Towards a Unified Field Theory of Defects and Stresses.

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(ricevuto il 1 Marzo 1982; manoscritto revisionato ricevuto il 20 Maggio 1982)

We propose a new, unified theory of defects and stresses in the continuum limit of solids. The total energy has a generally covariant form involving $G_{ij}G^{ij}$, where G_{ij} is the Einstein tensor of stress, and the scalar curvature R of the defects (which includes dislocations and disclinations).

The final form efficiently unifies two previously unrelated geometric formulations of defects and stresses.

In the continuum theory of defects and stresses in solids, geometry plays two important, separate roles. The first goes back to Kondo's observation (1), in 1952, that dislocations are the discrete version of Cartan's torsion (2) and has led to a co-ordinate-independent description of dislocations and disclinations in terms of a defect dreibein field $e^a{}_\alpha$ (*) (which denotes the tangents to the co-ordinate lines chosen arbitrarily in the crystal) and its metric $g_{\alpha\beta} = e^a{}_\alpha e_{a\beta}$ (3,4). If the connection is defined as usual for spaces with torsion by

$$\Gamma_{\alpha\beta}{}^\gamma = e^{a\gamma}\partial_\alpha e_{a\beta} = \left\{\begin{matrix}\gamma\\ \alpha\beta\end{matrix}\right\} + K_{\alpha\beta}{}^\gamma \tag{1}$$

with

$$K_{\alpha\beta}{}^\gamma = S_{\alpha\beta}{}^\gamma - S_\beta{}^\gamma{}_\alpha + S^\gamma{}_{\alpha\beta}\,, \qquad S_{\alpha\beta}{}^\gamma \equiv \tfrac{1}{2}(\Gamma_{\alpha\beta}{}^\gamma - \Gamma_{\beta\alpha}{}^\gamma)\,,$$

the torsion $S_{\alpha\beta}{}^\gamma$ is related to dislocations and the curvature $R_{\alpha\beta\gamma}{}^\delta = e^{a\delta}(\partial_\alpha\partial_\beta - \partial_\beta\partial_\alpha)e_{a\gamma}$ to disclinations. We can give an extremal principle for this structure by postulating the defect energy

$$F_{\rm def} = \int d^3x\,\sqrt{g}\,g^{\alpha\beta}R_{\alpha\beta}(g, K) \tag{2}$$

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(1) K. KONDO: *On the geometrical and physical foundations of the theory of yielding*, in *Proceedings of the II Japan National Congress on Applied Mechanics* (Tokyo, 1952).

(2) For a review see E. KRÖNER: Lectures presented at the *1980 Summer School on the Physics of Defects* in Les Houches.

(*) The indices « a » have the trivial metric $\begin{pmatrix}1&&\\&1&\\&&1\end{pmatrix}$, *i.e.* $e_{a\alpha} = e^a{}_\alpha$.

(3) I. E. DZYALOSHINSKY and G. E. VOLOVIK, *Ann. Phys.* (*N. Y.*), **125**, 67 (1980).

(4) B. JULIA and G. TOULESS: *J. Phys.* (*Paris*) *Lett.*, **16**, L395 (1979).

and defining

(3) $$-\frac{1}{2}\sqrt{g}\,\eta^{\alpha\beta}=\frac{\delta F_{\rm def}}{\delta g_{\alpha\beta}}\,,\quad -\frac{1}{2}\sqrt{g}\,\alpha^{\beta}{}_{\gamma}{}^{,\alpha}=\frac{\delta F_{\rm def}}{\delta K_{\alpha\beta}{}^{\gamma}}\,,$$

as the symmetric momentum tensor and the spin current, respectively. Performing the derivatives we find

(4) $$\alpha_{\alpha\beta}{}^{;\gamma}=2(S_{\alpha\beta}{}^{\gamma}+S_{\alpha}{}^{\gamma}S_{\beta\sigma}{}^{\sigma}-\delta_{\beta}{}^{\gamma}S_{\alpha\sigma}{}^{\sigma})\,,$$

