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Benefits and shortcomings of the continuous theory of dislocations

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Abstract

Out of the vast field of microstructural mechanical behaviour of solids, we choose the area of elastoplasticity of crystalline solids. It is emphasized that elastoplastic deformation proceeds through defects in the ordered crystalline structure. Most important, at least in our investigation, are the defects *dislocations* that produce plasticity by motion at all temperatures and, in addition, *point defects* that become active at a higher temperature. It is shown that for two reasons, the elastoplasticity of crystalline solids does not fit well into the scheme of continuum mechanics: (i) The conventional tensor of dislocation density counts only excess dislocations of one sign, whereas the observed hardening and softening is due to the dislocations of *two* signs. (ii) The motion of the typical defects in the crystalline structure destroys the particles that constitute the body whose particles, therefore, do not persist during the elastoplastic motion. For this reason, the elastoplastic crystalline solid is not a differentiable material manifold.

During the elastoplastic deformation, an irregular, often densifying dislocation network develops that can be seen in the electromicroscope and therefore is characteristic for the internal mechanical state. The network can be described by the infinite set on n-point correlation functions of dislocations. It is proposed that solutions are classified as of first, second, third, etc. order according to the highest order of correlation function which is included. The first-order theory is the so-called mean field theory, a well-known concept within the statistical physics. The two-point autocorrelation function gives the often used total length of dislocations in a unit volume, also a state quantity.

The present state of the theory, in particular of the dynamics, is still rather underdeveloped.

Keywords: Dislocations; Continuous theory; Crystalline solids

1. Introduction

In this article, we are concerned with the mechanics of solid media with microstructure, i.e. with *microstructure mechanics*. In the last decades, the investigation of such media has increased extraordinarily. This is not astonishing if one bears in mind that almost all (solid) matter possesses a microstructure and that the behaviour of such materials depends strongly on this structure, (Kunin, 1982; Capriz, 1989). The work (Capriz, 1989) contains a valuable classification of the various types of microstructure, according to the form of the *order parameter*, or of similar quantities, which are needed to classify the microstructure

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considered. Of interest are the structures on all possible length scales from atomic scale (e.g. crystals) to macroscopic scale (e.g. concrete or certain plastics).

The field of microstructure mechanics is atmost complex. This means that in an article of this size and character many topics cannot be discussed even though they might be very important in certain situations. So I shall be very brief on the thermodynamical aspects and even restrain from a deeper discussion of the dynamics.

A large part of the microstructured media can be described as ordered, however, with defects in this order. Then, ordinarily, the objects of interest are the defects since they, in a sense, bring the material to life. Therefore, a large part of research on materials with microstructure is concerned with the study of defects in ordered structures.

The term, or the object, ''defect'' has a meaning only in relation to the order prevailing in the considered solid. Once a specific order is defined, we can explain deviations from this order as defects. Most convenient for an explanation of such a situation is the example of crystalline matter, a structure particularly often found with metallic materials.

Mathematically, the most simple type of crystal, which we call point crystal, can be defined by requiring that at each material point (atom), three nonplanar vectors $(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)$ can be drawn which point to the next neighbour atoms in such a way that the vectors $\boldsymbol{e}_i$ $(i = 1, 2, 3)$ are Euclidean parallel in the whole specimen. The $\boldsymbol{e}_i$ play the role of the order parameter in the crystalline structure. By using experimental tools, e.g. electron microscopes, one can find local deviations from the Euclidean parallelism, and can then identify them in our case (point crystal) as defects named dislocations (line defects) or as point defects such as interstitials or vacancies or shear faults.

Besides the line and point defects, there also exist surface defects whose classification is not yet final. Twin and grain boundaries belong to this group.

In order to classify the defects in otherwise ordered structures it is necessary to distinguish between elementary and composed defects. This is a requirement similar as it is known from the theory of elementary particles. By this requirement, the number of different elementary defects (or particles) becomes finite, usually small.

In the crystals described so far, the particles are atoms, taken as material points. There also do exist the so-called molecular crystals, e.g. where the particles are extended to little rods (one may also think of more complex particles). Of course, in these cases, the order parameter, which was $(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)$ in atomic crystals is different now, and therefore, the defects also become different. The most prominent defect in rod crystals (in crystals where the particles are rods) is the dislination (a line defect), also called *spin disclination* to distinguish it from *orbit disclinations* which are defects in other structures, e.g. in atomic crystals. The orbit disclinations, however, are not elementary defects – they rather correspond to certain superpositions of dislocations. We mention in passing that the molecules of liquid crystals are often rod-like. Therefore, spin disclinations occur in liquid crystals, where they are elementary defects. In this article, however, we shall restrict ourselves to materials having a crystalline structure with point particles. Metals are the outstanding representatives of this group.

We have mentioned that it is the defects which bring life into ordered structures. The best example is again the dislocation, whose movement implies local plastic deformation at the momentaneous position of the dislocation. This is the reason why the connection between plastic flow and dislocation motion has been studied since the appearance in science of the dislocation in the year 1934. At that time, there was great hope that a future theory of dislocations could be ranged in the extremely successful continuum mechanics with its whole wealth of applications. This hope has been fulfilled only partially, and this will be a main point of this exposition.

All matter which we use in our daily life is built up from atoms or molecules. In many cases, their structure is crystalline, i.e. ordered, in others amorphous, i.e. disordered and in others, partially ordered (or partially disordered). The properties of these various groups of materials are very different, and to explain

this in detail is an important aspect of material science. In this paper, we shall not try to solve this problem but rather restrict ourselves to the field of plasticity, or better elastoplasticity, thereby emphasizing some principal features of such a theory. Going from simpler to more complex situations, we start in Section 2 with a brief remembrance of the classical theory of ideal plasticity as was developed in the last century. This theory neglects all effects of elasticity, with the consequence that the internal state of the trial body remains unchanged during the deformation. This means in particular that the body does not harden nor soften during the deformation.

In Section 3, we allow for elastic effects in a way which is suggested by the picture of continuum mechanics. We shall see that in this scenario, we have to allow for the incompatibility of both elastic and plastic parts of the deformation. In this theory where we are concerned essentially with the internal mechanical state, we do not speak of dislocations or other defects as yet. This means that we omit an important part of the phenomenon elastoplasticity.

In Section 4, we combine elastic and plastic deformation to give the total elastoplastic deformation. The composition is multiplicative in the nonlinear theory, but becomes additive in the linearized theory.

Section 5 essentially contains the elementary, linearized continuum theory of dislocations. Here it is shown that this theory is incomplete since the traditional tensor of the dislocation density, that appears here for the first time, contains dislocations of only one sign (plus or minus). This is a serious handicap to the theory.

Another handicap is described in Section 6. Here it is shown that, due to the dislocation motion, the structure of the solid suffers an internal renting to pieces. This implies that the crystal is not a (differentiable) material manifold.

The strong statistical components of the dislocation structure suggest a way out from this dilemma. This is to consider elastoplasticity as a problem of statistical physics. The dislocations are described in Section 7 as random functions of position (and perhaps time). All tools of statistical physics are now available. In Section 8, we show in particular that the dislocation correlation functions are helpful to describe the dislocation state. They enable one to proceed systematically to better approximations by including higher order correlations. First approximation is a mean field theory which is close to the elementary theory described in Section 5.

In Section 9, we illustrate that the greatest difficulty when developing a realistic theory of elastoplasticity is the complexity of the internal mechanical state. This is a problem completely absent, for instance, in the conventional elasticity or ideal plasticity theory. The problem with the internal mechanical state is closely connected with the response problem treated in Section 10. A crystalline solid with dislocations is no longer in the state of the ideal crystal. We shall argue in Section 5 that dislocations cannot approach each other closer than perhaps 20 Å, and this means that the largest volume part of the specimen will remain crystalline under the deformation, whereas dislocations occupy an only small part of the volume. But where the dislocations are, there is no longer a crystalline state, as the mutual relative positions of the atoms are principally different there. This clearly implies an elevated energy and, as a consequence hereof, a specific response to the presence of dislocations. It is argued that this response has the dimension of a moment stress.

