, and the same can be said about elementary defects in crystals, or, more generally, in any ordered structure (see below).

As the particles do in the universe, so also the defects surround themselves with physical fields (stresses) through which they interact during their motion in their world. Of course, this motion obeys physical laws in both cases. The detection and description of these laws is the primary goal of the theoretical physics of elementary defects.

There exists an interesting difference between the two situations just sketched. In our universe we are *internal observers* who do not possess the ability to realize *external* actions on the universe, if there are such actions at all. Here we think of the possibility that the universe could be deformed from outside by higher beings. A crystal, on the other hand, is an object which we certainly can deform from outside. We can also see the amount of deformation just by looking inside it, e.g., by means of an electron microscope. Imagine some crystal being who has just the ability to recognize crystallographic directions and to count lattice steps along them. Such an *internal observer* will not realize deformations from outside, and therefore will be in a situation analogous to that of the physicist exploring the world. This physicist clearly has the status of an internal observer.

The concept of internal observer is fundamental. Although he has no access to certain information, he does not miss that information which is really relevant for the physical situation. In our case of interest this is the knowledge about the defects and their "life." Note that the *topological observer* has even more restricted information. For instance, point defects in Bravais lattices escape completely his attention. One of the most important tasks of the internal observer is to find out about the possible elementary defects in his world. As in the elementary particle theory, this is not at all trivial. To find a new elementary defect has a similar significance for defect theory as the discovery of new elementary particles has for their theory.

The foregoing discussion suggests that the theory of defects be developed in the language of physical field theories. Such theories have been particularly successful with the so-called "gauge" or "gauge field"

approach. Application of this approach to defects in crystals seems to have first been proposed by Turski (1966). Others followed. It has been claimed by Kadic and Edelen (1983) and Edelen and Lagoudas (1988) that in this way a dislocation and disclination dynamics has been developed. In this respect one must raise the following doubts if this theory is supposed to describe the physical world of defects in solid or liquid crystals. As is well known, there exists a certain convertibility between dislocations and point defects such as vacancies and (self-)interstitials. For instance, dislocations moving perpendicular to their Burgers vector (so-called nonconservative motion) produce such point defects, and similar processes occur when dislocations cut each other. Both modes of motion are physically real and responsible for various effects. Point defects also migrate toward dislocations and annihilate there. Analogous effects exist with disclinations in liquid crystals. All these effects are not discussed by the mentioned authors and are not contained in their theory. A consequence of the facts sketched above is that there cannot exist a general theory, e.g., dynamics, of dislocations and disclinations which does not contain also the point defects. Recall that for some time the question of whether or not a closed theory of *electrodynamics* exists was unanswered. Meanwhile, incidentally thanks to the general gauge idea, it is known that indeed electrodynamics is not a closed theory, but rather forms a complex together with the theory of weak interactions.

The above remarks are not intended to dispute the value of the mentioned work, which has shown to a certain degree how the formalism of the gauge approach can be applied to the problem of defects in ordered structures. In particular, the above authors also have provided a mathematical apparatus which is not so commonly known among materials scientists and physicists. We can learn from all this the following: A mathematical formalism alone cannot lead to physically realistic theories. It has to be accompanied by physical investigations, and this requires good insight into the physical situation, in particular on the microscale. Only if the gauge approach is combined with this insight can it lead to progress in our field.

The noted gauge theories of defects also suffer from the neglected effect that the motion of the defects is always highly dissipative, so that a Lagrangian does not exist, at least not in the simple form as the gauge principle of minimal coupling would suggest. A way out might be Anthony's thermodynamics based upon a Lagrangian formalism (Anthony and Knoppe, 1987). We shall not go further into this question, but discuss a problem which in our opinion is basic to the desired defect theory, gauge approach or not. This is the field theory of point defects.

The theory of Kondo and Bilby *et al.*, being correct, makes it plausible that also point defects should fit into the scheme of differential geometry.

However, point defects have not yet been brought into connection with differential geometry in a final convincing manner, whereas the corresponding problem for dislocations is solved. It is the attempt of the present work to provide the desired connection. This will lead to the description of a new type of elementary point defect for which we propose the name *point stacking fault* or *elementary shear fault.*

2. VACANCIES AND SELF-INTERSTITIALS AS ELEMENTARY POINT DEFECTS IN BRAVAIS LATTICES

At present we are far from a general dynamical theory of defects. In this work we are satisfied to develop the geometrical part of the theory in which we describe the configurations of Bravais crystals with point defects in the language of differential geometry so that this theory can be combined with that of dislocations in a natural way. We restrict our investigation to the Bravais crystal, because this crystal has the smallest amount of different defect types, but enough to study the general principles. We shall first consider the elementary point defects, vacancy and self-interstitial, where the term "self" indicates that the atom sitting on an interstitial site is of the same sort as the atoms on the regular lattice sites. We have treated his problem recently (Kröner, in press); therefore, we restrict ourselves to a short review.