(5) $$\eta^{\alpha\beta}=\theta^{\alpha\beta}-\tfrac{1}{2}(D_{\gamma}+2S_{\gamma\sigma}{}^{\sigma})(\alpha^{\alpha\beta,\gamma}-\alpha^{\beta\gamma,\alpha}+\alpha^{\gamma\alpha,\beta})\,,$$

where

(6) $$\theta^{\alpha\beta}=R^{\alpha\beta}-\tfrac{1}{2}g^{\alpha\beta}R$$

is the Einstein tensor of the defect field and D_{γ} the covariant derivative. Linearizing and identifying (2) $e_{a\alpha}\equiv\partial_{\alpha}u_{a}(\boldsymbol{x})$ as the derivatives of the displacement field $u_{a}(\boldsymbol{x})$ of the crystal, the connection $\Gamma_{\alpha\beta\gamma}=\partial_{\alpha}e_{\gamma\beta}=\partial_{\alpha}\partial_{\beta}u_{\gamma}$ may be split into symmetric and antisymmetric parts as $\Gamma_{\alpha\beta\gamma}=\Gamma_{\alpha(\beta,\gamma)}+\Gamma_{\alpha[\beta,\gamma]}=\partial_{\alpha}u_{\beta\gamma}+\partial_{\alpha}\omega_{\beta\gamma}$ where $u_{\alpha\beta}\equiv(\partial_{\alpha}u_{\beta}+\partial_{\beta}u_{\alpha})/2$ is the strain and $\omega_{\alpha\beta}\equiv(\partial_{\alpha}u_{\beta}-\partial_{\beta}u_{\alpha})/2$ the local rotation. This can be brought to form (1) as

$$\Gamma_{\alpha\beta\gamma}=\tfrac{1}{2}(\partial_{\alpha}g_{\beta\gamma}+\partial_{\beta}g_{\alpha\gamma}-\partial_{\gamma}g_{\alpha\beta})+K_{\alpha\beta\gamma}$$

with a metric $g_{\alpha\beta}=2u_{\alpha\beta}$ and $K_{\alpha\beta\gamma}=\partial_{\alpha}\omega_{\beta\gamma}+\partial_{\gamma}u_{\beta\alpha}-\partial_{\beta}u_{\gamma\alpha}$ which, in this context, is commonly called contortion (5). From these identifications we can calculate, using (4),

(7) $$\alpha_{\alpha\beta}\equiv-K_{\alpha\beta}+\delta_{\alpha\beta}K_{\gamma\gamma}=\varepsilon_{\beta\gamma\delta}\partial_{\gamma}(u_{\delta\alpha}+\omega_{\delta\alpha})=\varepsilon_{\beta\gamma\delta}\partial_{\gamma}\partial_{\delta}u_{\alpha}\,,$$

where we have gone from antisymmetric tensor indices to vector indices via $\alpha_{\alpha\beta}\equiv\equiv\tfrac{1}{2}\varepsilon_{\alpha\gamma\delta}\alpha_{\gamma\delta,\beta}$, $K_{\alpha\beta}\equiv\tfrac{1}{2}K_{\alpha\gamma\delta}\varepsilon_{\gamma\delta\beta}$.

Equation (7) shows that the field spin specifies the failure of the translations to be integrable. This quantity is commonly called *dislocation* density. Similarly, from (6) we find

(8) $$\theta_{\alpha\beta}=\varepsilon_{\beta\gamma\delta}\partial_{\gamma}\partial_{\delta}\omega_{\alpha}\,,$$

which is the analogue quantity for the rotation field, the *disclination* density. Inserting these two relations into (5), we find the symmetric energy-momentum tensor

(9) $$\eta_{\alpha\beta}=\theta_{\alpha\beta}-\varepsilon_{\beta\gamma\delta}\partial_{\gamma}K_{\delta\alpha}=\varepsilon_{\alpha\gamma\delta}\varepsilon_{\beta\sigma\tau}\partial_{\gamma}\partial_{\sigma}u_{\delta\tau}\,,$$

which is the standard incompatibility of strains (2), also referred to as *defect* density (5).