In Section 11, we make some remarks on the problems that are very important for elastoplasticity, but were nevertheless omitted in this article that was not supposed to become a book. Topics here are the appearance of point defects and their integration into the general (field) theory, the gauge theories of defects which recently have gained some popularity, though they have not led to a breakthrough so far, the frequently observed development of dislocation patterns on a mesoscale and finally the field theoretical formulation of the theory in terms of affine differential geometry. Behind the latter stands an imposing mathematical formalism which in full generality takes care of all (the many) nonlinearities in our field.

One last word on the practiced mode of citation. We consider all quoted works as basic contributions to our field of investigation. I know that nevertheless my list is rather fragmentary, and I apologize to those who had deserved to be quoted and are not.

2. Ideal plasticity

The object of ideal plasticity (e.g. Geiringer, 1973) is a completely structureless medium, something that does not exist in reality. Its properties are the same at all points and times. In other words, such a body is homogeneous on all length and time scales. As far as mechanics is concerned, to which we limit ourselves, such a medium satisfies the equations

$$\rho\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t}-\operatorname{div}\boldsymbol{\sigma}=\boldsymbol{F}\qquad\text{(equations of motion)},\tag{1}$$

$$\rho\operatorname{div}\mathbf{v}+\frac{\mathrm{d}\rho}{\mathrm{d}t}=0\qquad\text{(equation of continuity)}.\tag{2}$$

Here ρ is the (scalar) matter density, $\mathbf{v}$, the velocity (vector) field, $\boldsymbol{\sigma}$, the stress (tensor) field, $\boldsymbol{F}$, the external force per unit volumes, ρ, v_i, σ_{ij} are 10 fields that determine the dynamical state of our medium. Eqs. (1) and (2) comprise four equations, so that we need six further equations for the determination of ρ, v_i, σ_{ij}. These equations must specify the particular physical situation of the medium. The situation is that of ideal plasticity and consists of two parts. The first part has five equations

$$\frac{1}{2}\left(\frac{\partial v_i}{\partial x_j}+\frac{\partial v_j}{\partial x_i}\right)=\lambda s_{ij}\quad(\lambda\geqslant 0),\tag{3}$$

which form the plastic flow law of de St. Venant and Lévy (1870) and von Mises (1913).

The second part is the scalar equation:

$$s_{ij}s_{ij}=2k^2,\ \ s_{ij}=\operatorname{deviator}(\sigma_{ij}),\tag{4}$$

and this is von Mises' (1913) law of yield limit. It implies that yielding sets in when the stress has reached a certain limit which is determined by the constant k. An extension of the theory would be that k and λ depend on the position in our medium. Obviously, Eq. (3) is Newton's law of viscosity, whereas Eq. (4) is the typical law of a plastic body. Hence, a material obeying Eqs. (1)–(4) could also be classified as (ideally?) viscoplastic. Eq. (3) implies that this flow is volume conserving. It may be expected that the laws characterizing viscosity and plasticity like those in Eqs. (3) and (4) should also flow into more complex theories of plasticity or viscoplasticity. This is the main reason why we have this section.

The laws of ideal plasticity and simple extensions thereof have been applied a lot in theory and practice, sometimes with considerable success. However, real materials show the phenomena of strength, hardening and softening which lead to a change of the internal mechanical state of the body. It is obvious that such a behaviour cannot be described by the Eqs. (1)–(4). Since the named phenomena are at the root of our understanding of the notion of plasticity, our aim must be to develop a plasticity theory of real bodies, and this means to study strength, hardening and softening as well as their basic sources. In many cases, such research has shown that the basic sources are the defects, in particular the dislocations, so that their study appears to be unavoidable. It is helpful, however, to postpone this study a bit and first to see what happens when we extend the ideal plasticity to a plasticity combined with elasticity. We shall then speak of elastoplasticity.

3. Mathematical theory of internal stress

Now, the role of the internal mechanical state is fundamental. This is the state of self-stresses (eigenstresses) in which the stress sources are *internal* to the body, in contrast to what we have in more conventional applications of elasticity theory, where the stress sources are volume and surface densities of the *external* forces.

To find out more about the internal stress sources consider the medium at rest, i.e. the static situation. Let us compare the scenarios with external and internal stress sources. The theory with external stress sources is the conventional elasticity theory which in linear approximation obeys the equations of equilibrium

$$\partial_i \sigma_{ij} = -F_j \quad (\operatorname{div} \boldsymbol{\sigma} = -\boldsymbol{F}), \tag{5}$$

compatibility

$$\epsilon_{ikm}\epsilon_{jln}\partial_k\partial_l\varepsilon_{mn} = 0 \quad (\operatorname{inc} \boldsymbol{\varepsilon} = 0), \tag{6}$$

and the stress–strain law

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl} \quad (\boldsymbol{\sigma} = \boldsymbol{c\varepsilon}). \tag{7}$$

Eqs. (5)–(7) is the *linearized form* of the laws of (static) elasticity theory, where we have omitted the surface equations for simplicity. Note that at this stage of development of the theory many essential points arise already from the linearized theory. It is a minor task to write down Eqs. (5)–(7) also in the frame of the nonlinear theory.

In Eq. (6), ε_{mn} is the elastic strain tensor, and "inc" (read "incompatibility of") is the tensor operator of incompatibility, defined by

$$(\operatorname{inc})_{ijmn} = \epsilon_{ikm}\epsilon_{jln}\partial_k\partial_l, \tag{8}$$

so that $\operatorname{inc} = 0$ means compatibility. c_{ijkl} is the, in general anisotropic, material tensor of the linearized elasticity theory.

The external volume force F_j in Eq. (5) is mostly given in the statement of the problem. In particular it can be equal to zero. If in this case, we require that instead of obeying the compatibility law the elastic strain tensor is incompatible, we arrive at the equations of equilibrium

$$\partial_i \sigma_{ij} = 0 \quad (\operatorname{div} \boldsymbol{\sigma} = 0), \tag{9}$$

incompatibility

$$\epsilon_{ikm}\epsilon_{jln}\partial_k\partial_l\epsilon_{mn} = \eta_{ij} \quad (\operatorname{inc} \boldsymbol{\varepsilon} = \boldsymbol{\eta}), \tag{10}$$

and the stress–strain law which conveniently is formulated in the inverse form

$$\varepsilon_{ij} = s_{ijkl}\sigma_{kl} \quad (\boldsymbol{\varepsilon} = \boldsymbol{s\sigma}). \tag{11}$$

Obviously, the Eqs. (9)–(11) permit stresses when the "incompatibility tensor" $\boldsymbol{\eta}$ is nonzero. Since

$$\operatorname{div}\operatorname{inc} \equiv 0, \tag{12}$$

we can satisfy Eq. (9) by

$$\boldsymbol{\sigma} = \operatorname{inc} \boldsymbol{\chi}, \tag{13}$$

so that $\boldsymbol{\varepsilon} = \boldsymbol{s} \operatorname{inc} \boldsymbol{\chi}$ and

$$\operatorname{inc} \boldsymbol{s} \operatorname{inc} \boldsymbol{\chi} = \boldsymbol{\eta}. \tag{14}$$

This equation is brought into a more convenient form by introducing the auxiliary tensor $\boldsymbol{\chi}'$ through (Kröner, 1954)

$$\chi_{ij} = 2\mu\left(\chi'_{ij} + \frac{\nu}{1-\nu}\chi'_{kk}\delta_{ij}\right), \tag{15}$$

with inverse

$$\chi'_{ij} = \frac{1}{2\mu}\left(\chi_{ij} - \frac{v}{1+2v}\chi_{kk}\delta_{ij}\right), \tag{16}$$

where μ and v are shear modulus and Poisson's ratio. Of course, Eqs. (15) and (16) are useful for isotropic elasticity only.