The basic idea is that the very definition of the Bravais crystal requires step counting along crystallographic directions. We distinguish between primitive crystallographic (p.c.) directions, well defined in any Bravais lattice, and nonprimitive ones (n.p.c.). To give an example: In the frequently encountered face-centered cubic (fcc) crystal, the base vectors of the p.c. directions are $\frac{1}{2}$ [110], $\frac{1}{2}$ [101], $\frac{1}{2}$ [011], where the figures in brackets are Cartesian vector components, i.e., referring to the Cartesian base vectors [100], [010], [001]. The directions defined by the latter vectors are n.p.c. Another n.p.c. system of base vectors is $[\bar{1}11]$, $[1\bar{1}1]$, $[11\bar{1}]$, where $\bar{1}$ stand for -1. This notation is very common in crystallography and physics.

In the following we shall treat the continuized crystal as described, but keep in mind always the real crystal with nonvanishing lattice constant. In the ideal crystal, which is the undeformed and defect-free crystal, the distance between two lattice points can easily be defined just by the step-counting procedure along three allied crystallographic directions. Of course, we require that the distance of two lattice points be invariant with respect to the choice of the "crystallographic system," a notion which is self-explanatory.

We are particularly interested in the distances of lattice points which are infinitesimal neighbors judged from the macroscale. If dx^k specifies the

relative position of such points in any crystallographic coordinate system, then the law of distance is given by

$$ds^2 = a_{kl}\, dx^k\, dx^l \tag{1}$$

In the fcc crystal we have for the (nonprimitive) Cartesian coordinates $a_{kl} = \delta_{kl}$, whereas for the p.c. system defined we have, from $a_{kl} = \mathbf{e}_k \cdot \mathbf{e}_l$ (scalar product of the base vectors)

$$(a_{kl}) = \frac{1}{4}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix} \tag{2}$$

We remark that noncrystallographic coordinate systems have no meaning for the description of a crystal, at least not from the standpoint of the internal observer who sees the atoms, but not the space in between.

Imagine now that vacancies of a certain density are distributed in the crystal. Usually, such densities, given by the ratio of vacancies to atoms in the unit volume, are very low, e.g., do not reach more than 10^{-3}, say, in thermal equilibrium just below melting temperature. Now the frequency of seeing a vacancy along a crystallographic path, measured by lattice steps between neighboring vacancies, is the same in the real and in the continuized crystal. This is due to the requirement that the content of mass and defect is not changed in the limiting process. We conclude that the number of vacancies along a crystallographic path between two lattice points of macroinfinitesimal distance is infinite if the real vacancy density is finite. The ratio of vacancies over the step number between the two points, however, is finite. Introducing the convention that vacancies are omitted from counting, we see that each vacancy means one step less.

Now each vacancy sits on a crystallographic lattice site, and thus at the junction of three crystallographic direction lines. These might be chosen p.c. or not. For the already mentioned p.c. coordinates in fcc crystals we have calculated the metric tensor which takes account of the vacancies as

$$g^{-}_{kl} = (1 - N^{-})^2 a_{kl}(\text{p.c.}) \tag{3}$$

where N^{-} is the number density (number per unit volume of crystal) of vacancies (Kröner, in press). Transformation into Cartesian coordinates yields

$$g^{-}_{kl} = (1 - N^{-})^2 \delta_{kl} \tag{4}$$

which shows that the vacancy, being a crystallographic defect, is isotropic in fcc crystals, and more generally in any Bravais crystal.

If interstitials rather than vacancies are considered, then a slight complication arises, because the interstitials are never on lattice sites, and thus

not in the junction of the p.c. coordinates. However, it is possible to find allied crystallographic coordinate lines with junctions on interstitial sites. It then makes sense to count an extra step at each interstitial in these coordinates. In this way one arrives at a metric tensor for a crystal with interstitials,

$$g_{kl}^{+} = (1 + N^{+})^2 a_{kl} \tag{5}$$

where, as derived, the k, l refer to any coordinates having junctions at the interstitial sites. Transformation to Cartesian coordinates yields

$$g_{kl}^{+} = (1 + N^{+})^2 \delta_{kl} \tag{6}$$

so that also the interstitial appears as an isotropic defect.

We emphasize already here that the action of an interstitial can well be anisotropic. This, however, is to be described by means of the response law whose derivation requires energetic considerations and therefore goes beyond the presently employed differential geometry.

If vacancies and (self-)interstitials are present simultaneously, then the resulting metric tensor is

$$g_{kl} = (1 - N^{-} + N^{+})^2 a_{kl} \tag{7}$$

Obviously, (7) contains the mutual annihilability of vacancies and self-interstitials.

The square root of the determinant of the metric tensor $\mathbf{g}$ is equal to the volume V of the unit cube, after one atomic volume has been subtracted for each vacancy and added for each interstitial. Since the volume V_0 of the unit cube without defects equals the square root of the determinant of $\mathbf{a}$, we can prove with help of (7) that

$$V = (1 + \Delta N) V_0, \qquad \Delta N \equiv N^{+} - N^{-} \tag{8}$$

Equations (7) and (8) give a nice picture of how vacancy and interstitial are described in the language of differential geometry.

