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Continuum mechanics and range of atomic cohesion forces

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Abstract

The conventional continuum theories of solid state physics are based on the supposition of an infinitesimal range of the atomic cohesion forces. Hence, these theories are not the right tool for handling problems in which experimental or model lengths which are not large compared with the range R of these forces play a role. Problems of this kind deal primarily with crystal defect interaction phenomena which strongly influence the macroscopic properties of solids.

Since a finite force range is not in contradiction with the continuum idea itself, the local theories can be generalized as to include the nonlocal phenomena in solids. The theory is given for the property of elasticity. Other properties would lead to similar theories. The resulting integral equation has been solved rigourously for one class of problems with the following result: The displacement field due to a point force in a medium which responds locally and the displacement field in a medium responding nonlocally, in which the acting forces are distributed over the range of the cohesion forces, are the same. Thus it is shown that the nonlocal theory deviates to a considerable degree from the local theory in the case of far-reaching atomic forces. Furthermore it is emphasized that for a medium responding nonlocally the situation in a surface layer of thickness R is quite different from that in the interior of the body.

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1. Introduction

To any crystalline solid one can assign two characteristic lengths[2] which strongly influence its physical properties:
(1) the lattice parameter a,
(2) the range parameter R of the atomic cohesion forces.

In situations where all occuring lengths are large compared with a and R, the finiteness of a and R has been neglected and continuum theoretical methods were applied with great success.

In recent time, continuum theories were often used, even if the above assumption is not fulfilled necessarily, namely in cases where lengths with the magnitude of R or even smaller become important. Examples for such lengths are the radius of curvature of notches or of a strong lattice bending or torsion produced in some way, the wave length of high-frequency sound waves, the distance between two dislocations or other lattice defects, the thickness of a surface layer etc. Some of these lengths are essential for the phenomenon of fracture. Here, also the so-called surface of fraoture plays a role, the "thickness" of which is very small.

The application of continuum theoretical methods is justified as long as the smallest characteristic length of the experiment, which will be called the smallest "test length" L, is sufficiently large compared with the lattice parameter. This situation will be assumed in the following. In contrast to the conventional theories, however, allowance will be made for ranges R which are comparable with or even larger than L. The author believes that this situation will hold in a number of applications in solid state physics or materials sciences, especially those concerning interaction of crystal defects.

We shall confine ourselves to the property of elasticity but will keep in mind that similar considerations apply to other physical properties as well. As for electrodynamics, cf. (1). It is easily seen that the conventional concept of stress, one of the fundaments of elasticity theory, breaks down when cohesion forces of a finite range are accounted for.

To this end consider the usual idea which leads to the definition of stress. Separate two parts I and II of the body by a cut, i.e. remove the forces acting between I and II. Assume that by the cut no displacement in I, say, is to happen. Then the compensatory forces dp per area element dS which

2. Instead of one lattice and range parameter several parameters may occur. The limitation to one is for simplicity of representation only. The theory itself does not contain this restriction.

correspond exactly to the response forces exerted on I by II before cutting must be applied along the surface of I. Hence the stress tensor σ defined by $dp = dS \cdot \sigma$ measures the response at point r of the uncut body.

This definition of stress implies that it is possible to apply forces in the cut face such that no displacement occurs in I. Obviously this assumption is not justified if the cohesion forces have a finite range. The forces exerted by II on I then also act in the interior of I. If we separate II from I, then the compensatory forces must be applied inside I too. In this way, the definition of stress above breaks down. It will be shown in the next section how elasticity theory can be generalized to include the effect of a finite range of atomic forces.

2. Nonlocal elasticity

The characteristic feature of a finite range of cohesion forces implies the interaction between two volume elements dV and dV', say, situated at positions r and r'. The internal energy of the body then has the form

$$U' = \frac{1}{2}\iint dV\, dV'\, u(r,r') \tag{1}$$

where u(r,r') is a two point energy density.

