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ELASTICITY THEORY OF MATERIALS WITH LONG RANGE COHESIVE FORCES*

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Abstract—The strain energy of a deformed material with spatial interaction can be written either in a differential (*multipolar*) form, i.e. as a single volume integral containing displacement gradients up to infinite order, or in an integral (*non-local*) form, e.g. as a double volume integral summing up the interactions of pairs of mass elements. The linear theory is derived from lattice theory and the following insights have been gained: (1) The differential theory, though in principle applicable to any (analytic) elastic long range problem, is mainly convenient in describing range effects on a very small (nearly atomic) scale. (2) The effects of the electric cohesive forces can be comprised in the two-point material tensors (kernels) of the non-local theory. In this way, the macroscopical theory becomes purely elastic. (3) Van der Waals cohesive forces give rise to elastic range effects under certain inhomogeneous stress conditions, in particular in defect interaction and diffusion problems.

1. INTRODUCTION

THE two most important classical approaches to the mechanical behaviour of solids are the mass point approach—especially the atomic lattice theory—and the continuum theories, e.g. elasticity theory. As is well-known, the theory of elasticity‡—in contrast to lattice dynamics—is based on the concept that the response (or internal) forces of the body are contact forces, i.e. have a zero range.§ This means a certain limitation for the applications since the cohesive forces in real materials have a finite or even infinite rather than a zero range.

The range of forces and the continuity of matter are two different concepts. It therefore appeared promising to attempt a "non-local" elasticity theory, i.e. a continuum theory which takes into account the finite range of the cohesive forces [2, 3]. As will become clear later in this work, the theory is closely related to the multipolar elasticity theory of the first kind proposed by Green and Rivlin [4, 5]. Lattice theory takes into account a finite range of the interparticle forces from the very beginning. This fact suggests to derive the mentioned non-local elasticity theory directly from the lattice theory. By such a procedure one obtains not only the macroscopic form of the theory but also the material properties expressed in terms of interparticle potentials which are relatively well-known for many materials. In this way a reasonable estimate can be given of the size of the expected effects.

The here implied task of a rigorous conversion of lattice theory into a continuum theory has been treated successfully by Krumhansl [6]. This author arrives at a generalization of elasticity theory which is characterized by the occurrence in the internal energy of

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‡ We restrict ourselves to elastic phenomena in this paper. The possibility for extension to non-elastic phenomena of the present ideas is seen immediately.

§ This important aspect of elasticity theory is discussed in [1], p. 225 ff.

displacement gradients up to infinite order. This theory is equivalent to the (linear) multipolar elasticity theory of the first kind of [4].

Whereas Krumhansl was concerned with situations in which the (multipolar) internal energy sum converges rapidly we shall focus our investigation on situations where this does not apply. In such cases the differential theory considered in Section 2 is replaced conveniently by an integral theory as explained in Section 3.

The main part of Section 2 is concerned with questions of convergence in the (linear) differential theory. For simplicity, the investigation is performed in one dimension. It will be apparent from our treatment that the main results of this investigation apply correspondingly in three dimensions, too.

The integral theory of Section 3 goes beyond the representation in [3] in so far as boundary conditions are considered explicitly and as the role of higher displacement gradients in the long range energy expression is clarified.

Among other things, the problem of self-strain under non-local conditions is discussed in Section 4. Section 5 contains concluding remarks referring in particular to actual material behaviour.

2. THE DIFFERENTIAL THEORY

In this section we consider the one-dimensional problem. We imagine a crystal the atoms of which are displaced in x-direction by amounts $u(x)$ which do not depend on the other cartesian coordinates y and z. For the sake of simple language we shall speak of a "chain of identical particles" at equidistant points x in the reference state, but we keep in mind that these "particles" are lattice planes rather than mass points. The force law between two particles at x and x' shall depend on their distance $|x'-x|$ alone. The (statical part of the) increase in internal energy by an elastic deformation, i.e. the strain energy, is, in the framework of linear theory,

$$E = \frac{1}{2} \sum_{x,x'} \Phi(|x'-x|)(u'-u)^2 \tag{1}$$

where $u' = u(x')$ and the coupling parameters $\Phi(|x'-x|)$ contain the material information.

The question under which circumstances long range interactions have to be included can be discussed directly by use of equation (1). Consider an asymptotic behaviour of Φ as $|x'-x|^{-m}$ (m positive, finite, integer). For a homogeneously strained crystal ($u = ax$) the strain energy becomes

$$E = \frac{a^2}{2} \sum_{x,x'} \frac{1}{|x'-x|^{m-2}} \tag{2}$$

which shows that farther distant particles contribute essentially to the energy if $m \leqq 3$. Van der Waals interactions are characterized by $m = 5$.* Hence they are, so to speak, short range under homogeneous strain. In contrast to this, the increase in interaction energy $e(x)$ of one particle with all the others diverges for the infinite chain with $m = 3$.†

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* The interaction energy of two induced dipoles at distance r decays as r^{-5} and the 3-dimensional coupling parameters as r^{-7}. The one-dimensional parameters are obtained by integration over y, z, hence the decay as $|x'-x|^{-5}$. [See the *Note added in proof* (i) at the end of the paper.]