3. POINT STACKING FAULTS AS ELEMENTARY POINT DEFECTS

In the last section we introduced a step-counting procedure which allowed us to define and measure distances between lattice points with the help of a metric tensor. If vacancies and/or interstitials are present, then this leads to a change of the metric tensor (a_{kl}) in absence of these defects [equation (7)]. This change, however, has the quality of an isotropic tensor, i.e., of a scalar. If elementary point defects disturb the step counting, thus the metric, then it is suggestive to expect a full tensor rather than an isotropic

one as a measure of the point defects. So the question arises of whether there are perhaps further elementary point defects. We try to show in the following that there does in fact exist a further type of point defect, later called a "point stacking fault." This defect can be related to a general volume-conserving metric tensor so that a full metric tensor is required to take into account all elementary point defects.

A *point* stacking fault is created if the *surface* defect stacking fault shrinks to a point. In other words: the (surface) stacking fault can be considered as surfacewise composed from the elementary point stacking faults. For detailed descriptions of the concept of stacking fault see, e.g., Seeger (1955), Diehl (1965), and Friedel (1967).

In this section we investigate the so-called conservative stacking faults originally studied by Heidenreich and Shockley (1948). They are of fundamental importance in fcc and close-packed hexagonal crystals. These crystals can be described as stacks of close-packed planes of spheres with a stacking sequence ABCABCABC... for the fcc lattice (Figure 1) and ABABAB... for the hexagonal lattice. The stacked planes are (111), i.e., their normal is the vector [111]. Atoms lying in the same plane are specified by the same symbols (A, B, C) in Figure 1. In the full stacking sequence the planes specified by A follow one from the other by translations [111]. The corresponding applies to the planes B and C. Figure 2 shows one of the planes $(1\bar{1}0)$ of the crystal of Figure 1. The intersection of this plane with the

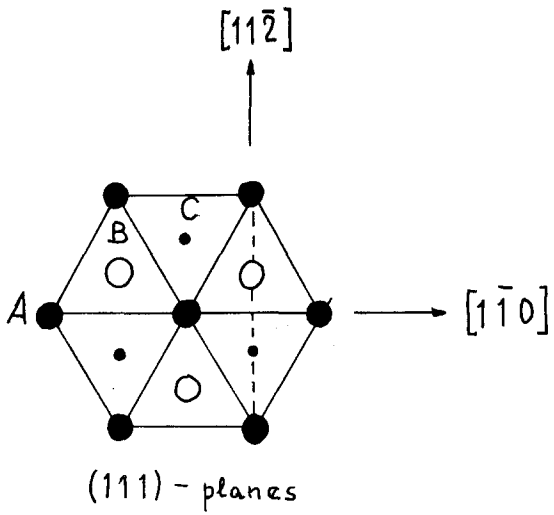

Fig. 1. Stacking sequence (3 planes) of an fcc crystal. A, B, C denote the three positions for dense packing of {111} planes.

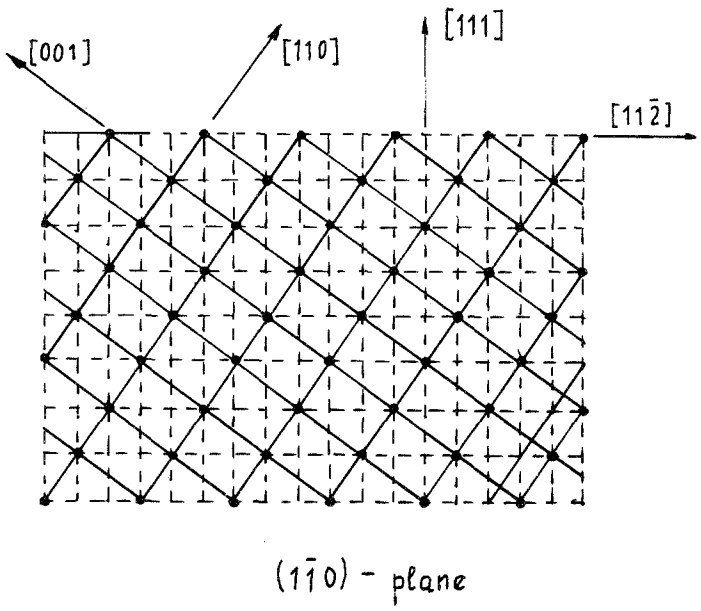

Fig. 2. Defect-free (1$\bar{1}$0) plane of the crystal of Figure 1. Shown are the underground net (n.p.c., dashed) and the p.c. coordinate net.

drawing plane of Figure 1 is given as a dashed line in Figure 1. The crystal is in its ideal state. Figure 3 exhibits the crystal represented by the plane of Figure 2 after the upper half has been parallel-displaced relative to the lower half by the vector $\frac{1}{6}[11\bar{2}]$. In this way we have produced a surface defect of which we see the trace only in Figure 3. This defect is the Shockley stacking fault.