The conservation laws following from the symmetry of action (2) are

(10) $$(D_{\mu}+2S_{\mu\sigma}{}^{\sigma})\theta_{\lambda}{}^{\mu}+2S_{\nu\lambda}{}^{\varkappa}\theta_{\varkappa}{}^{\nu}-\tfrac{1}{2}\alpha^{\nu}{}_{\varkappa}{}^{;\mu}R_{\lambda\mu\nu}{}^{\varkappa}=0\,,\quad (D_{\mu}+2S_{\mu\sigma}{}^{\sigma})\alpha^{\lambda\varkappa,\mu}=\theta^{\lambda\varkappa}-\theta^{\varkappa\lambda}$$

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(5) R. DE WITT: *Solid State Phys.*, **10**, 249 (1960); *J. Res. Nat. Bur. Stand. Sect. A*, **77**, 49, 359 (1973).

and reduce, in linear approximation, to the well-known relations [5]

$$\partial_\beta \theta_{\alpha\beta} = 0\,, \qquad \partial_\beta \alpha_{\alpha\beta} = \varepsilon_{\alpha\gamma\delta}\theta_{\gamma\delta}\,, \tag{11}$$

which state that disclination lines must be closed, while dislocation lines can only end on disclinations.

The field equations for η and α are $\eta = 0$, $\alpha = 0$ such that defects are absent at zero temperature. If the system is heated, however, fluctuations may cause a nonzero average defect density, due to the nonlinearity of the energy (2).

The second place at which a geometric description arises is the physics of internal stresses [6]. This is completely independent of the first, since it holds also in the absence of defects. It is based on the observation that, without external-body forces, the symmetric stress tensor σ_{ij} is divergenceless and may be identified with $\mu l^2/\gamma$ times the Einstein curvature tensor

$$G^{ij} = \tfrac{1}{4}\varepsilon^{ikl}\varepsilon^{jmn}R_{klmn} \tag{12}$$

of a Riemannian space with dreibeins $e^\alpha{}_i(x)$ and a stress metric $g_{ij} = e^\alpha{}_i(x)e_{\alpha j}(x)$, where l is the lattice spacing, γ measures the nonlinearities of the crystalline forces and μ is the shear module. If we use the Poisson number ν as the second elastic constant, the stress energy takes the form

$$F_S = \frac{\mu l^4}{4\gamma^2}\int \mathrm{d}^3x\sqrt{g}\left(G_{ij}G^{ij} - \frac{\nu}{1+\nu}\,G_i{}^{i2}\right), \tag{13}$$

which is invariant under general local co-ordinate transformations

$$\delta_E e^\alpha{}_i = \xi^j\partial_j e^\alpha{}_i + \partial_i\xi^j e^\alpha{}_j\,. \tag{14}$$

Also it is trivially so under local rotations

$$\delta_R e^d{}_i(x) = \omega^d{}_\beta e^\beta{}_i(x) \tag{15}$$

since F_S is a functional of $g_{\mu\nu}$ only.

The relation between these two approaches has remained a challenging open problem (see ref. [2]). It is the purpose of this note to propose a possible solution which may eventually be extended to a proper unified geometric theory of defects and stresses.

The basic idea goes back to a recent observation, made in the context of a theory of melting, that a grand canonical ensemble of fluctuating random loops of dislocations

([6]) H. Schaefer: *Z. Angew. Math. Mech.*, **33**, 356 (1953); S. Minagawa: *RAAG Memoirs of the Unifying Study of Basic Problems in Engineering and Physical Sciences by Means of Geometry*, edited by K. Kondo, Vol. **3** (1962), p. 193; K. Kondo: *RAAG Memoirs of the Unifying Study of Basic Problems in Engineering and Physical Sciences by Means of Geometry*, edited by K. Kondo, Vol. **3** (1962), p. 148; Y. Yamamoto: *RAAG Memoirs of the Unifying Study of Basic Problems in Engineering and Physical Sciences by Means of Geometry*, edited by K. Kondo, Vol. **2** (1958), p. 165; S. Amari: *RAAG Memoirs of the Unifying Study of Basic Problems in Engineering and Physical Sciences by Means of Geometry*, edited by K. Kondo, Vol. **4** (1968), p. 153. See also E. Kröner: *Kontinuumstheorie der Versetzungen und Eigenspannungen*, in *Ergebnisse der Angewandten Mathematik*, Vol. **5**, edited by L. Lösch and F. Lösch (Heidelberg, 1958); Lectures presented at the *1980 Summer School on the Physics of Defects* in Les Houches.