In view of Eqs. (15) and (16) one finds that Eqs. (9)–(11) are satisfied by the solutions of the equations (Kröner, 1954)

$$\nabla^4 \boldsymbol{\chi}' = \boldsymbol{\eta}, \quad \operatorname{div} \boldsymbol{\chi}' = 0. \tag{17}$$

In possession of $\boldsymbol{\chi}'$, the stress follows easily from Eqs. (15) and (13).

The equations of this section are useful when the stresses due to a given "dislocation distribution" are to be calculated. The connection to dislocation theory is given by the equation

$$\boldsymbol{\eta} = -(\boldsymbol{\alpha} \times \nabla)_{\mathrm{sym}}, \tag{18}$$

where "sym" denotes symmetrization and $\boldsymbol{\alpha}$ is the tensor of dislocation density as introduced in Section 5. So, the presence of dislocations implies incompatibility.

4. Elastoplasticity – preliminary thoughts

We now show that the basic Equations (9)–(11) of the internal stress state are well prepared to adapt plastic deformation into the theory. For this task we need a deeper understanding of the concept of incompatibility. To achieve this, we divide, in a thought experiment, the medium into its little volume elements which first might be finite, but then become infinitesimal under a suitable limiting process. Imagine that we cut the medium along all boundaries between adjacent volume elements. We now give to every volume element some plastic deformation in such a way that in the mentioned limiting process a continuous plastic strain, say $\varepsilon^{\mathrm{p}}_{ij}$, arises. It is possible that after the performance of this process the volume elements fit together perfectly. This is the case when the macroscopic function of plastic strain is compatible, i.e. satisfies

$$\operatorname{inc} \boldsymbol{\varepsilon}^{\mathrm{p}} = 0. \tag{19}$$

In fact, in this case the strain $\boldsymbol{\varepsilon}^{\mathrm{p}}$ can be derived from a plastic displacement field; therefore, it is a compatible strain field. That is so in the situation of ideal plasticity. In general, however, $\boldsymbol{\varepsilon}^{\mathrm{p}}$ can be any function, so that $\boldsymbol{\varepsilon}^{\mathrm{p}}$ will, in general, be an incompatible strain. This case occurs in reality when we perform plastic deformation on the body. Now, the real deformations of interest are those which leave the body intact, i.e. lead from one compact state to another compact state. For a medium that is capable of elastic and plastic deformation, the condition that the body remains compact under the action of elastic and plastic deformation is that their incompatibilities are equal but of opposite sign, so that they cancel for the sum $\boldsymbol{\varepsilon}^{\mathrm{e}} + \boldsymbol{\varepsilon}^{\mathrm{p}}$. Thus, the condition that the body remains compact in the combined elastoplastic deformation reads

$$\operatorname{inc} \boldsymbol{\varepsilon}^{\mathrm{e}} = -\operatorname{inc} \boldsymbol{\varepsilon}^{\mathrm{p}}, \tag{20}$$

where we now use $\boldsymbol{\varepsilon}^{\mathrm{e}}$ for "elastic strain". Also, this equation can easily be transformed into the nonlinear form.

Eq. (20) is necessary but not sufficient for the purpose, what we can see as follows: Define total, elastic and plastic deformation gradients by

$$\mathrm{d}x^k = F^k_K \,\mathrm{d}X^K, \quad \mathrm{d}x^k = F^{\mathrm{e}k}_{\kappa}\,\mathrm{d}x^{\kappa}, \quad \mathrm{d}x^{\kappa} = F^{\mathrm{p}\kappa}_{K}\,\mathrm{d}X^K. \tag{21}$$

In Eq. (21), X^K are the material coordinates, x^k the space coordinates and $\mathrm{d}x^k$ are the anholonomic coordinate differentials of a fictive intermediate state which would arise if, as discussed above, a pure plastic deformation would be applied to the initial state.

Obviously,

$$F_K^k = F_\kappa^{\mathrm{e}k} F_K^{\mathrm{p}\kappa}. \tag{22}$$

e and p denote, as before, "elastic" and "plastic". Eq. (22) is the rule showing how the total deformation gradient decomposes into elastic and plastic part. If we linearize Eq. (22) by introducing the, now infinitesimal, distortion tensor

$$\beta_K^k = F_K^k - \delta_K^k, \tag{23}$$

then Eq. (22) becomes

$$\beta_K^k = \beta_K^{\mathrm{e}k} + \beta_K^{\mathrm{p}k}. \tag{24}$$

Thus, the decomposition of the (total) deformation into elastic and plastic part is multiplicative in the nonlinear case, but reduces to an additive law in the linear form. We use the term "distortion" rather than "displacement gradient", because the β's are gradients only if the corresponding deformations are compatible. The case of interest is that elastic and plastic distortions are incompatible, whereas the total distortion is compatible. This is so because we assume that during the elastoplastic deformation, the body is not torn into pieces, i.e. remains compact. We may now write $\beta_{ij} = \partial_i u_j$ with u_j the total displacement field, but corresponding equations do not exist for β_{ij}^{e} and β_{ij}^{p}. This implies that the forms with $F_k^{\mathrm{e}k}$ and $F_K^{\mathrm{p}k}$ in Eq. (21) are, in general, Pfaffian forms.

For simplicity, our arguments were partly based on the linearized theory of elasticity. They can also be used analogously in the frame of the nonlinear theory, which, however, is much more complex.

In the preceding text, we have sketched a continuous medium that can undergo deformations composed from elastic and plastic parts. These deformations connect compact states of the medium and can be described in terms of a displacement field. Allowing now also for motion, we identify a body, say B, with a three-dimensional material manifold whose motions are families of time-dependent diffeomorphisms $\boldsymbol{\chi}$ of B into the Euclidean space E_3.

A consequence of these statements is that

$$\boldsymbol{x} = \boldsymbol{\chi}(\boldsymbol{X}, t), \tag{25}$$

where $\boldsymbol{x}$ denotes the position in E_3 of the particle labelled by $\boldsymbol{X}$ in some reference configuration which we may choose as stress-free. The existence of Eq. (25) with differentiable $\boldsymbol{\chi}$, which is called "motion", implies that we have sketched a theory which fits into the conventional continuum mechanics. We shall come back to Eq. (25) in Section 6.

5. Dislocations – elementary approach

The result that the total distortion $\boldsymbol{\beta}$ must derive from a displacement field can also be written as

$$\operatorname{curl} \boldsymbol{\beta} = 0, \tag{26}$$

or, with Eq. (24)

$$\operatorname{curl} \boldsymbol{\beta}^{\mathrm{e}} = -\operatorname{curl} \boldsymbol{\beta}^{\mathrm{p}}, \tag{27}$$

which, of course, is related to Eq. (20).

Now, consider the surface integral

$$\int_S \mathrm{d}S \cdot \operatorname{curl} \boldsymbol{\beta}^{\mathrm{p}} = \oint_C \mathrm{d}x \cdot \boldsymbol{\beta}^{\mathrm{p}} \equiv \oint_C \mathrm{d}\boldsymbol{b} = \boldsymbol{b}_C, \tag{28}$$

over a surface S inside the medium, where S is bounded by the circuit C. A part of Eq. (28) can be rewritten as

$$\int_S \mathrm{d}S \cdot \boldsymbol{\alpha} = \boldsymbol{b}_C, \quad \boldsymbol{\alpha} \equiv \operatorname{curl} \boldsymbol{\beta}^{\mathrm{p}}. \tag{29}$$

It is suggestive to interpret $\boldsymbol{\alpha}$, which obviously describes a line density, as the tensor of dislocation density, because the line integrals in Eq. (28) are Burgers circuits as used to define the Burgers vector in the elementary dislocation theory (Burgers, 1939a,b). There is one Burgers vector for each circuit C, namely $\boldsymbol{b}_C$. This is a measure of the number of dislocations piercing through the surface S. Incidentally, this number is the same for all surfaces S that have the same circuit C as boundary. Note that $\operatorname{div} \boldsymbol{\alpha} = 0$ from the definition (29) of $\boldsymbol{\alpha}$. Of course,

$$\operatorname{curl} \boldsymbol{\beta}^{\mathrm{p}} = \boldsymbol{\alpha} \quad \text{(definition)}, \tag{30}$$

$$\operatorname{curl} \boldsymbol{\beta}^{\mathrm{e}} = -\boldsymbol{\alpha} \quad \text{(law)}, \tag{31}$$

where the sign is conventional.