In Figure 3 is also sketched (dashed) an underground orthogonal net which can be used as a crystallographic coordinate net with primitive base vectors $\frac{1}{6}[11\bar{2}]$ and $\frac{1}{3}[111]$. Another orthogonal net with base vectors $\frac{1}{2}[110]$ and [001] is also shown. Looking at the plane only, this net can be understood as (two-dimensional) primitive crystallographic with respect to the atomic positions. In three dimensions, of course, the primitive base vectors of the fcc lattice are all of type $\frac{1}{2}\langle 110\rangle$.

Figure 4 shows the same crystallographic plane with three stacking faults arranged above each other. We have chosen a periodic sequence of these faults mainly for illustration. In fact, a random sequence would finally lead to the same general result. The underground net is as before. Note that not all junctions of this net are occupied by atoms. The disturbance of the lattice by the stacking faults is shown by the primitive, originally

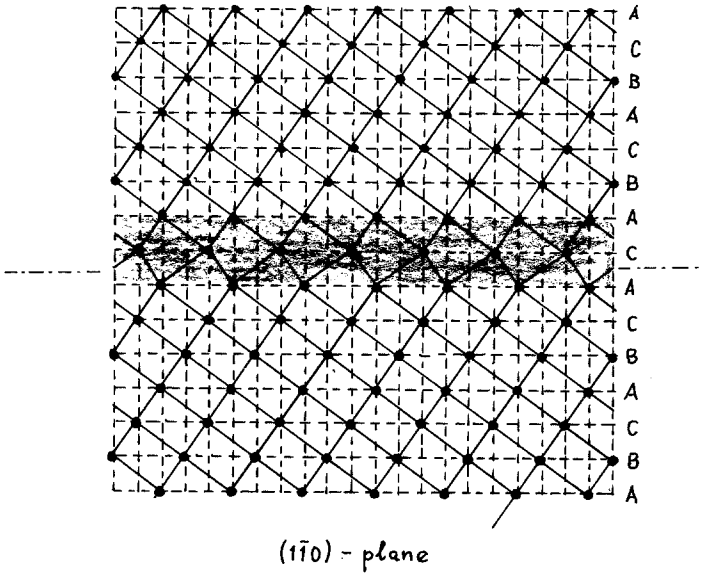

Fig. 3. Crystal of Figure 2, with one surface stacking fault.

rectilinear, net. This net is now rectilinear only *between* the stacking faults. Here the base vectors are still $\frac{1}{2}$ [110] and [001], whereas in the stacking faults we see base vectors $\frac{1}{3}$ [221] and $\frac{1}{6}$ [114] (check!).

In Figure 4 we have also drawn two straight lines which go through lattice points in equal distances, namely 8, if we count atoms along the distorted p.c. coordinate lines. Eight is the periodicity number of the stacking faults.

Both of the straight lines belong to one of the distorted (p.c.) coordinate lines. We can draw the corresponding lines for each distorted line and so obtain an oblique rectilinear coordinate net (Figure 5). This net is crystallographic with respect to the defected crystal. It shows that by the introduction of the stacking faults the crystal has undergone shearings whose average is specified by the deviation from the original net of the now oblique new net. The base vectors of this net can be read off from Figure 4. Giving the vectors, say $\mathbf{e}_{i'}$, between equivalent points along the oblique axes the length 8 (the periodicity length), we obtain

$$\begin{aligned} \mathbf{e}_{1'} &= \tfrac{1}{8}(\tfrac{3}{2}[11\bar{2}]+\tfrac{8}{3}[111]) = \tfrac{1}{48}[25, 25, \bar{2}] \\ \mathbf{e}_{2'} &= \tfrac{1}{8}(-\tfrac{5}{2}[11\bar{2}]+\tfrac{8}{3}[111]) = \tfrac{1}{48}[1, 1, 46] \end{aligned} \tag{9}$$

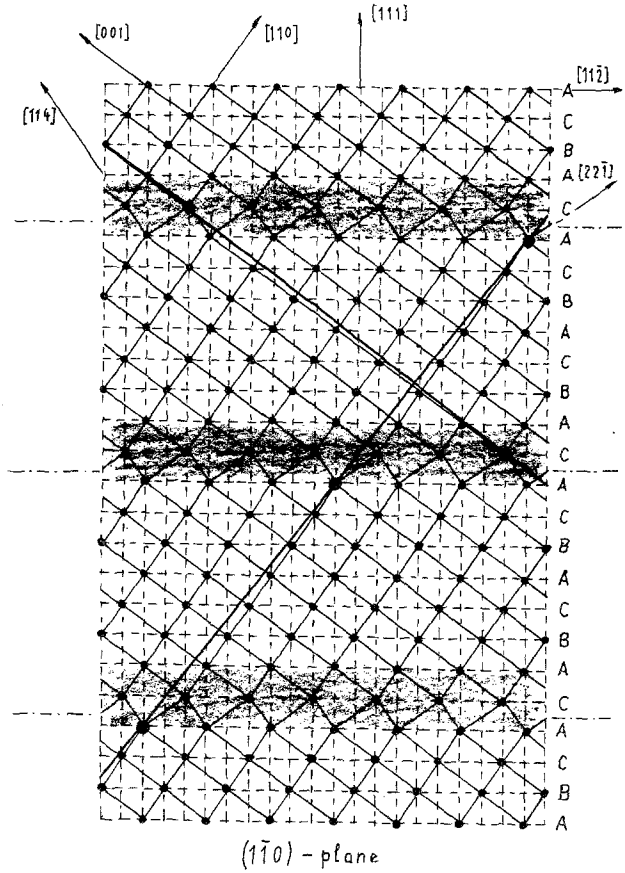

Fig. 4. Crystal of Figure 2 with three periodically arranged surface stacking faults.