† The same applies for the interaction energy itself. As a consequence of this, infinite crystals of this kind would not be stable. A different question is whether materials with such interactions ($m = 3$) do exist or not. If they do exist they at least do not belong to the main standard types.

Consider now a sinusoidal displacement field $u = u_0 \cos kx$. By use of simple trigonometric formulas one obtains for $e(0)$, e.g.

$$e(0) = u_0^2 \sum_{x'} (\cos kx' - 1)^2 / |x'|^m. \tag{3}$$

Here, the largest contribution is not from neighbour particles but, as one finds, from particles at approximate distance $\lambda/4$ for $m = 3$, e.g. which is a macroscopic distance if the wave length λ is macroscopic. This result shows that a non-local theory is adequate for treating wave propagation in this type of crystal.

In the case of Van der Waals interaction ($m = 5$) the contribution to $e(0)$ decreases monotonically, but slowly, with distance $|x'|$ which shows that no big range effects are expected for wave propagation in Van der Waals crystals. A more thorough investigation (Appendix 2), nevertheless, reveals that range effects are not always negligible in crystals with Van der Waals interactions.

We now return to the theory. Following Krumhansl we imagine a continuous displacement field $u(x)$ which at the lattice points assumes the values u of the displacements of the particles concerned. The displacement u' in (1) can now be developed into a Taylor series around point x by which equation (1) becomes

$$E = \frac{1}{2} \sum_x \sum_{p,q=1}^{\infty} C^{(pq)} u^{(p)} u^{(q)}, \tag{4}$$

$$C^{(pq)} = \sum_{x'} \Phi(|x'-x|)(x'-x)^{p+q}/p!q!. \tag{5}$$

In equation (4) the p-th derivatives of u are denoted by $u^{(p)}$.

If the particle chain is of infinite length then the summation over x in equation (5) can be converted exactly into the corresponding integral:

$$E = \frac{1}{2h} \int \mathrm{d}x \sum_{p,q=1}^{\infty} C^{(pq)} u^{(p)} u^{(q)} \tag{6}$$

where h is the lattice parameter.

In the finite chain small additional terms would appear according to the Euler–Maclaurin sum formula. We shall consider these terms in the next section.

Equation (6) together with the values (5) of the elastic parameters $C^{(pq)}$ can be considered the basis of a one-dimensional multi-polar elasticity theory (of the first kind) of materials of the space differential type, speaking in the terminology of Green and Rivlin [5]. The work of Krumhansl implies that the solutions of the continuum theory derived with the aid of equation (6) are exact solutions also of the lattice theory based on equation (1).

Of course, this continuum theory can only work if the energy in the form (6) converges. Two sources of divergencies can easily be imagined: (a) the sums in (5) giving the elastic parameters $C^{(pq)}$ can diverge and (b) the sum in equation (6) can possibly diverge even if the $C^{(pq)}$ are finite. (a) The sums in (5) can only diverge if the chain is infinite (assuming that Φ is finite at all lattice points). In the infinite chain any Φ ($|x'-x|$) the asymptotic behaviour of which is given by $|x'-x|^{-m}$ will cause a divergence of those elastic parameters $C^{(pq)}$ for which $p+q-m \geqq -1$. Hence these divergencies also occur in the case of Van der Waals forces and stronger decay (but not with an exponential force law). For many strain states the various divergencies in the sum will cancel under a Van der Waals law. In the other cases, the infinite body is a bad image of the real finite body with the corresponding strain: long range forces are now important also in Van der Waals crystals (Appendix 1, 2). (b) As shown in Appendix 1, the strain energy per unit length of a sinusoidal displacement field of wave length λ in a finite chain of finite power m converges for $\lambda > 2h$ (probably for $\lambda = 2h$, too) when calculated from equations (5), (6). This result is satisfactory because in a chain of lattice parameter h the smallest physically meaningful wave length is $2h$. A similar result applies for an exponential displacement field. Since any reasonably behaved displacement field can be built up by superposition of sinusoidal or exponential displacements this means that—with the above restriction—the strain energy per unit length as calculated from equations (5), (6) is always convergent.

For waves in a Van der Waals crystal we have calculated from equations (5), (6) the contributions to the energy of the displacement gradients of various order. Even for macroscopic wave lengths one finds higher order contributions which are larger than the energy due to the first gradient (the ordinary elasticity term). However, this is no physical effect. It rather has to do with the fact that the Taylor series of a sinus converges very slowly. In fact, the higher gradient contributions cancel to the largest extent if one includes a sufficient number of them.