can be described by a field theory, whose coupling to the stresses is gauge invariant. Upon further study ([8]), this gauge invariance revealed itself as a limiting form of general co-ordinate invariance in the low-temperature limit ([*]) in which the spin of the dislocation fields $s \sim b\mu l^2/T$ grows to infinity such that its spatial components commute. In this theory, the dislocation density of linear elasticity (where the indices a and i are the same) turns out to be simply the canonical spin current density

(16) $$\alpha^{ai} = \tfrac{1}{2}\varepsilon^{abc}S_{bc,}{}^{i}$$

with $S_{bc,}{}^{i} = -(i/2)\pi^i S_{bc}\varphi$ in terms of matter fields φ, $\pi \equiv \partial f_m/\partial\partial_i\varphi$, and spin matrix $S_{ab}(f_m$ is the matter energy density). The divergence of this object can be calculated, since spin plus orbital angular currents are conserved, as

(17) $$\partial_i\alpha^{ai} = -\tfrac{1}{2}\varepsilon^{abc}\partial_i(x^b\theta^{ci} - x^c\theta^{bi}) = \varepsilon^{aic}\theta^{ic},$$

where θ^{ab} is the canonical momentum tensor. This is to be compared with the present defect formulae (11), such that the disclination density turns out to be simply the canonical momentum tensor of the defect field theory. Thus the fluctuating disclinations are automatically included in this theory. Moreover, relation (5) is reproduced: it is the standard connection between the symmetric Belinfante momentum tensor (here η_{ij}) and the canonical one (here θ_{ij}), both differing by pure gradient terms involving the spin current (here α_{in}). Thus (2) is an acceptable defect field theory in the continuum limit.

But then there is no problem in coupling defects and stresses. According to our work in ref. ([7,8]), defects move under stress as if they were spinning external particles in a curved space. It is well known how to introduce spin into a gravitational field ([9]).

For this we go to nonholonomic co-ordinates defined differentially via $\partial_a \equiv h_a{}^\alpha\partial_\alpha$, where $h_\alpha{}^\alpha(\boldsymbol{x})$ are orthonormal dreibein fields, just as $e_a{}^\alpha(\boldsymbol{x})$, and

$$\overset{h}{g}_{ab} = h_a{}^\alpha h_b{}^\beta g_{\alpha\beta}(\boldsymbol{x}) = \begin{pmatrix}1 & & \\ & 1 & \\ & & 1\end{pmatrix}_{ab}$$

just as $g_{ab} = e_a{}^\alpha e_b{}^\beta g_{\alpha\beta}(\boldsymbol{x})$. The only difference between $e_a{}^\alpha$ and $h_a{}^\alpha$ is that, when calculating connections $\overset{h}{\Gamma}_{\alpha\beta}{}^\gamma$ as in (1) but using $h_a{}^\alpha$, we allow only the torsion to be nonzero, while the curvature vanishes, $\overset{h}{R}_{\alpha\beta\gamma}{}^\delta = 0$. The defect energy can be expressed entirely in terms of $h_a{}^\alpha$ and $K_{\alpha\beta}{}^\gamma$ in the form

(18) $$F_{\text{def}}[h, K] = \int d^3x \sqrt{\overset{h}{g}}\, h^{a\alpha}h^{b\beta}R_{\alpha\beta ab},$$

where

(19) $$R_{\alpha\beta ab} = \partial_\alpha A_{\beta ab} - \partial_\beta A_{\alpha ab} - [A_\alpha, A_\beta]_{ab}$$

([*]) Which usually comprises the melting point, *i.e.* at $T = T_{\text{melt}}$, the value of s is still quite large. For a Lindemann parameter $L = 120$ one has $s = 60$ and s grows like L^2 ([8]).