The values for the metric

$$g_{k'l'} = \underset{k'}{\mathbf{e}} \cdot \underset{l'}{\mathbf{e}}$$

of the oblique net are

$$\begin{aligned} g_{1'1'} &= 1254/48^2, \qquad g_{2'2'} = 2118/48^2 \\ g_{1'2'} &= g_{2'1'} = -42/48^2 \end{aligned} \tag{10}$$

and

$$|\underset{1'}{\mathbf{e}}| = 0.738, \qquad |\underset{2'}{\mathbf{e}}| = 0.959 \tag{11}$$

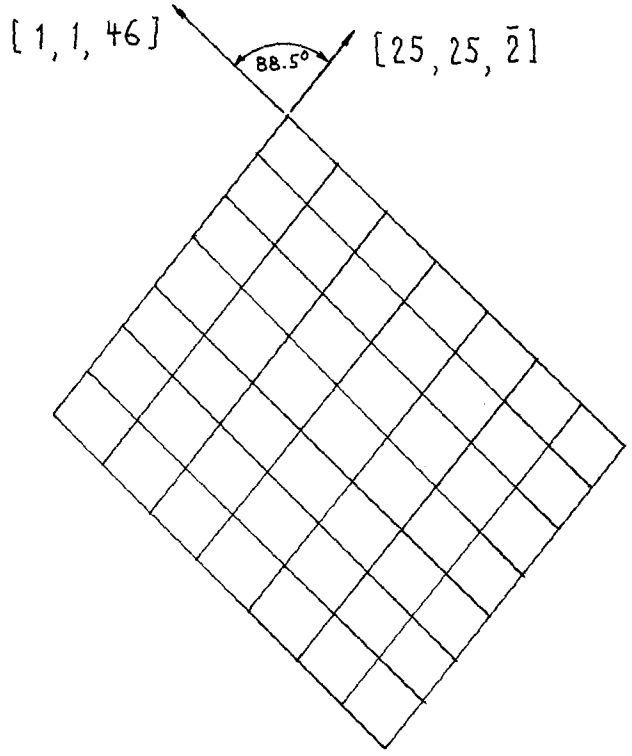

Fig. 5. The p.c. coordinate net of the distorted crystal of Figure 4. The net is not orthogonal.

Comparing this with

$$|\underset{1}{\mathbf{e}}| = 1/\sqrt{2}, \qquad |\underset{2}{\mathbf{e}}| = 1$$

which is the corresponding base of the undefected crystal, we see that $|\underset{1'}{\mathbf{e}}|$ is somewhat longer than $|\underset{1}{\mathbf{e}}|$ and $|\underset{2'}{\mathbf{e}}|$ slightly smaller than $|\underset{2}{\mathbf{e}}|$, as is also proved by Figure 4. The angle, say α, between $\underset{1'}{\mathbf{e}}$ and $\underset{2'}{\mathbf{e}}$ is determined from

$$\cos\alpha = (\underset{1'}{\mathbf{e}} \cdot \underset{2'}{\mathbf{e}})/(|\underset{1'}{\mathbf{e}}||\underset{2'}{\mathbf{e}}|) = 0.026 \tag{12}$$

so that $\alpha \approx 88.5°$.

The shearing of the originally unperturbed crystal can be described by means of a matrix $B \equiv (B^i_{i'})$ defined by

$$\underset{i'}{\mathbf{e}} = B^i_{i'}\underset{i}{\mathbf{e}}, \qquad B^i_{i'} = \underset{i'}{\mathbf{e}} \cdot \overset{i}{\mathbf{e}} \tag{13}$$

where the meaning of $\underset{i}{\mathbf{e}}$ and $\overset{i}{\mathbf{e}}$ is evident.

Obviously, B and its transpose B^t are the sums of three dyadics:

$$B = B^{i}_{i'} \underset{i}{\mathbf{e}} \overset{i'}{\mathbf{e}}, \qquad B^t = B^{i}_{i'} \overset{i'}{\mathbf{e}} \underset{i}{\mathbf{e}} \tag{14}$$

and

$$B \cdot B^t = B^{i}_{i'} B^{j}_{j'} a_{ij} \overset{i'j'}{\mathbf{e}\,\mathbf{e}} = g_{i'j'} \overset{i'j'}{\mathbf{e}\,\mathbf{e}} \equiv \mathbf{g} \tag{15}$$

so that the metric tensor $\mathbf{g}$ can be calculated if the matrix B is known (compare a corresponding formula in nonlinear elasticity theory.) It is not possible to calculate B completely from $\mathbf{g}$, because the rotation part of B does not contribute to $\mathbf{g}$. We shall return to this problem later.