The slow convergence in this case only occurs when one includes formally interactions over large distances, i.e. if one extends the x'-sums in equation (5) over all particles, as it was meant in this formula. In reality, only near neighbour interactions contribute essentially (see also appendix). If we restrict to these in equation (5) then we obtain a rapid convergence for the wave in the Van der Waals crystal. Only for wave lengths comparable to the lattice parameter can a contribution to the energy of the second or third displacement gradient possibly be detected, as was pointed out by Krumhansl. One could call the latter effect a "true" or "physical" multipolar effect, in contrast to the "apparent" or "mathematical" effect due to the poor convergence of the Taylor series of a wave.

We learn from this consideration that the energy expression (5), (6) is, in general, not a convenient starting point for handling wave problems even though it finally leads to correct results. The multipolar theory is only convenient when fast convergence of the energy expression is secured. This occurs certainly very seldom in materials with basically long range interactions. Instead of going from equation (1) to equations (5), (6) by use of a Taylor expansion, one treats these materials better by converting directly equation (1) into a continuum form. In this way one arrives at the theory originally called "non-local" by the author [2]. We shall see how this theory can be derived from the lattice theory in a rather rigorous way. In contrast to sums, integrals are easily treated in three dimensions. Hence we develop everything in three dimensions from now on.

3. THE INTEGRAL THEORY

We consider a primitive cubic crystal which allows us to use cartesian coordinates x_i in a very simple manner. Derivatives are written in comma notation or by using the symbol $\partial_i = \partial/\partial x_i$. The results can easily be generalized as to apply to any Bravais crystal. It is wise to limit oneself to Bravais lattices because in non-primitive structures multipolar effects of "not the first kind" come in which are better treated separately.

The three-dimensional analogue to equation (1) is in our example the formula

$$E = \frac{1}{2}\sum_{\mathbf{r},\mathbf{r}'} \Phi_{ik}(\mathbf{r}-\mathbf{r}')(u_i'-u_i)(u_k'-u_k) \tag{7}$$

in an obvious notation, where $\Phi_{ik} = \Phi_{ki}$. We split the cohesive forces into a short range part treated by the differential theory and a long range part more suitable for the integral theory. This separation is not unique. It is favourable to let the long range part $\Phi_{ik}^{\mathrm{long}}$ of the coupling parameters Φ_{ik} become smooth for $\mathbf{r} \to \mathbf{r}'$, as we shall see.

In the integral theory we renounce the Taylor expansion. We prefer to convert directly the sums in (7) into integrals by use of the Euler–Maclaurin formula. For any function $f(x)$ this formula has the form

$$\sum_{x=a}^{b} f(x) = \frac{1}{h}\int_{a}^{b} f(x)\,\mathrm{d}x + \tfrac{1}{2}[f(a)+f(b)] + \dots \tag{8}$$

where h is the lattice parameter and the omitted terms (infinite in number) are derivatives of increasing order at the boundaries a, b of the "chain" multiplied by constant coefficients.

A three-dimensional formula of this type seems not available, so we apply equation (8) in three directions successively. For a lattice, the boundaries of which are composed of primitive cubic lattice planes, the application of equation (8) gives exactly

$$\sum_{V} f(\mathbf{r}) = \frac{1}{V_0}\int f(\mathbf{r})\,\mathrm{d}V + \frac{1}{2}\sum_{S} f(\mathbf{r}) + \dots \tag{9}$$

where V_0 is the volume of the primitive cell (the "average volume" of the particle) and the omitted terms are, as before, given by derivatives at the surface of f with increasing order. Since a crystal of arbitrary shape can be approximated by the above described crystal, we conclude that within this approximation equation (9) applies to primitive cubic crystals of any shape. In this way we obtain

$$\sum_{V} f(\mathbf{r}) = \frac{1}{V_0}\int f(\mathbf{r})\,\mathrm{d}V + \frac{1}{2}\int_{S} \frac{1}{S_0(\mathbf{r})} f(\mathbf{r})\,\mathrm{d}A + \dots \tag{10}$$

where $S_0(\mathbf{r})$ is the "average area" occupied by the particle at point $\mathbf{r}$ on the surface. The error is of the importance of the discontinuity of a surface of a crystal, i.e. negligible in most circumstances.

The approximation implied by omitting the derivative terms in (10) depends on the behaviour of $f(\mathbf{r})$. For our application the critical quantity is $\Phi_{ik}^{\mathrm{long}}(\mathbf{r}-\mathbf{r}')$. Since we have decided to include the fast varying part of $\Phi_{ik}(\mathbf{r}-\mathbf{r}')$ into the short range energy, we expect rapid convergence of the sum (10) in our application. In many cases even the first surface integral will be negligible. We include it, nevertheless, since in this way we shall gain some additional insight.