Eq. (31) is the law that ensures that the body does not break into pieces under the action of the elastoplastic deformation. It contains how the elastic distortion must develop to keep the body compact.

Eq. (31) appears as a relatively easily handleable differential equation with a well understandable meaning.

However, the situation is by far more complex than it appears here. The point is that only the *resulting* Burgers vector is measured by Eq. (29), see e.g. (Kroupa (1964)). This means that the positive and negative dislocations cancel to a large degree. For instance, the resulting Burgers vector turns out to be as zero, if an equal number of positive and negative dislocations pierce through S even if this number is very large. This is not at all an academic situation, but occurs frequently in practice. A prominent example is simple tension, where for reasons of symmetry equal numbers of positive and negative dislocations are produced, so that $\boldsymbol{b}_C = 0$ for each C. Nevertheless, experience shows that many materials harden or soften strongly under simple tension, which means that the internal mechanical state changes inspite of the absence of a macroscopic dislocation density $\boldsymbol{\alpha}$. In other cases, e.g. bending and torsion, excess dislocations of one sign are produced, but their number is usually so small that the change of state from them is much less than that due to the simultaneously produced dislocations of both signs.

If we now argue in terms of dislocations, then we should be aware that dislocations do not form nice line densities, as for instance electrons in conductors do, but rather they form multiply interconnected networks. This is in agreement with our former findings that dislocations occur in roughly equal numbers of both signs.

In the undeformed crystal, one normally sees a quite loose dislocation network that densifies (sometimes looses) strongly during the deformation. It is of great significance that there is an upper limit to the density of dislocations. In fact, when dislocations of opposite signs approach each other below a critical distance, then they suddenly hasten onto each other and annihilate. The critical distance, say d_{cr}, is somewhat different for screw and edge dislocations, 20 atomic distances might be of a typical value (Differt and Essmann, 1993; Essmann and Differt, 1996). Note that this distance is very small on the macroscopic scale.

There are two limiting cases in this respect. The mean diameter of the Burgers circuit C which we use to detect the dislocations (i) is (much) smaller than the critical distance d_{cr}, or (ii) it is (much) larger than the critical distance d_{cr}.

Both cases are up to our convenience. That means they are legitimate for the corresponding experiments. Let us first discuss case (i). Of course, the Burgers circuit of such a smallness will surround either none or one dislocation. With the help of many small Burgers vectors we can then measure the course of all dislocations, and these will occur as separate lines that form an interconnected network. A dislocation which passes through a point $\boldsymbol{x}$ in the direction given by the unit vector $\boldsymbol{t}(\boldsymbol{x})$ is then described by the dyadic $\boldsymbol{t}(\boldsymbol{x})\boldsymbol{b}$. Here, $\boldsymbol{b}$ does not depend on the position, because $\boldsymbol{b}$ is always constant along a dislocation line. Note that there can exist in a crystal several different Burgers vectors, all however connected with the lattice structure. Therefore, the number of Burgers vector types is always small and can often be taken into account by simple addition. In the following, we assume that there exists only one type of Burgers vector in our medium.

In our present case, description by single lines, we do not have a dislocation *density* but single (separate) dislocations characterized by $\boldsymbol{t}(\boldsymbol{x})\boldsymbol{b}$. Formally, however, we can introduce a dislocation density also in the case of single dislocations. This density has the form

$$\boldsymbol{\alpha}(\boldsymbol{x}) = \boldsymbol{t}(\boldsymbol{x})\boldsymbol{b}\delta(\rho). \tag{32}$$

Here $\delta(\rho)$ is a delta function which is infinite along the course of all dislocation lines and zero otherwise. ρ is the shortest distance of a point from the dislocation line L.

Eq. (32) leads to the correct Burgers vector of a dislocation piercing through a small area s perpendicular to the dislocation line. In fact, the integration over s gives

$$\int \alpha_{il}\,\mathrm{d}S_i = \int t_i b_l \delta(\rho) t_i\,\mathrm{d}S = b_l, \tag{33}$$

where $\int \delta(\rho)\mathrm{d}S = 1$ has been used.

Dislocation densities of the just considered type are frequently used in model calculations where one is concerned with the problems of separate dislocations, in particular calculations of stress and strain. Of interest are singular dislocations, two, three or more single dislocations and their interaction, often straight, sometimes circular and other dislocations.

As mentioned (case ii), to measure the Burgers vectors, we can choose the circuits C also large. We then measure excess dislocations of one sign per circuit C. This means that we get a dislocation density $\bar{\boldsymbol{\alpha}}$ that is the average of the microscopic density $\boldsymbol{\alpha}$ considered so far. Whereas the microdensity describes the dislocation exactly, the macrodensity does not. It is simpler instead.

In the problems of type (i), the dislocation distribution is given, e.g. by the model. This is, of course, not the general problem of elastoplasticity, where we want to calculate elastic and plastic strain, dislocation distribution, stress, hardening etc. Nevertheless, it is very useful to be able to calculate the stress and strain distribution due to a given dislocation arrangement. The *given distribution of dislocations* makes the problem deterministic, whereas the problem of *given external forces* rather than given dislocations belongs to the statistical physics. This is so because the dislocation network developing under these conditions is a random network.

6. Differentiable material manifold – a nonappropriate picture

The findings of the last section imply that the Eqs. (26)–(29) give an only incomplete picture of the geometry, or kinematics, of dislocations, and this insofar as these equations do not describe sufficiently the internal mechanical state. In fact, only excess dislocations of one sign are included into Eq. (29), and we know that this state is described essentially by the positive and negative dislocations together. There is another circumstance which lets us suspect that not everything is in order with the theory of Section 5.

In Section 4, we have recalled that in continuum mechanics the motion $\boldsymbol{\chi}$ of a particle, labelled by $\boldsymbol{X}$ in some reference state can be written as

$$\boldsymbol{x} = \boldsymbol{\chi}(\boldsymbol{X}, t). \tag{34}$$

This equation gives us the trajectories of the particles during their motion. This motion can be described as a change of placement, i.e. a displacement, which depends on position and time. The existence of the function $\boldsymbol{\chi}$ is in accordance with Eq. (26) which implies the existence of a displacement field, say $\boldsymbol{u}$, as a solution of Eq. (26):

$$\boldsymbol{\beta} = \operatorname{grad} \boldsymbol{u}. \tag{35}$$

We now argue that this equation, and together with it, also Eq. (34) cannot strictly describe the plastic deformation by dislocations. As a consequence, plastic deformation does not fit too well into continuum mechanics.