It is interesting to note that, with

$$a_{ij} = \underset{i}{\mathbf{e}} \cdot \underset{j}{\mathbf{e}}$$

we have

$$\det\{g_{i'j'}\} = \det\{a_{ij}\} \tag{16}$$

which expresses the fact that the Shockley stacking faults do not change the volume. Equation (16), which is exact, can be verified generally. As an example, the numerical values of (10) may be used.

If vacancies and interstitials as well as point stacking faults are present, then all these together can be described by the full metric tensor $\mathbf{g}$, whose determinant takes care of the (excess) vacancy–interstitial density, whereas the remainder is representative of the point stacking faults. Above we have proved this in a two-dimensional simplification illustrated by Figure 4. There is no doubt that the result extends to three-dimensional crystals.

So far we have treated surface stacking faults, whereas the main interest of this work lies in elementary defects, and thus in point stacking faults. However, if the internal observer runs along the distorted crystallographic lines, it is not important that the deviations from the undisturbed crystallographic lines occur in equal distances nor that neighboring distorted lines have their deviations mutually correlated. This means that as far as length measurement is concerned, it makes no essential difference whether the elementary point stacking which builds up the surface stacking fault really forms a surface fault or is distributed, e.g., at random in the volume of the crystal. Hence, the results gained for the surface stacking faults apply immediately to three-dimensional densities of point stacking faults. Figure 6 shows how a distribution of point stacking faults can be represented in a somewhat idealized picture. The symbols, double-sided arrows, indicate the elementary shears.

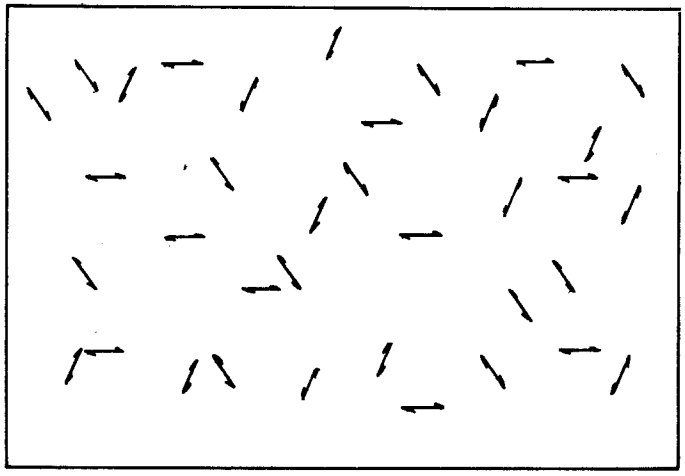

Fig. 6. Example for the density of point stacking faults (schematic).

The results of this section were illustrated on the fcc lattice. There do exist stacking faults in other types of Bravais lattices as well. The theory is the same, only the numerical values change.

4. DIFFERENTIAL GEOMETRY OF DISLOCATIONS AND POINT DEFECTS

We shall now show how the elementary point defects can be embedded into the differential geometry of affinely connected spaces. As indicated in Section 1, we consider flat crystals, i.e., demand that the material geometry possesses teleparallelism.

An essential part of this geometry can be incorporated into Cartan's structure equations, which we copy from Edelen and Lagoudas (1988). A collection of exterior forms

$$\nu \in \Lambda^1_{r,1}, \qquad \Gamma \in \Lambda^1_{r,r}, \qquad \Sigma \in \Lambda^2_{r,1}, \qquad \Theta \in \Lambda^2_{r,r} \tag{17}$$

forms a complete differential system of degree 1 and class r if and only if

$$d\nu + \Gamma \wedge \nu = \Sigma \tag{18}$$

$$d\Sigma + \Gamma \wedge \Sigma = \Theta \wedge \nu \tag{19}$$

$$d\Gamma + \Gamma \wedge \Gamma = \Theta \tag{20}$$

$$d\Theta + \Gamma \wedge \Theta = \Theta \wedge \Gamma \tag{21}$$

The mathematical symbols in these equations represent $(r \times r)$ matrices (Γ, θ) and $(r \times 1)$ matrices (ν, Σ) of differential forms of degree 1 (ν, Γ) and

2 (Σ, θ). Here d is the symbol for exterior derivation. If we consider ν and Γ as *a priori* given quantities, then equations (18) and (20) are definitions of Σ and Θ and equations (19) and (21) are integrability conditions which are satisfied identically by (18) and (20). The geometrical meaning of the occurring quantities is: Γ, linear connection; Σ, torsion; Θ, curvature; ν, some matrix to be discussed later.

Here we are interested in flat spaces, i.e., $\Theta = 0$. Hence equation (21) disappears identically, (20) is the teleparallelism equation, and (19) is satisfied identically by (18). Equations (20) and (18) are the equations of main interest.