With the help of equation (10) the long range part of the internal energy (7) becomes

$$\begin{aligned} E^{\mathrm{long}} = {} & \frac{1}{2V_0^2}\int_V\int_V \mathrm{d}V\,\mathrm{d}V'\,\Phi_{ik}^{\mathrm{long}}(\mathbf{r}-\mathbf{r}')(u_i'-u_i)(u_k'-u_k) \\ & + \frac{1}{4V_0}\int_V\int_S \mathrm{d}V\,\mathrm{d}A'\,\frac{1}{S_0(\mathbf{r}')}\Phi_{ik}^{\mathrm{long}}(\mathbf{r}-\mathbf{r}')(u_i'-u_i)(u_k'-u_k) \\ & + \frac{1}{4V_0}\int_V\int_S \mathrm{d}A\,\mathrm{d}V'\,\frac{1}{S_0(\mathbf{r})}\Phi_{ik}^{\mathrm{long}}(\mathbf{r}-\mathbf{r}')(u_i'-u_i)(u_k'-u_k) \\ & + \frac{1}{8}\int_S\int_S \mathrm{d}A\,\mathrm{d}A'\,\frac{1}{S_0(\mathbf{r})S_0(\mathbf{r}')}\Phi_{ik}^{\mathrm{long}}(\mathbf{r}-\mathbf{r}')(u_i'-u_i)(u_k'-u_k). \end{aligned} \tag{11}$$

We now introduce a two-point tensor $t_{ikjl}(\mathbf{r}-\mathbf{r}') = t_{kijl}(\mathbf{r}-\mathbf{r}')$ defined by the set of equations

$$\partial_j \partial'_l t_{ikjl} = -\Phi^{\text{long}}_{ik}/V_0^2 \tag{12}$$

$$n_j \partial'_l t_{ikjl} = +\Phi^{\text{long}}_{ik}/2S_0(\mathbf{r})V_0 \tag{13}$$

$$\partial_j n'_l t_{ikjl} = +\Phi^{\text{long}}_{ik}/2S_0(\mathbf{r}')V_0 \tag{14}$$

$$n_j n'_l t_{ikjl} = -\Phi^{\text{long}}_{ik}/4S_0(\mathbf{r})S_0(\mathbf{r}'). \tag{15}$$

n_j is the external normal unit vector of the surface S. From equations (12), (13) follows $\partial'_l t_{ikjl}$, from equations (14), (15) follows $n'_l t_{ikjl}$ and from these two expressions one obtains t_{ikjl}. If we substitute equation (12) into equation (11) we find after some partial integrations

$$E = \frac{1}{2}\int_V \int_V \mathrm{d}V\,\mathrm{d}V' t_{ikjl}(\mathbf{r}-\mathbf{r}')u_{i,j}(\mathbf{r})u_{k,l}(\mathbf{r}'). \tag{16}$$

All other integrals vanish due to the boundary conditions (13)–(15).

Equation (16) shows that only that part of t_{ikjl} which is symmetric with respect to interchange of the subscripts pairs ij and kl contributes to the energy. Hence we can (and will) require t_{ikjl} to possess this symmetry which also implies the symmetry $t_{ikjl} = t_{iklj}$.

We decompose $u_{i,j}$ in equation (16) into strain ε_{ij} and rotation ω_{ij} and do the same with $u'_{k,l}$. Provided the cross terms vanish we can write

$$\begin{aligned} t_{ikjl}u_{i,j}u'_{k,l} &= t_{(ikjl)}\varepsilon_{ij}\varepsilon'_{kl} + e_{ijm}e_{kln}a_{mn}\omega_{ij}\omega'_{kl} \\ &= (t_{(ikjl)} + e_{ijm}e_{kln}a_{mn})u_{i,j}u'_{k,l} \end{aligned} \tag{17}$$

where e_{ijm} is the permutation tensor, $t_{(ikjl)}$ is the totally symmetric part of t_{ikjl} and a_{mn} is a symmetric tensor depending on $\mathbf{r}-\mathbf{r}'$. This consideration shows that equations (12)–(15) have solutions of the symmetry*

$$t_{ikjl} = t_{jlik} \tag{18}$$

which is closely related to the well-known Huang symmetry in lattice dynamics. Incidentally, a corresponding result would be obtained if Φ_{ik} depended on $\mathbf{r}$, $\mathbf{r}'$ separately (but symmetrically) rather than on $\mathbf{r}-\mathbf{r}'$ alone.

Even with all mentioned symmetry restrictions on t_{ikjl} this tensor is not defined uniquely by equations (12)–(15). Nevertheless, the energy (16) appears determined uniquely which is all we need at present. We shall come back to an implication of the non-uniqueness of t_{ikjl} in Section 4.