This problem was first investigated independently by Anthony (1993) and Kunin (1990) with practically identical results. The arguments are as follows:

Relation Eq. (34) implies that the body is built up from particles specified by $\boldsymbol{X}$. It is tacitly or expressis verbis assumed that these particles persist during the whole motion of the body. Just this assumption is invalid for the plastic deformation of crystalline bodies. Firstly, consider the choice that the particles $\boldsymbol{X}$ are identified with the atoms (or molecules) of the lattice. Now, to a large extent, the plastic deformation proceeds through the motion of groups of dislocations along the lattice planes. On its path, each dislocation causes a relative shift of the neighbouring atoms by one lattice distance. Since as a rule, groups of 20 or more dislocations pass along one glide plane, originally neighbouring atoms are separated through the dislocation motion by many atomic distances. This means that the motion of the atoms during plastic deformation is extremely discontinuous and in this picture not treatable in a continuum theory. Anthony et al. (1998) and Anthony and Azirhi (1998), speak of an "internal tearing", a rather vivid picture.

The only alternative I can think of is to declare infinitesimal volume elements as the particles of our body. This is in more accordance with the continuum picture. However, now the dislocations will pass through these new particles thereby destroying them such that a volume element in some current state cannot be identified materially with a volume element of any previous state. This means that there are no trajectories $\boldsymbol{\chi}$ that describe the motion of particles along any path, because such identifiable particles do not exist. Hence, the basic Eq. (34) together with Eq. (26) breaks down, and there is no continuum theory of elastoplasticity in the strict sense.

These findings are rather unfortunate because continuum mechanics is well developed and easy to handle. So one might ask oneself how big the error is when Eq. (34) or Eq. (26) are used inspite of their strict invalidity. There is some hope that this error is not too large since the separation of atoms resulting from the gliding of groups of dislocation is very small on the macroscopic scale, which is the scale of interest in many applications. In fact, 100 atomic distances which might be an upper limit for this effect is quite small on the macroscale. The fluctuations that arise from this effect are usually not mentioned, but they cause an uncertainty that is difficult to estimate. After accepting such a procedure Eq. (34) should be interpreted in a statistical sense: $\boldsymbol{\chi}$ would then be an average motion rather than a deterministic motion. Unfortunately, the statistical basis for this averaging is not very well defined.

7. Dislocation statistics

As is well known, the dislocation network under plastic deformation is very irregular, in fact random in the sense of probability theory. In the theory of Section 5, we had prescribed the course of all dislocations and from there calculated everything in a deterministic way. We now recognize that the former theory

should be interpreted as the deterministic microscopic theory which underlies the macroscopic statistical theory.

Within the frame of the statistical theory the dislocations, as other variables like stress, elastic and plastic strain, become random variables. We write $\boldsymbol{t}(\boldsymbol{x})\boldsymbol{b}$ for the value of the dislocation at point $\boldsymbol{x}$ where, as mentioned before, the dimensionless vector $\boldsymbol{t}(\boldsymbol{x})$ gives the line direction at $\boldsymbol{x}$, and $\boldsymbol{b}$ the constant Burgers vector. For the following investigation it is convenient to use $\boldsymbol{t}(\boldsymbol{x})\boldsymbol{b}$ as a measure of dislocation rather than to use the density $\boldsymbol{t}(\boldsymbol{x})\boldsymbol{b}\delta(\rho)$.

Except for very simple dislocation configurations, e.g. a few straight dislocation lines, it will be difficult to calculate stress and strain, given $\boldsymbol{t}(\boldsymbol{x})\boldsymbol{b}$, as functions of position in a deterministic theory. In fact, we deal here with a many-defect problem comparable in complexity with the many-body problem of solid state or particle physics. For this, special methods have been developed in statistical physics. In the following, we show how such methods can also be applied to our dislocation problem. We do this again by the example of the statistical theory.

Basic random objects in the physical particle theory are for instance the electrons which often distribute themselves over random positions in the solid. In our many-defect problems with dislocations the objects are described by $\boldsymbol{t}(\boldsymbol{x})\boldsymbol{b}$, and are also distributed at random in the body. There is a constraint that must be observed later in the practical calculations, namely the constraint that dislocations do not end in the interior of the body, but rather are nonending lines (therefore $\operatorname{div}\boldsymbol{\alpha} = 0$). Since we are up to a statistical theory, we use the ensemble picture. Hence, we do not look at a single specimen, but study the behaviour of an ensemble consisting of many, many repetitions of the original (real) system. We perform the same experimental test on all these repetitions and use the results to say something about the average behaviour of the ensemble.

The basic experimental test consists in the measurement of $\boldsymbol{t}(\boldsymbol{x})\boldsymbol{b}$ at a point $\boldsymbol{x}$ in each member of the ensemble, such that $\boldsymbol{x}$ is a common point for each member, i.e. the coordinates of $\boldsymbol{x}$ remain the same when going from one member to the next. Having done that with point $\boldsymbol{x}$, which we now also call $\boldsymbol{x}_1$, we do the same with points $\boldsymbol{x}_2, \boldsymbol{x}_3$, etc. Often, however, it will not be necessary to do this with more than one point, namely, when we know that the specimen is statistically (or macroscopically) homogeneous. In that case, we expect the same result in the following average procedure which gives us the ensemble average $\langle \boldsymbol{t}\boldsymbol{b} \rangle$ over the numerical results of the measurements at the various members of the ensemble.

To arrive at a manageable statistical theory it is necessary to assume the validity of an ergodic hypothesis which in our case (statics) states that the volume average of a random function equals the ensemble average of the same function. In mathematical language,

$$\bar{f}(\boldsymbol{x}) \equiv \frac{1}{\Delta V}\int_{\Delta V} f(\boldsymbol{x})\,\mathrm{d}V, \quad \langle f(\boldsymbol{x})\rangle \equiv \lim_{N\to\infty}\sum_{N} f(\boldsymbol{x}). \tag{36}$$

(volume average) (ensemble average)

Here $f(\boldsymbol{x})$ is the basic random function, ΔV is the representative, or macroscopic, volume element which is infinitesimal on the macroscale, but very large on the microscale. N is the number of members in the statistical ensemble on which the test measurements are performed.

The literature on statistical physics is full of discussions of the ergodic hypothesis so that we can renounce a longer exposition on this subject. Qualitatively, the following statement is valid: physical systems obey the ergodic hypothesis when the situation is *sufficiently* random. That means for instance that we cannot expect an ergodic situation when the disorder in the systems consists of small deviations from order, e.g. if we have a chessboard pattern with slight disturbances.

We shall now try to become more acquainted with the ergodic theory by considering some examples. The random function is represented by the numerical values at the points in the members of the ensemble, i.e. by the values of the dislocation tensors $\boldsymbol{t}(\boldsymbol{x})\boldsymbol{b}$. For simplicity we consider only one Burgers vector $\boldsymbol{b}$,

which is constant in our dislocation network. That means the random variable proper is $\boldsymbol{t}(\boldsymbol{x})$. In the microscopic picture $\boldsymbol{t}$ will vary widely from point to point. In particular, $\boldsymbol{t}$ may also equal zero. Note that $\boldsymbol{t}(\boldsymbol{x})\boldsymbol{b}$ is not a dislocation density but gives the numerical values of the dislocations themselves at the points $\boldsymbol{x}$.

Taking the ensemble average of $\boldsymbol{t}(\boldsymbol{x})\boldsymbol{b}$ as defined in Eq. (36) we have, with constant $\boldsymbol{b}$

$$\langle \boldsymbol{t}(\boldsymbol{x})\boldsymbol{b}\rangle = \langle \boldsymbol{t}(\boldsymbol{x})\rangle \boldsymbol{b}. \tag{37}$$

To calculate this we must know the components of $\boldsymbol{t}(\boldsymbol{x})$. Since $\boldsymbol{t}(\boldsymbol{x})$ is a unit directional vector tangential to a dislocation line which can point in any direction, we can specify $\boldsymbol{t}(\boldsymbol{x})$ in terms of its components

$$(t_1, t_2, t_3) = (\sin\vartheta\cos\varphi, \sin\vartheta\sin\varphi, \cos\vartheta), \tag{38}$$

where ϑ and φ are spherical coordinates.