We now use a well-known result of differential geometry, namely that any linear teleparallel connection can be represented in the form

$$\Gamma^{k'}_{ii'} = A^{k'}_{\alpha}\partial_i A^{\alpha}_{i'}, \qquad A^{k'}_{\alpha}A^{\alpha}_{i'} = \delta^{k'}_{i'}, \qquad A^{k'}_{\alpha}A^{\beta}_{k'} = \delta^{\beta}_{\alpha} \tag{22}$$

where $A^{k'}_{\alpha}$ is any $(n \times n)$ matrix (in our case of interest 3×3), and ∂_i denotes partial differentiation with respect to some coordinate system (i) which we shall take to be crystallographic and representative for the ideal crystal. Also, (i') and (α) relate to coordinate systems, about which we speak later. Equation (22) is easily verified by insertion into (20).

Using the notation of (22) also in (18) and writing B instead of ν to conform with our earlier papers, we obtain after a routine calculation, with

$$B^{i}_{k'}B^{i'}_{i} = \delta^{i'}_{k'}, \qquad B^{i}_{i'}B^{i'}_{k} = \delta^{i}_{k}, \qquad \partial_{l'} \equiv B^{i}_{l'}\partial_i \tag{23}$$

the fundamental equation

$$-B^{i'}_{i}\partial_{[l'}B^{i}_{k']} + A^{i'}_{\alpha}\partial_{[l'}A^{\alpha}_{k']} = \Sigma^{i'}_{l'k'} \tag{24}$$

which can also be found in Schouten (1954), equation (III. 9.3). Identifying B with the matrix of equation (14), we have the additional equation [cf. (15)]

$$B^{i}_{i'}B^{j}_{j'}a_{ij} = g_{i'j'} \tag{25}$$

According to (13), the matrix $B^{i}_{i'}$ transforms a system $\underset{i}{\mathbf{e}}$ of base vectors into a system $\underset{i'}{\mathbf{e}}$. If $\underset{i}{\mathbf{e}}$ and $\underset{i'}{\mathbf{e}}$ are material vectors, then $\overset{i}{B}$ is a distortion (or deformation) from $\underset{i}{\mathbf{e}}$ to $\underset{i'}{\mathbf{e}}$. The distortion is a physical process, i.e., independent of what system we choose as (i). We may take, for instance, the Cartesian system and obtain from (25)

$$B^{i}_{i'}B^{i}_{j'} = g_{i'j'} \tag{26}$$

(sum over i from 1 to 3)

Thus, if $B^{i}_{i'}$ is given, we can easily obtain the metric tensor for the (dragged along) coordinate system (i'). In Section 3 we introduced this tensor as a measure of elementary point defects.

The matrix $B^{i}_{i'}$ has to do with elementary point defects, whereas the matrix $A^{\alpha}_{k'}$ introduced in (22) is related to dislocations. It is instructive to

investigate the point defects in the absence of dislocations ($A^{\alpha}_{k'} = \delta^{\alpha}_{k'}$) and vice versa ($B^{i'}_{i} = \delta^{i'}_{i}$). The latter study is found in many texts on the differential geometry of dislocations (e.g., Kröner, 1981).

With $A^{\alpha}_{k'} = \delta^{\alpha}_{k'}$ the defect equations (24) and (25) become

$$-B^{i'}_{i}\partial_{[l'}B^{i}_{k']} = \overset{(B)}{\Sigma}{}_{l'k'}{}^{i'} \tag{27}$$

and

$$B^{i}_{i'}B^{j}_{j'}a_{ij} = g_{i'j'} \tag{28}$$

where the latter can also be written as

$$B \cdot B^{t} = \mathbf{g} \tag{29}$$

[cf. (15)]. If our former results are physically sound, then $\overset{(B)}{\Sigma}{}_{l'k'}{}^{i'}$ and $g_{i'j'}$ must be representative of the point defects. "No point defects" means that the right-hand side of (27) vanishes and that of (28), (29) becomes the unity tensor. The general solution of (29) then reads $B = R$, where R is any rotation matrix. Substituting this in equation (27) with vanishing right-hand side leads easily to the result that R is a spatially constant rotation matrix. The occurrence of this matrix is not completely understood. However, it is clear that $\overset{(B)}{\Sigma}$ and $\mathbf{g}$ together represent the point defects except those perhaps contained in the constant rotation matrix. It seems that for some reason they cannot be seen by the internal observer.

It is convenient to use for the coordinate net (i') the dragged along coordinates belonging to (i). Then it is evident that B describes a kind of deformation of the crystal, which accompanies the introduction of the elementary point defects. This deformation, considered as a field, might well be incompatible. In such a case, B contributes to the torsion according to (27).