([7]) H. KLEINERT: Berlin preprint (June 1981) (September 1981). Lecture presented at the *Conference of the European Physical Society, Lisbon, July 1981*, *Phys. Lett. A*, **89** 294, (1982).

([8]) H. KLEINERT: *Lett. Nuovo Cimento*, **34**, 471 (1982),

([9]) F. W. HEHL, P. VAN DER HEYDE and G. D. KERLICK: *Rev. Mod. Phys.*, **48**, 393 (1976).

is the covariant curl of the gauge field $A_{\alpha ab} \equiv (A_\alpha)_{ab} = K_{\alpha ab} - \overset{h}{K}_{\alpha ab}$ and K is the original contortion (indices can be changed from α to a via $h_a{}^\alpha$). Similarly, the stress energy can be brought to co-ordinates $\overset{s}{h}{}^\alpha{}_i$ by simply replacing g_{ij} by $\overset{s}{h}{}^\alpha{}_i \overset{s}{h}_{\alpha j}$ in (13), *i.e.* $F_s[\overset{s}{h}{}^\alpha] \equiv F_s[g_{ij} \equiv \overset{s}{h}{}^\alpha{}_i \overset{s}{h}_{\alpha j}]$. Now the movement of the spinning defect particles $h_a{}^\alpha$ in the stress field $\overset{s}{h}{}^\alpha{}_i$ can simply be obtained by adding $F_s[\overset{s}{h}]$ and $F_{\text{def}}[h, K]$ with $h^a{}_\alpha$ replaced by $\tilde{h}^a{}_\alpha \equiv h^a{}_\beta h^\beta{}_i$:

$$F[\overset{s}{h}, h, K] = F_s[\overset{s}{h}] + F_{\text{def}}[h, \overset{s}{h}, K - \overset{h}{K}] . \tag{20}$$

Minimization with respect to $\overset{s}{h}{}^\alpha{}_i$ leads to

$$\varepsilon_{\alpha\gamma\delta}\,\varepsilon_{\beta\sigma\tau}\,\partial_\gamma\,\partial_\sigma\,\sigma_{\delta\tau} - \frac{\nu}{1+\nu}\,(\delta_{\alpha\beta}\,\partial^2 - \partial_\alpha\,\partial_\beta)\,\sigma_{\gamma\gamma} = 2\mu\eta_{\alpha\beta} + \text{nonlinear terms},$$

which is the well-known source equation for stress in the presence of defects.

Minimization with respect to $h^a{}_\beta$ and $K_{\alpha\beta}{}^\gamma$ gives the field equations of defects $\alpha = 0$, $\eta = 0$, where α and η are given by (4) and (5) except that all quantities are expressed in terms of « stressed » dreibeins $\tilde{h}$ rather than h.

The theory can be completed by adding torsion terms to the stress energy, but due to their experimental smallness we have not yet done so.

It was shown before (7,8) how the fluctuations in the defect field correspond to summing over all closed defect loops. Notice that there still is freedom in adding interactions among the defects which will play a crucial role in the study of phase transitions such as melting (7).

In conclusion we see that, in the absence of stress, the field theory (20) has all the properties of our defect field theory except for its spin s having the specific value $s = 2$. Previously, (7,8) we had required s to be large. In order to understand the difference with the present treatment, we must remember that, in our previous theory, the largeness was due to the finiteness of the Burgers vector $\boldsymbol{b}$. In the present proper continuum theory, $\boldsymbol{b}$ goes to zero. In order to cope properly with the noncommutative aspects of defects, however, it is essential that the spin does not become completely zero. The value $s = 2$ seems to be the smallest possibility capable of realizing the nontrivial algebraic aspects of the defect structure in a true continuum theory.