Of course, we shall never know the values of ϑ, φ at all points in the specimen. This implies that we never shall know the microscopic dislocation distribution in the medium, except when we prescribe it in some model picture. Nevertheless, one important result can be established without calculation. If the network is macroscopically isotropic and homogeneous, then the components t_1, t_2 and t_3 of $\boldsymbol{t}$ will be equal in the average. Herefrom, it follows that in this case $\langle \boldsymbol{t}\rangle = 0$, the macroscopic dislocation value in zero. A similar situation was mentioned already in Section 5.

The findings of the last paragraph constitute a rigorous, but not very helpful partial solution of our problem. Another, maybe a bit more useful solution will be described now.

8. Correlation functions

For the next consideration we need an important concept of statistical physics, namely the concept of correlation function. We assume that this concept is not completely strange to the reader. Therefore, we shall keep short the explanations referring to this. The tests relevant to the concept are an extension of the tests introduced in the last section. Instead of making measurements at one point $\boldsymbol{x}$ (or $\boldsymbol{x}_1$) in all members of the ensemble, we now make *simultaneous* measurements at two points, multiply the outcomes in each member and take the ensemble average. We obtain for a random variable $f(\boldsymbol{x})$, say

$$\langle f(\boldsymbol{x}_1) f(\boldsymbol{x}_2)\rangle \equiv \langle f(\boldsymbol{x}_1) f(\boldsymbol{x}_1 + \Delta\boldsymbol{x})\rangle, \quad \Delta\boldsymbol{x} = \boldsymbol{x}_2 - \boldsymbol{x}_1. \tag{39}$$

This result is a macroscopic function of $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$, and can also be written in the form:

$$\int f_1 f_2 P_2(f_1, f_2)\,\mathrm{d}f_1\,\mathrm{d}f_2. \tag{40}$$

Here P_2 is the two-point probability density. $P_2\,\mathrm{d}f_1\,\mathrm{d}f_2$ is the probability for finding f in the range $\mathrm{d}f_1$ around f_1 and simultaneously in $\mathrm{d}f_2$ around f_2, when performing the mentioned test. Expressions (39) and (40), whose identity we shall not prove here, are known as two-point correlation functions.

In an analogous way, one may define three-point, four-point etc. generally q-point correlation functions. The three-point function is for instance

$$\langle f(\boldsymbol{x}_1) f(\boldsymbol{x}_2) f(\boldsymbol{x}_3)\rangle, \quad \text{or} \quad \int f_1 f_2 f_3 P_3(f_1, f_2, f_3)\,\mathrm{d}f_1\,\mathrm{d}f_2\,\mathrm{d}f_3, \tag{41}$$

and the correlation functions of higher order read correspondingly. They all together establish the complete (infinite) set of correlation functions if, for reason of convenience, we declare the function $\langle f_1\rangle$ as the one-point correlation function. The great importance of the correlation functions rests on the following two properties. (i) Since the correlation functions connect points such as $(\boldsymbol{x}_1, \boldsymbol{x}_2), (\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3)$ etc. of the ensemble, they play a distinguished role in theories of the interaction of particles, defects, etc. (ii) The full set

of correlation functions (including that for $q = 1$) gives the complete macroscopic information for the random variable in question, if certain criteria for convergence are fulfilled. This result is a consequence of the fact that by definition all correlation functions are also ensemble averages. The complete macroscopic information is less than the microscopic one which gives the value of the random variable at each point in the real specimen in a deterministic way.

Note that in the present investigation, we restrict ourselves to two scales, namely microscopic and macroscopic. In many practical problems, more than two scales must be regarded, and then the situation becomes much more involved. As an example consider polycrystalline aggregates, in which traditionally one distinguishes between three scales for the stresses, the stresses of the first, second and third kind. The first of these stresses is the macroscopic one, the second one that of the grains and the third one relates to microscopic fluctuations as caused by dislocations and other defects. If we deal with single crystals rather than with polycrystals, then the stresses of second kind are absent. This is the case of the two-scale statistics, which we shall treat furthermore.

We now discuss the role of the two-point correlation function in the dislocation description. As before, our random variable will be $\boldsymbol{t}(\boldsymbol{x})\boldsymbol{b}$. Then, according to the previous definition, the two-point correlation function is

$$\langle t_i(\boldsymbol{x}_1) b_j t_k(\boldsymbol{x}_2) b_l \rangle, \tag{42}$$

where again we take $\boldsymbol{b}$ as a constant vector. $\boldsymbol{t}$ is defined as in Section 6. As a fourth rank tensor which relates to two points ($\boldsymbol{x}_1$ and $\boldsymbol{x}_2$) Eq. (42) is a complicated object. We simplify our task by considering only a scalar part of Eq. (42), i.e. a part which is invariant with respect to the coordinate transformation. This is the so-called autocorrelation function

$$\langle t_i(\boldsymbol{x}) b_j t_i(\boldsymbol{x}) b_j \rangle = b^2 \langle t_i(\boldsymbol{x}) t_i(\boldsymbol{x}) \rangle = b^2 \langle t^2(\boldsymbol{x}) \rangle, \tag{43}$$

where $b = |b|$ and $t = |t|$.

According to the definition of the ensemble average, we have

$$\langle t^2(\boldsymbol{x}) \rangle = \lim_{N \to \infty} \sum_N \frac{1}{N} t^2(\boldsymbol{x}). \tag{44}$$

Now, $t^2(\boldsymbol{x}) = 1$ because $\boldsymbol{t}$ is a unit vector. The sum in Eq. (44) goes over the members of the ensemble. Depending on whether a dislocation passes through the point $\boldsymbol{x}$ of an ensemble member or no dislocation is at $\boldsymbol{x}$, the contribution of the member to the sum is 1 or 0. Let n denote the number of positive events in the sum over the members, then the sum is equal to n and the chosen invariant of the two-point correlation function becomes

$$(n/N) b^2, \tag{45}$$

where for practical purposes N needs not to be infinity, but should be large so that the averaging has a meaning. Note that n in Eq. (45) depends on the chosen size of N, so that for large N, Eq. (45) does practically not depend on N.

Obviously, n/N is the probability of finding that a dislocation goes through some point $\boldsymbol{x}$. If the distribution of dislocations is macroscopically homogeneous, then n/N is the same for each $\boldsymbol{x}$.

In the derivation of Eq. (45) we have utilized the ensemble theory. It is also possible, and for the interpretation perhaps useful, to work with the volume averages. For convenience we divide the specimen into a great number M of atomic cells of size b^3. If m is the number of cells met by a dislocation and $\bar{l}$ is the average length within a cell of such a dislocation, then obviously the total length of all dislocations in a volume of size Mb^3 is

$$L = m\bar{l}. \tag{46}$$

Since the volume average equals ensemble average, the invariant part of the two-point correlation function can be written as

$$k_0 \equiv \overline{t_i(\boldsymbol{x})b_j t_i(\boldsymbol{x})b_j} = \frac{1}{Mb^3}\left(\sum_{\text{cells}} t^2\right) b^5 = \frac{1}{Mb^3} m b^5 = (m/M)b^2, \tag{47}$$

very close to Eq. (45). Inserting m from here into Eq. (46) we obtain

$$L = M\bar{l}k_0/b^2. \tag{48}$$

This is the total length of all dislocations in the volume Mb^3. Since $M, \bar{l}, b$ do not change during the experiment, we find that L is given essentially by the autocorrelation function k_0 of the dislocation distribution. This result is remarkable, because L is heuristically found, long used measure of the dislocation state. It represents a state quantity in the sense of thermodynamics since it can be measured, e.g. by electron microscope, without knowing anything about the past of the specimen.

L, often also named ρ, is frequently used in theories with dislocations. It is a convenient measure of the dislocation density. Its increase under deformation implies the densification of the dislocation network. But as a single scalar function it is of course a very modest description of the network. In fact, a complete (macroscopic) description would require not a single correlation function, but the whole set of correlation functions of the order $q = 1$ to ∞. This means that the number of internal variables of such a medium is infinite, in a strict sense, as surmised early by Drucker (1960).