If no point defects are introduced, we have $B^{i'}_{i} = \delta^{i'}_{i}$ and the defect equation (24) becomes

$$A^{i}_{\alpha}\partial_{[l}A^{\alpha}_{k]} = \overset{(A)}{\Sigma}{}_{lk}{}^{i} \tag{30}$$

Equation (25) is no longer needed. Note that we have replaced the primed coordinate net (i') by the unprimed (i). This is legitimate because the material coordinate system (i') is obtained from that of the defect-free crystal by the introduction of point defects. If there are no point defects, then $(i') = (i)$.

Equation (30) is a basic equation of the theory of Kondo (1952) and Bilby *et al.* (1955), who interpret Σ as the dislocation density. Again it is convenient to consider the coordinate system (i) as crystallographic in the

ideal crystal. If (α) is a crystallographic coordinate system after dislocations have been introduced, then (α) is anholonomic, as is the system (i') if it is chosen crystallographic in the case of incompatible B.

In the absence of dislocations, (30) has the general solution $A_k^\alpha = \partial_k \phi^\alpha$ with an arbitrary field ϕ^α. This A_k^α describes a distortion from the ideal to a deformed state without dislocations. In this case (α) is holonomic and the distortion is identified as compatible, elastic. This follows from the well-known theory of dislocations (e.g., Kröner, 1981).

Obviously, ϕ^α does not contribute to Σ in (30). It follows that only six of the nine functions A_k^α contribute to the defects, whereas all nine functions $B_{i'}^i$ imply defects. Thus, the totality of elementary point and line defects is represented by 15 functions of positions. The defect equations (24) and (25) express the fact that the defects can be produced by certain distortion operations A and B which are not elastic.

5. CONCLUSION

The defect equation (24) contains two contributions, where the first one results from an incompatible distribution of point defects and the second one is the dislocation density in the usual meaning. Both terms look relatively symmetric, but they are not, because $\partial_{l'}$ contains B, but not A. Incidentally, the first term, but not the second, has the form of an anholonomic object (Schouten, 1954). There is the possibility that $A = B$, so that $\Sigma = 0$. This means that certain distributions of elementary point defects can annihilate dislocation densities. Further investigation is needed to see whether this annihilation is related to the one postulated at the beginning of this paper. Whereas Σ, like $\mathbf{g}$, is a tensor, and thus capable of describing physical quantities, the two separate terms in (24) are not. The reason is that in the presence of point defects, the dislocations are not, in general, autonomous physical objects, but they mix with point defects, and only the sum of the two terms in (24) represents a physical object. So we come to the conclusion that Σ and $\mathbf{g}$ have to be combined into a quantity $\{\Sigma, \mathbf{g}\}$ which then represents the elementary pointline defects. This reminds us of our early discussion according to which point and line defects can mutually convert. It also seems to be related to a discussion by Kunin (1986), who distinguishes an *affine* connection $\{\Gamma, \mathbf{h}\}$ from a *linear* connection Γ, emphasizing that the linear connection misses some degrees of freedom. The quantity $\mathbf{h}$ is called a tensor by Kunin. We are inclined to compare it with our B. The identification of $\mathbf{h}$ with point defects, however, is not done by Kunin. Detailed investigation of these questions is urgent.

The theory was developed for an internal observer who has a few clearly defined abilities. It is not difficult for him to find the metric tensor

in a certain situation with point defects (for dislocations the analogous problem was solved long ago). In fact, the internal observer is able to recognize the vacancy and the interstitial when, on his step-counting path, he arrives at one of the atoms adjacent to the vacancy or interstitial. As described, these objects are *length* defects. Similarly, we have introduced the point stacking faults as *angle* defects, also seen by the internal observer. To specify the defect state of his world, this observer only has to count the frequency with which all these defects separately appear on his counting path. This frequency determines the densities of the defects. The metric tensor describing this follows easily.

We have not discussed the mechanical stability of the point stacking faults. These might well be unstable in many cases, depending on the material, temperature, pressure, etc. The existence of surface stacking faults shows that several or many point stacking faults can mutually stabilize in the form of surface stacking faults. There might be other cases where point stacking faults really exist.

In our investigation of point stacking faults we have omitted the second type of defects, the so-called Frank stacking faults. These are related to plane arrays of vacancies or interstitials, and hence they are not elementary defects. In the transition to point stacking faults they become elementary, however related to the vacancies and interstitials, and thus also contained in the metric $\mathbf{g}$. The Frank stacking faults often form small tetrahedra. If these composed defects shrink to a point, they become single vacancies or interstitials, so that also the stacking fault tetrahedra fit in our picture. It would be possible to develop our analysis without speaking explicitly of vacancies and interstitials, just by including Frank's stacking faults.

The investigation of this work shows that there is no closed theory of elementary point defects and no closed theory of elementary line defects (dislocations) in Bravais crystals. The theoretical proposition, represented in particular by the defect equations (24) and (25), implies a unification of the older incomplete theories. To achieve this unification, we had to introduce elementary defects which so far have hardly, if at all, been discussed. They seem to be closely related to a defect called "Verhakung" by Dehlinger (1929). This defect was later discarded in favor of the dislocation.

In this paper the theory was developed for the ordered structure "Bravais crystal." It is evident that similar investigations should be done for other ordered structures as well.

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