In view of the symmetry (18), we can replace (and find it convenient) the tensor $t_{ikjl}(\mathbf{r}-\mathbf{r}')$ by a tensor $c_{ijkl}(\mathbf{r}-\mathbf{r}')$ through

$$t_{ikjl} = (c_{ijkl} + c_{jkil})/2, \qquad c_{ijkl} = t_{ikjl} + t_{jkil} - t_{jilk}. \tag{19}$$

Observing the symmetries of $c_{ijkl}(\mathbf{r}-\mathbf{r}')$

$$c_{ijkl} = c_{jikl} = c_{ijlk} = c_{klij} \tag{20}$$

equation (16) is transformed into

$$E = \frac{1}{2}\int_V \int_V \mathrm{d}V\,\mathrm{d}V' c_{ijkl}(\mathbf{r}-\mathbf{r}')\varepsilon_{ij}(\mathbf{r})\varepsilon_{kl}(\mathbf{r}'). \tag{21}$$

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* See the *Note added in proof* (ii) at the end of the paper.

The convenience of equation (21) consists in the fact that the strains alone contribute to the internal energy.

The total internal energy is the sum of the short and long range energies. So we obtain*

$$E = \frac{1}{2}\int_V \mathrm{d}V\, C_{ijkl}\varepsilon_{ij}(\mathbf{r})\varepsilon_{kl}(\mathbf{r}) + \frac{1}{2}\int_V\int_V \mathrm{d}V\,\mathrm{d}V'\, c_{ijkl}(\mathbf{r}-\mathbf{r}')\varepsilon_{ij}(\mathbf{r})\varepsilon_{kl}(\mathbf{r}'). \tag{22}$$

We expect this expression to be very accurate except for describing phenomena on a scale which is comparable to the lattice parameter. As mentioned, we can allow for these phenomena by including higher displacement gradients into the short range energy. This is the most convenient thing to do in most circumstances. It is not necessary, however. Keeping the short range energy in the local form [first term of equation (22)] would mean that the convergence of equation (10), when applied to smaller scale problems, decreases, i.e. the above omitted derivative terms in the long range integral have to be included now. It can easily be seen that the long range energy can then be written in form of a double integral which contains higher order displacement gradients. The corresponding two-point material tensors follow from boundary value problems similarly as $t_{ikjl}(\mathbf{r}-\mathbf{r}')$ did. So we see: for small scale phenomena we need higher (than first order) displacement gradients either in the short range or in the long range energy.

From now on we restrict ourselves to phenomena on a larger scale so that equation (22) represents the increase of internal energy in a reasonable accuracy. The rest is very simple: we introduce the stress tensor σ_{ij} as the variational derivative $\delta E/\delta\varepsilon_{ij}$ of E:

$$\sigma_{ij}(\mathbf{r}) = C_{ijkl}\varepsilon_{kl} + \int_V c_{ijkl}(\mathbf{r}-\mathbf{r}')\varepsilon_{kl}(\mathbf{r}')\,\mathrm{d}V'. \tag{23}$$

This equation is our constitutive law. The moment equilibrium condition implies the symmetry of the stress tensor and is satisfied by the symmetry properties of the material tensors. The equations of motion and the boundary conditions follow most easily from the Lagrange formalism:

$$\partial_i\sigma_{ij} + \rho F_j - \rho\ddot{u}_j = 0 \tag{24}$$

$$n_i\sigma_{ij} = t_j \tag{25}$$

where ρ is the mass density and F_j and t_j are the external forces per unit mass and unit area respectively. Inserting the constitutive law (23) with $\varepsilon_{ij} = (u_{i,j}+u_{j,i})/2$ into the equations of motion, one obtains three simultaneous Fredholm integro-differential equations of the second kind for the displacements, the solution of which is standard.

Often it may be good enough to include just the first integral in (11) into the internal energy. The equations of motion then become

$$C_{ijkl}u_{k,lj} + \int_V \Phi^{\mathrm{long}}_{ik}(\mathbf{r}-\mathbf{r}')u_k(\mathbf{r}')\,\mathrm{d}V' + F_i - \rho\ddot{u}_i = 0, \tag{26}$$

i.e., somewhat simpler than equation (24) with equation (23) substituted. The particular advantage of this formulation is that it is not necessary to solve the boundary value problem in order to obtain $c_{ijkl}(\mathbf{r}-\mathbf{r}')$ from $\Phi_{ik}(\mathbf{r}-\mathbf{r}')$, since we do not need $c_{ijkl}(\mathbf{r}-\mathbf{r}')$.

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* The calculation of the tensor C_{ijkl} from coupling parameters Φ_{ik} is found in the standard texts on lattice theory. It goes via a tensor T_{ikjl} which is related to C_{ijkl} in the same way as is t_{ikjl} to c_{ijkl}.

4. COMMENTS

(a) *Many-particle forces*

In the simplest case, namely three-particle interactions, a sum extended over $\mathbf{r}, \mathbf{r}', \mathbf{r}''$ has to replace the sum in equation (7). In the linear theory where bilinear terms alone in the displacements are admitted, this sum can always be reduced to a sum over $\mathbf{r}$ and $\mathbf{r}'$. A corresponding statement applies to arbitrary n-particle forces ($n > 3$). Hence, the linear theory need not be modified in order to allow for many-particle forces.