Let $\Delta U'$ be the increase in energy over the energy U_0 of the nondeformed body. Then $\Delta u = 0$ for zero strain. We shall denote the strain tensor in cartesian cordinates by ε_{ij}. In a linear theory $\Delta u(r,r')$ is proportional to $\varepsilon_{ij}(r)$ and $\varepsilon_{kl}(r')$, hence

$$\Delta U' = \frac{1}{2}\iint dV\, dV'\, c_{ijkl}(r,r')\, \varepsilon_{ij}(r)\, \varepsilon_{kl}(r') . \tag{2}$$

The proportionality quantities $c_{ijkl}(r,r')$ will be called the (nonlocal) elastic moduli of the material, since they are the quantities which specify the elastic properties of the material. To give the theory a simpler form we shall restrict ourselves to moduli of the form[3]

$$c_{ijkl}(r,r') = K(|r-r'|)\, C_{ijkl} \tag{3}$$

3. The general case can easily be treated in the same way.

where the C_{ijkl} are constant in any cartesian frame. The function $K(|r-r'|)$ gives the decrease of the cohesion forces with distance. An especially simple form of K would be the delta-function $\delta(|r-r'|)$. In this case, one integration in (2) can be performed, and one falls back to the local theory.

Next we replace the strains by displacements $s_j(r)$ using the well-known formula $\varepsilon_{ij} = \frac{1}{2}(\partial s_j/\partial x_i + \partial s_i/\partial x_j)$ and obtain

$$\Delta U' = \frac{1}{2}\iint dV\, dV' C_{ijkl}\, K(|r-r'|) \frac{\partial s_j(r)}{\partial x_i} \frac{\partial s_l(r')}{\partial x'_k} . \qquad (4)$$

The potential energy of external volume and surface force densities F(r) and A(r) resp. can be written

$$\Delta U'' = \int F_j(r)\, s_j(r)\, dV + \int A_j(r)\, s_j(r)\, dS. \qquad (5)$$

The kinetic energy is, using ϱ for mass density,

$$T = \frac{1}{2}\varrho \dot{s}_j \dot{s}_j . \qquad (6)$$

Applying the well-known variation formalism to the Lagrangian $L = T-\Delta U'-\Delta U''$ we obtain the equations of motion

$$\int dV' K(|r-r'|) P_j(r') - \int dS' K(|r-r'|) Q_j(r') = \varrho \ddot{s}_j(r) + F_j(r) \qquad (7)$$

and the boundary conditions

$$\int dV' K(|r-r'|)\, n_i\, C_{ijkl} \frac{\partial s_l(r')}{\partial x'_k} = A_j(r) \qquad (8)$$

where n_i denotes the external surface normal.

In (7), the following abbreviations have been used:

$$C_{ijkl} \frac{\partial^2 s_l(r')}{\partial x'_i\, \partial x'_k} = -P_j(r'), \quad n_i(r')\, C_{ijkl} \frac{\partial s_l(r')}{\partial x'_k} = Q_j(r) \qquad (9)$$

Eqs. (9) are the static equilibrium and boundary conditions of the local elasticity theory, if P_j and Q_j are interpreted as volume and surface force densities.

The appearance of the surface integral in eq. (7) shows the important fact that the equations of motion have a very

different form near the surface and in the interior of the body, i.e. in distances from the surface which are larger than the effective range of the cohesion forces. So it turns out that the surface layer can have quite special properties.

We shall confine ourselves to static situations and will not consider boundary problems. In many cases of practical importance as often in the defect interaction problem the boundary effect is negligible, i.e. the body can be considered infinite. The basic eqs. (7,8) then reduce to a single set of three equations:

$$\int dV' K(|r-r'|)\, P_j(r') = F_j(r). \qquad (10)$$

These are Fredholm integral equations of first kind with Kernel K for the determination of forces $P_j(r)$ which produce the same displacement field in a body responding locally, with elastic moduli C_{ijkl}, as do the forces $F_j(r)$ in material responding nonlocally. By solving this integral equation for P_j, the problem can obviously be reduced to one of local elasticity.