Of course, nobody likes to handle an infinite number of variables. Fortunately, experience with statistical physics tells us that in normal situations the significance of the correlation functions decreases with increasing order, so that for many problems it should suffice to include correlation functions upto the order of 2, 3 or 4.

Physicists are used to deal with complex statistical problems and have developed sophisticated methods for this. In particular, correlation functions are introduced in many disciplines of physics. Their value rests not only on their theoretical treatability, but also on their experimental accessibility.

9. Micro- and macrodescription

So far we have discussed a microscopic and a macroscopic picture of the dislocation state. In the microscopic picture the dislocation state is described deterministically and completely by the values of $\boldsymbol{tb}$ over the whole specimen. In the macroscopic picture, ensemble averages which are used in a systematic way give finer and finer details about the macroscopic dislocation distribution. The outstanding tool for this is found in the concept of dislocation correlation functions of order 1 to ∞. Both $\boldsymbol{tb}$ and the correlation functions are state variables in the sense of general thermodynamics because they permit measurements without any knowledge of the past.

Both $\boldsymbol{tb}$ in the microtheory and the q-point correlation functions, say k_q $(q = 1 \ldots \infty)$ in the macrotheory play the role of dynamical variables in the two theories, and the k_q are ensemble averages. At the same time, they are independent variables to be used in the energy expression if one wants to develop a dynamical theory. To this end, several researchers have proposed the Lagrange formalism, but encountered various difficulties. I mention recent work of Maugin (1993), Naghdi and Srinivasa (1993, 1994), Le and Stumpf (1994), Anthony et al. (1998) and Anthony and Azirhi (1998). Most serious is perhaps that the Lagrange formalism was not invented to treat problems with dissipation. Maybe a proposal of Anthony might help here. Anthony et al. (1998) and Anthony and Azirhi (1998), introduce complex fields instead of the real physical fields, for instance ψ for T, the temperature, where ψ has some analogies to the complex Schrödinger ψ-function. It is perhaps too early to give a final judgement for this proposal.

The other great problem consists in the necessity for a good description of the dislocation state. In the microscopic approach we have ***tb***. But only when this is simple enough, e.g. for straight dislocations, will a solution be possible. This is in fact the reason why we try to develop a macroscopic theory. Such a theory is certainly simpler than the deterministic (microscopic) theory, but still too complex as to do something useful with it. Except perhaps, if one omits the correlation functions of higher order and satisfies oneself with the remaining functions, e.g. k_1, k_2. A step to a better description was done by Anthony who, as others, proposes to describe the (macroscopic) dislocation state by giving separate numbers for each type of glide system, e.g. 12 numbers L_1–L_{12} which represent the total lengths of dislocations in the unit volume, but now per glide system. Unfortunately, already in this case, where the description of the dislocation state is still rather poor, results a quite involved calculation.

Today, statistical problems are often solved by numerical methods. Under certain presuppositions it then suffices to make a calculation with only one realization (member) of the ensemble. The number of included points with ***tb*** should then be very large. For instance when developing such an algorithm one could methodologically profit a lot from the molecular dynamics. A specific difficulty however will remain, namely that the ***tb***'s have to connect themselves along lines that do not end in the interior of the body. This problem requires a theory for itself.

10. The response problem

In the (linearized) theory of elasticity the potential energy density W is a function, in more complex situations (e.g. nonlocal theory) a functional, of the elastic distortion

$$W = W[\beta^{\mathrm{e}}_{ij}]. \tag{49}$$

A more complex situation prevails also when we introduce the dislocation density $\boldsymbol{\alpha} = \operatorname{curl}\boldsymbol{\beta}$, as in Section 5. The form of $\boldsymbol{\alpha}$ suggests that we use, in addition to $\boldsymbol{\beta}$, also $\operatorname{curl}\boldsymbol{\beta}$ as independent variable in W. A linearized theory results when W is quadratic in the independent variables. That means we use

$$W = A\beta^2 + B(\operatorname{curl}\beta)^2, \tag{50}$$

where A, B are constant material tensors. For simplicity we have omitted a term mixed in $\boldsymbol{\beta}$ and $\operatorname{curl}\boldsymbol{\beta}$. In the following coarse estimate we assume that A and B are of the similar order of the magnitude. Comparing the dimensions, we note that $\boldsymbol{\beta}$ is dimensionless and $\operatorname{curl}\boldsymbol{\beta}$ has the dimension $1/\text{length}$. This means that the second energy term in Eq. (50) contains a factor $1/l^2$ when compared with the first one. This factor is related to the distance between dislocations which in typical cases is of the order 10^{-4} cm. So the second energy term contains a quantity of the order 10^{-8} cm^2 that is very small on the macroscale. For this reason the dislocation term in Eq. (50) is usually omitted. However, the reality of dislocations in plastically deformed solids is different. Due to their strong far-reaching interactions, dislocations form particular locally varying low energy arrangements so that the first part of the energy decreases distinctly. The two energy terms then become of the same order of magnitude so that none of them may be neglected.

Response quantities are usually defined as the variational derivatives of the energy density W with respect to the independent variables. In our case,

$$\sigma_{ij} = \delta W/\delta\beta_{ij}, \quad \tau_{ij} = \delta W/\delta(\operatorname{curl}\beta)_{ij}. \tag{51}$$

Obviously, τ_{ij}, the specific response to a dislocation density, has the dimension of a moment stress.

We had argued before that in the macroscopic theory, the tensor $\boldsymbol{\alpha}$ of dislocation density misses an essential part of the dislocation distribution. Therefore, also the response quantities as defined in Eq. (50) will be incomplete when Eq. (50) is understood as macroscopic. To obtain a more complete description of

the macroresponse, here we can also introduce the correlation functions this time on the stress side of the theory.

If Eq. (50) is interpreted as equation of the microscopic theory in the deterministic approach, then $\boldsymbol{\beta}$ and $\boldsymbol{\alpha}$ represent completely the geometric (or kinematic) degrees of freedom. Then also $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$ are a complete description of the static response. $\boldsymbol{\tau}$ will be zero where $\boldsymbol{\alpha} = 0$, that means, $\boldsymbol{\tau}$ will be nonzero only along the delta lines of the dislocations. This is an exact statement for our model with delta function. Of course, this picture is not consistent with the real world, namely that our crystals possess a smallest, but finite length, the lattice parameter. This fact was taken into account by Peierls (1940) who was able, by a nonlinear model, to calculate the dislocation core. In our context, it is remarkable that the theory of Peierls contains a moment stress as the response quantity (Kröner, 1992). This supports our finding that moment stress is the specific response to the presence of a dislocation density. This fact establishes a certain proximity between dislocation theory and the theory of Cosserat media, and this has been investigated by various authors, e.g. Epstein and de León (1994, 1995). Not everything is clear, however.

11. Conclusion

In our presentation of the continuous theory of dislocations, we have discussed problems that must be kept in the mind of those who are up to the development of a theory that permits macroscopic applications in the field of elastoplasticity of solids. We have restricted ourselves to the deformation of crystalline solids, a field which in itself is huge so that many problems had to be omitted.

Elastoplastic deformation has an immense potential for practical applications. In this respect, it can be compared with the theory of electromagnetism. Here, one knows that all electromagnetic phenomena have to fit into the frame of Maxwell's equations. It is then suggestive to look for a set of equations that have to be obeyed in all processes of elastoplastic deformation. These equations could be comprised under the name elastoplastodynamics. We know, however, that the elastoplastic deformation proceeds by the motion of defects, essentially dislocations, so that also dislocation dynamics would be a good name. Since the behaviour of crystalline matter is determined by many defects, one may also speak of a many-defect theory, in analogy to many-particle or many-body theories in other parts of physics.