(b) *Surface tension*

Equations (1) and (7) apply to a deformation from an equilibrium state, otherwise terms linear in the displacements had to be included. On the other hand, it was assumed in Sections 2 and 3 that the particles form a perfect lattice in the reference state. To meet both requirements, external forces, say, P_i, acting on the particles must be present.

We imagine that additional forces $-P_i$ (closely related to the surface tension) which cancel the forces P_i are applied. If the deformation from the reference state (as defined above) to the unloaded state is (practically) infinitesimal then an external force density, F_i, acting on the crystal in the reference state, first, and in the unloaded state, second, will cause the same displacements. This is no longer true if the deformation from reference to unloaded state is finite. When in such a case we want to apply the theory to deformations from the unloaded state then we first have to correct the formulas obtained above for c_{ijkl} which requires the solution of the nonlinear surface tension problem and is rather involved.

(c) *Self strain*

It was noted in Section 3 that equations (12–15) together with the symmetry conditions for t_{ikjl} do not define the tensor field $t_{ikjl}(\mathbf{r}-\mathbf{r}')$ uniquely. To achieve uniqueness we must infer the additional relations

$$e_{mnj}\partial_n t_{ikjl} = 0, \qquad e_{pql}\partial'_q t_{ikjl} = 0 \tag{27}$$

assuming that t_{ikjl} goes to zero for $\mathbf{r}-\mathbf{r}' \to \infty$.

Imagine a tensor field $\bar{t}_{ikjl}(\mathbf{r}-\mathbf{r}')$ satisfying the set of homogeneous equations obtained by setting zero the right sides of equations (12–15) and which also satisfies the inhomogeneous equations corresponding to equation (27). This tensor when added to t_{ikjl} in equation (16) will not contribute to the energy. It would contribute, however, when the displacement gradients are replaced by more general second rank tensors sometimes called dipolar displacements or distortions. The occurrence of these tensors implies a violation of the elastic compatibility law and indicates a situation of self strain, as is well-known. This result shows that the constitutive law being identical for load strains and self strains in the local theory differs in the non-local theory. Clearly, the reason is that in the local theory the strain at a point alone determines the stress at this point whereas in the non-local theory it is the strain at all points. Hence it makes a difference in the constitutive law whether or not this strain varies compatibly.

The energy expression (22) can be generalized to include self strain situations by adding a tensor $\bar{c}_{ijkl}$ to c_{ijkl} which is related to $\bar{t}_{ikjl}$ as was c_{ijkl} to t_{ikjl}. $\bar{t}_{ikjl}$ certainly does not depend on Φ_{ik}. It should be an interesting problem to determine $\bar{t}_{ikjl}$ from fundamental observations on an atomic scale.

(d) *Multipolar elasticity theory*

In their multipolar continuum mechanics Green and Rivlin [5] have defined, besides the mentioned materials of the space differential type, materials of the space functional type in which the stress multipoles are space functionals of the displacement gradients. A material of which the internal energy has the form (16) would belong to this group. By Taylor development of $u'_{k,l}$ around point $\mathbf{r}$ the energy (16) can easily be transformed in a convergent space differential form, i.e. into a single volume integral containing higher displacement gradients. Hence the specification of a material as "of the space differential type" or "of the space functional type" can be misunderstood. The fundamental physical criterion for the two types of materials in question is whether they have short range or long range cohesive forces.

5. CONCLUSION

The importance of long range interactions in ionic crystals has been emphasised by Born and Huang in [1], p. 225 ff. The solution of the problem offered there implies the combination of elasto- and electrodynamics and has local constitutive equations including elastic–electric cross terms. Since the forces exerted on the particles by the internal electric field determine the response of the body, one has to calculate these fields which involves a volume (and perhaps a surface) integration. This part of the task is incorporated into the material tensors $c_{ijkl}(\mathbf{r}-\mathbf{r}')$ in our formulation of the theory. It means that in a way we have eliminated the electric part of the theory at the expense of the locality of the constitutive laws. Both approaches may have their advantages in certain situations.

Ionic crystals are not Bravais crystals but have at least two different atoms in an elementary cell. Hence the results of the present investigation are not immediately applicable. The appropriate differential theory is a multipolar theory of the second kind to which an integral (non-local) theory can be constructed in a way similar to that which we have developed for the Bravais crystal. The details of this theory are not yet worked out. It is clear from the work of Mindlin [7] that this theory will show an essential feature of ionic crystals, namely the decomposition of the wave spectrum into an optical and an acoustical branch.

In passing, we should mention that the above long range theory is certainly applicable to gravitational interaction which is important in solids of stellar size.