3. An exact solution

The methods for solving Fredholm integral equations are highly developed. We shall not use these methods here, but rather guess a certain class of solutions. Let P_j be a single force acting in the origin. Then $P_j(r') = P^\circ_j\, \delta(r')$ where the constants P_j give direction and size of the force. Introducing this into eq. (1o) the integration can be performed, which yields

$$F_j(r) = P^\circ_j\, K(|r|) \qquad (11)$$

for any K.

We see: The force density $P^\circ_j K(|r|)$ in the "nonlocal" body produces the same displacement field as a single force with magnitude and direction of P°_j does in the corresponding "local" body. Hence considerable effects of nonlocality occur if the range of the cohesion forces is large.

4. Stress in the nonlocal theory

We now return to the concept of stress. In the local theory the stored energy is

$$\Delta U' = \frac{1}{2}\int \sigma_{ij}(r)\, \varepsilon_{ij}(r)\, dV. \qquad (12)$$

We decide that this equation is true in the nonlocal theory too. This implies a new definition of stress σ_{ij}. By comparison with eq. (2) we find the nonlocal stress-strain relation

$$\sigma_{ij}(r) = \int c_{ijkl}(r,r')\,\varepsilon_{kl}(r')\,dV'. \qquad (13)$$

Observing that the nonlocal stresses have the same dimension as the local ones, we obtain the following physical meaning of the $\sigma_{ij}(r)$: they measure the resultant of all forces which tug at an area element at point r. These forces are the interaction forces between the area element considered and all the volume elements. In this way the concept of nonlocal stress appears as a natural generalization of the concept of local stress.

Introducing Fourier transforms for the quantities appearing in eq. (13) we arrive at elastic moduli which depend on the wave vector k. This dependence is due to the nonlocality of the response. Hence, the response to a spatially periodic strain depends on the wave length. In the case of time-periodic processes the elastic moduli, of course, depend on the frequency ω, too.

Similar phenomena have been studied recently in electrodynamics. Especially the k- and ω- dependent dielectric constant of the electron gas has been discussed extensively (see e.g. (2)). The origin of the k-dependence is again the finite range of interactions, namely of the Coulomb interaction between electrons.

5. Conclusion

Nonlocal theories have been considered in several branches of physics, especially in modern quantum field theories. Here we suggest that nonlocal theories, mechanical as well as electromagnetical, shall be applied for the explanation of the behaviour of actual materials. Of course, not all materials behave the same way in this respect. It will be one of the main problems of the near future to find out which materials react more local and which less. This means that one needs estimates of the nonlocal moduli c_{ijkl}, e.g. It is clear that this information does not evolve from the present theory, but rather from a more fundamental atomic theory. In some cases this problem could be solved by the crystal lattice theory.

Two further results of nonlocal elasticity might also be mentioned. (i) The theory can easily be formulated for incompatible problems. In that case stress functions are introduced instead of displacements. This formulation, which will be given elsewhere, is convenient for problems with continuous

defect distributions and perhaps for temperature stress problems.

(ii) If the cohesion forces are rather short-range, only volume elements in closer vicinity contribute to the energy. One can then develop $\varepsilon(r')$ in terms of $\varepsilon(r)$ and its derivatives. The integration over r' can now be performed formally and leads to a number of spatially constant material tensors which are assigned to ε and its various derivatives. Formally defined response tensors then appear as local stresses of higher order (multipole stresses). Cutting off the development after the second derivative of ε leads to a couple stress theory as discussed by Toupin (3) and the author (4). The couple stresses do in fact take into account to first order the effect of the nonlocality of the response.

In conclusion one more remark: I do not think that all former results on defect interaction etc. are essentially wrong. However, one has to be aware of the finite range of the cohesion forces which exists in all real materials and which sets definite bounds to the applicability of the local theories. In extreme cases, conclusions drawn from these theories may be in error even qualitatively.

It is hoped that the solution of problems by the nonlocal theory will further clarify the situation.

This work was supported by the Deutsche Forschungsgemeinschaft.

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