When developing a dynamical theory it is important from the beginning to specify the degrees of freedom of the considered physical system. In a way, this then defines the problem that one is going to treat. In our case, we know that dislocations play a decisive role in the elastoplastic deformation of crystalline bodies. We also know that the distribution of the dislocations has a great influence on the state of the medium. This implies that it is possible to introduce certain dislocation-related quantities as state variable beside the elastic strain. The question is whether this leads to a complete representation of the state on the geometrical, or kinematical, side. We have seen that this is in fact possible. A closer inspection shows us, however, that this is possible only under one condition, namely that no point defects migrate. Indeed, when they do migrate they help to change the state of the body and, therefore, have to be included as (internal) dynamical variables.

Contrary to the dislocations point defects move under thermal activation and therefore their motion is restricted to higher temperature. Now, dislocations are able to move in glide planes, but also out of glide planes, a motion known as climb. For topological reasons this motion is possible only if at the same time point defects are created or annihilated. Hence, at higher temperature the system gains degrees of freedom, namely those of the point defects. The situation is again similar to that of electrodynamics. At high energy supply, the system gains the new degrees of freedom of the weak interaction. That means that electrodynamics in itself is not a closed theory since it gains new degrees of freedom at high-energy supply.

In the mechanical analogue, high temperature implies high energy supply, and again this leads to new degrees of freedom. That means that the pure dislocation theory of elastoplasticity is valid only at suffi-

ciently low temperature. Of course it has been attempted to introduce point defects into the theory, which, however, does not become simpler in this way. Thus, we have omitted that.

Also omitted in this article is the dynamical part of the theory, because a convincing such theory does not exist. There is some hope, however, that the so-called gauge field theoretical approaches discussed at late will bring progress for the dynamic theory of defects. Gauge theoretical methods have been most utile in fundamental physical field theories. The first person who proposed to apply such methods to the defect problem in solids seems to have been Turski (1966). For quick information to the reader, we give in the following the titles of a few relevant papers or books on gauge theories: *Variational principle for equilibrium and incompatibility equations in dislocation theory* (Turski, 1966), *On the gauge transformation admitted by the equations of defect dynamics* (Golebiewska-Lasota and Edelen, 1979), *A gauge theory of dislocations and disclinations* (Kadić et al., 1983), *Gauge theory and defects in solids* (Edelen and Lagoudas, 1988), *Gauge theories in mechanics* (Kunin and Kunin, 1986), *Gauge theories and densities of topological singularities* (Dzyaloshinskii and Volovick, 1980), *Elastic behaviour of crystalline solids: A dynamic gauge model* (Popov, 1994), *Gauge fields in condensed matter* (Kleinert, 1989).

In these works, the results of the older defect theories were widely confirmed. Further work however is needed to bring the dynamic theory in a good state. So far, solved problems of moving dislocations are restricted essentially to single dislocations whose motion is prescribed. Wanted is then for instance to learn about the radiation of sound waves from these dislocations. Typical problems of this kind were treated by Callias and Markenscoff (1988) e.g. on singular asymptotics of integrals and the near-field radiated from nonuniformly moving dislocations (Callias and Markenscoff, 1988). This has to do with the damping or dissipation of moving dislocations and therefore deserves some attention also for elastoplastic deformation. On the other hand, it is certainly remote from the dynamics of a dislocation network, which must include creation and annihilation of dislocations. One of the great problems is obviously the development of the dislocation state under the elastoplastic deformation. For instance, it is observed that under large deformations the dislocations develop complex patterns on a mesoscale, i.e. between macro and micro (Mughrabi et al., 1979; Walgraef and Aifantis, 1985; Woo and Frank, 1987). Typical are cell patterns, ladder patterns and many others. A good theory should be able to predict such sequences of patterns that have a great influence on the properties of the material. For this problem, methods have been developed which resemble those in the field of synergetics, or self-organization or chaos.

Omitted is also the differential geometry of defects which was initiated independently by Kondo (1952) and by Bilby et al. (1955) in the fifties (also my own presentation of this topic Kröner (1981)). The great finding of these authors was that Cartan's circuit in differential geometry, by which Cartan defined the *torsion* of a space, is just the continuum version of the discrete circuit defining the Burgers vector in crystal physics. This cognition allows one to utilize the powerful complex mathematical formalism of differential geometry also to dislocation problems. It is interesting to note that the differential geometry of affinely connected spaces is particularly adapted to describe crystalline materials. For this reason the gauge theories of defects are often formulated in the language of differential geometry which also permits to draw analogies to fundamental physical field theories like gravitation or cosmical string theories. For a recent comprehensive survey on this see Hehl and coworkers (1995).

Unfortunately, the differential geometry of dislocations suffers from the same shortcomings as does the more conventional theory. Above all, Cartan's torsion tensor, identified as the tensor of dislocation density, is an average quantity only. Hence, the main impediment of the application of this formalism is again the complexity of the internal mechanical state (the defect state). Nowadays, the part of differential geometry which has to do with torsion (dislocations) is called Riemann–Cartan geometry. The general differential geometry of affinely connected spaces has in addition to Riemann–Cartan geometry the *nonmetric* degrees of freedom. These again are fully adapted to describe point defects in crystalline matter, as was recognized by Bilby et al. (1957). To understand this, note that the crystal is a perfectly metric body in which distances are measured by counting atomic steps along the lattice lines. The presence of point defects, however,

implies that when counting lattice steps one encounters, from time to time, a point defect which obviously disturbs the counting, thus, the measurement of distances. This effect was made quantitative by Kröner (1990).

Major part of this article was concerned with geometry or kinematics. However, there exists an interesting development in statics which, in the sense of Hamilton's mechanics, is dual to the geometrical theory. Originally, Schaefer (1953) established an analogy between the static part of elasticity theory and (linearized) Riemannian geometry. Stojanović (1963) and Kröner (1963) showed that this analogy continues when moment stresses, as occur in dislocation theory, are introduced. Instead of the Riemann curvature tensor one then needs the (linearized) Riemann–Cartan curvature tensor formed with the linear connection containing torsion.

Ben-Abraham (1970) realized that the analogy goes much further, namely is valid also when point defects are introduced, i.e. the geometry is built with a connection containing torsion and "nonmetricity". Ben-Abraham found in particular that the statical equilibrium conditions of the theory with dislocations *and* point defects have the form of the Bianchi identities of the general curvature tensor. This establishes a new differential geometry on the statical side of the theory. Here the stress functions χ_{ij}, considered in Section 3 in a linearized form, play the role of the metric tensor. One realizes that in this formalism, the geometry and the statics of the defect theory have the status of mutually *dual* formulations. The fact that all this is valid for arbitrary large stress and strain was shown by Kröner (1987). Kleinert (1989) has utilized the duality for the development of his so-called double gauge theory. He also proposed to take care of the discreteness of real dislocations by some quantization procedure, an attractive thought.

In this article it was not our aim to develop a complete theory of the elastoplastic behaviour, in particular of crystalline matter. This would have been impossible because the final, fully developed theory does not exist. Instead, we wanted to show that the existing theory, on the benefit side, permits the solution of many important problems, in particular the treatment of the interaction of dislocations. A convenient tool for this is the microscopic theory of dislocations (Section 5) which also acts as the basis for the later treatment of dislocations as random variables.

We also wanted to show the obvious shortcomings of the present theory of elastoplasticity. The greatest shortcoming is that the dislocation density tensor $\boldsymbol{\alpha}$, no matter whether introduced through differential geometry or in the conventional way, measures the *average* dislocation density only and therefore, regards the internal mechanical state utmost incompletely. In principle, this shortcoming could be overcome by reorientation of dislocation theory towards a statistical theory, but only with highest expenditure of computation. Is it worthwhile to try that?

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