In Appendix 2 we have shown that Van der Waals forces have to be treated as "long range" in certain situations of monotonically varying strain. Hereto belong displacement fields around lattice defects. In [3] the force between two isotropic point defects (centers of dilatation) was found to vary with distance r as $\mathrm{d}g(r)/\mathrm{d}r$ where $g(|\mathbf{r}-\mathbf{r}'|)$ is the variable part of the reciprocal kernel of $c_{ijkl}(|\mathbf{r}-\mathbf{r}'|)$. Since the latter quantity varies as $|\mathbf{r}-\mathbf{r}'|^{-5}$ in the case of Van der Waals forces, one also has (asymptotically) $g(r) \propto r^{-5}$ and the force between the two defects decays as $1/r^6$ as does the force between the molecules in a Van der Waals gas. Local theory gives a zero force in our situation which shows once more that range effects can be important in crystalline materials which have Van der Waals interactions. Many materials belong to this type.

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APPENDIX 1

Convergence of the Multipolar Energy

The interaction energy $e(x)$ of the particle at x with all the other particles follows from equations (4), (5):

$$e(x) = A\sum_{x'}\sum_{p,q=1}^{\infty}\frac{1}{p!q!}\frac{(x'-x)^{p+q}}{|x'-x|^m}u^{(p)}u^{(q)} \tag{A1}$$

where we have taken $\Phi = A|x'-x|^{-m}$. We show that $e(x)$ is convergent for any physically reasonable analytic strain state in a finite chain.

Consider a displacement field $u_0\exp(+x/ah)$ (the same result would be obtained from $u_0\exp(-x/ah)$. The summation over the values $x' < x$ converges so rapidly that only a few particles need to be included. Hence a divergence could only arise in the summation over $x' > x$ and for this sum we obtain after a slight rearrangement in the summations and setting $|x'-x| = nh$

$$\frac{Au_0^2}{h^m}\sum_{p+q=2}^{\infty}\left(\sum_{q=1}^{p+q-1}\frac{1}{p!q!}\right)\left(\sum_{n=1}^{N(x)}n^{p+q-m}\right)\left(\frac{1}{a}\right)^{p+q}. \tag{A2}$$

Here $N(x)$ is the number of particles with coordinates $x' > x$.

For the convergence behaviour only the terms with large $p+q$ are important. Using Legendre's duplication formula for the gamma function we find that for large $p+q$ the first parenthesis is smaller than $(p+q)\,.\,2^{p+q}/2\pi(p+q)!$. For positive values of $p+q-m$ the second parenthesis gives $(B_{p+q-m+1}(N+1)-B_{p+q-m+1}(0))/(p+q-m+1)$, with B the Bernoulli polynomials. Hence the expression (A2) converges a little better than the Bernoulli series

$$\sum_{p+q}^{\infty}\frac{B_{p+q}(N+1)}{(p+q)!}\left(\frac{2}{a}\right)^{p+q} \tag{A3}$$

which is absolutely convergent for $a > 1/\pi$ and finite N. If we set $ah = \lambda/2\pi i$ we have a sinusoidal displacement, and convergence occurs for a wave length $\lambda > 2h$.

APPENDIX 2

Range Effects in Van der Waals Crystals

Since we are content with a rough estimate, we replace (for $p+q \geqq 6$) the sums over n in equation (A2) by $n^{p+q-6}/(p+q-6)$, which is too small a value. Hence we shall certainly underestimate the contributions of the higher terms when we replace (A2) by

$$\begin{aligned}\frac{Au_0^2}{h^5N^4}\Bigg[&\left(\sum_{n=1}^{N}\frac{1}{n^3}\right)N^2\left(\frac{N}{a}\right)^2+\left(\sum_{n=1}^{N}\frac{1}{n^2}\right)N\left(\frac{N}{a}\right)^3+\frac{7}{12}\left(\sum_{n=1}^{N}\frac{1}{n}\right)\left(\frac{N}{a}\right)^4\\&+\frac{1}{4}\left(\frac{N}{a}\right)^5+\sum_{p+q=6}\left(\sum_{q=1}^{p+q-1}\frac{1}{p!q!}\cdot\frac{1}{p+q-4}\right)\left(\frac{N}{a}\right)^{p+q}\Bigg].\end{aligned}\tag{A4}$$

A maximum term is found near $p+q = N/a$. If the values of N and N/a are such that this term equals the first term in the bracket—the term which represents the local theory—then certainly the long range contributions to the interaction energy $e(x)$ are several times larger than the local term. For $N = 10^7$, for example, this occurs roughly at $N/a = 50$. If the length of the specimen is 10^8 particles, then $e(x)$ when calculated by the local theory may be wrong by an order of magnitude in 9/10 of the specimen provided $ah < 2.10^5$ lattice spacings.

Exponentially varying displacement fields can be produced in many ways. Among the most important possibilities are the application of an exponentially varying temperature field or an exponential distribution of foreign atoms as obtained by diffusion. It is interesting to note that although the energy per particle obtained by omitting the long range contributions may be very wrong, the local energy when summed up over all particles nevertheless approaches the correct total strain energy very well.* This indicates that the solution of problems of this kind based on the local energy expression may be better than one would expect at a first glance. Nevertheless, the range effect can be important, as is shown clearly in the point defect problem mentioned in Section 5.

The effect discussed above is due to the monotonical and sufficiently strong increase of the displacement field over a long distance. In a sinusoidal displacement field the increase is nowhere stronger than $\propto x^2$. This is too weak to give an appreciable long range effect in Van der Waals crystals.

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Notes added in proof

(i) By error the Van der Waals energy was taken to decay a r^{-5} instead of r^{-6}. All qualitative conclusions about Van der Waals forces, nevertheless, remain valid.

(ii) It is difficult to verify the vanishing of the cross terms in (17). For an infinite continuum a rigorous proof of the statement referring to equation (18) has been based on equation (12) and will be published in the Sedov anniversary volume. It is highly probable that the statement applies to a finite continuum too.

Résumé—L'énergie de tension d'un matériau déformé avec interaction spatiale peut s'écrire soit sous une forme différentielle (*multipolaire*), c'est à dire comme intégrale à un seul volume contenant des gradients de déplacement à un ordre infini, ou sous une forme intégrale (non locale), par exemple une intégrale à double volume résumant les interactions de paires d'éléments de masse. La théorie linéaire est derivée de la théorie des treillis, et l'on en retire les aperçus suivants:

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* To see this, calculate the energy by going in the $-x$-direction instead of in the $+x$-direction as we did before.

(1) La théorie différentielle, quoiqu'en principe applicable à tout problème d'élasticité (analytique) à grand rayon d'action, est commode principalement pour décrire des effets de rayon d'action à une échelle très réduite (presque atomique).

(2) Les effets des forces électriques de cohésion peuvent être comprises dans les éléments des tenseurs du matériau à deux points (noyaux) de la théorie non locale. De cette façon la théorie microscopique devient purement élastique.

(3) Des forces de cohésion de Van der Waals donnent lieu à des effets de rayon d'action d'élasticité dans certaines conditions de tension non homogènes, en particulier dans des problèmes d'interaction de défauts et de diffusion.

Zusammenfassung—Die Verzerrungsenergie eines verformten Materials mit räumlicher Wechselwirkung kann in zwei Weisen geschrieben werden: entweder in einer Differentialform (*multipolar*), d.h. als einzelnes Volumintegral, das die Verschiebungsgradienten bis zu unendlich hoher Ordnung enthält; oder in einer Integralform (*nichtlokal*), z.B. als ein doppeltes Volumintegral, das die Wechselwirkungen von Paaren von Volumelementen aufsummiert. Die lineare Theorie wird aus der Gittertheorie abgeleitet, und die folgenden Einsichten werden gewonnen:

(1) Zwar ist die Differentialtheorie im Prinzip auf jedes (analytische) Problem mit endlicher Reichweite der Kohäsionskräfte anwendbar; bequem ist sie aber hauptsächlich für eine Beschreibung von Reichweiteeffekten auf einer sehr kleinen (nahezu atomaren) Skala.

(2) Die Auswirkungen der elektrischen Kohäsionskräfte können in den Zweipunkt-Materialtensoren (Kernen) der nichtlokalen Theorie erfaßt werden. Auf diese Art wird die makroskopische Theorie rein elastisch.

(3) Van der Waalssche Kohäsionskräfte verursachen elastische Reichweiteeffekte unter gewissen Bedingungen inhomogener Spannung, insbesondere bei Problemen der Wechselwirkung und Diffusion von Gitterfehlern.

Абстракт—Энергия деформации деформированного материала с пространственным взаимодействием может бытв описана или в дифференциальной (многополюсной) форме, зналцм как объемный интеграл, содержающий градиенты перемещений вплоти до бесконечного порядка, или в интегральной (нелокальной) форме, напр. как двойной объемный интеграл, суммирующий взаимодействия пар элементов массы. Линейная теория выводится из теории решетки и получены слебующие познанил:

(1) Дифференциальная теория, несмотря на то, что в основном применимая к любой (аналитической) задаче непокапною ьзаидоуецстьил, является глаьныд образод удобной при описании эффектов ьзацдоуецстьцл в очень маленьким (почти атомным) масштабе.

(2) Эффекты электрических сил притяжения можна представить в виде двухточечных материальных тензоров (ядра) нелокальной теории. Этим путем макроскопическая теория переходит в чистую теорию упругости.

(3) Силы притяжения Ван-дер-Ваальса вызывают упругце эффекты нелокалного ьзацдобецстьцл под влиянием некоторых условий неоднородного напряжения, в частности, при взаимодействии деффектов и проблемах диффузии.