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ON DYNAMIC PROPERTIES OF DISCLINATIONS IN THE CONTINUUM MODEL

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1. What is said today being a disclination essentially is the same as Volterras distorsion of 4., 5. or 6. kind. Volterras distorsion of 1., 2. or 3. kind are well known as dislocations. Experimentally they were detected in crystals in 30s, and the continuum theory of dislocations was given by Kroner, Bilby, Bullough and Smith and Kondo et al. in 50s.

At latest from the experiments of Trauble and Essmann (1) we known, that disclinations really exist in crastals too. In the continuum model of the crystal at first by Anthony (2) was given a field theory of static disclinations. This theory enables us to calculate stress fields created by a disclination located at a fixed place. It is an extension of dislocation theory in geometrical terms, that means an extension of the theory with distant parallelism, describing dislocations, to a theory with non vanishing curvature. The main point is, that disclinations can be set in a one to one correspondence to curvature tensor, in formulas

$$E_{ij} = -\nu_{ij} \tag{1}$$

with

$$E_{ij} \underset{Df}{=} R_{nij}{}^{n} - \frac{1}{2} g_{ij} R_{npq}{}^{n} g^{pq},$$

$$g_{ij} = \sigma_{ij} - 2\epsilon_{ij}, \qquad \epsilon_{ij} = \text{elastic strain},$$

$$R_{ijk}{}^{l} = \Gamma^{l}_{jk,i} - \Gamma^{l}_{ik,j} + \Gamma^{r}_{jk}\Gamma^{l}_{ir} - \Gamma^{r}_{ik}\Gamma^{l}_{jr},$$

$$\Gamma^{l}_{ik} = \{^{l}_{ik}\} + T_{ik}{}^{l} + T^{l}{}_{ik} + T^{l}{}_{ki}$$

with Chirstoffel – affinity $\{^{i}_{kl}\} = \frac{1}{2} g^{ir} (- g_{kl,r} + g_{kr,l} + g_{rl,k})$ and torsion $T_{ik}{}^{l} = \frac{1}{2}(\Gamma^{l}_{ik} - \Gamma^{l}_{ki})$. According to Anthony ν_{ij} describes the disclination density and in general is followed by a non vanishing $T_{ik}^{(v)l}$. The torsion parts $T_{ik}^{(v)l}$ describes dislocations, and the separation $T_{ik}{}^{l} = T_{ik}^{(v)l} + T_{ik}^{(\nu)l}$ can be done unique.

As for dislocations only, the equations for moving disclinations can be followed by a geometrical generalization of (1), cf. Gunther [3], [4]. We here only need the linearized equations. Together with the linearization of (1) they read, cf. [3], [4].

$$\text{a)}\ \epsilon_{ij,rr} + \epsilon_{rr,ij} - \epsilon_{ri,rj} - \epsilon_{rj,ri} = -\frac{1}{2}(\nu_{ij} + \nu_{ji}) + \delta_{ij}\nu_{rr} + \frac{1}{2}[\in_{riq}\alpha_{qj,r} + \in_{rjl}\alpha_{qi,r} + \in_{jrq}\alpha_{qr,i} + \in_{irq}\alpha_{qr,j}]$$

$$\text{b)}\ \alpha_{kl,0} + \in_{ijk} J_{il,j} = \delta_{kl} S_{rr} - S_{lk},$$

$$\text{c)}\ \alpha_{ri,r} = -\in_{irs}\nu_{rs}$$

$$\text{d)}\ \epsilon_{ik,0} - \frac{1}{2}(v_{k,i} + v_{i,k}) = -\frac{1}{2}(J_{ik} + J_{ki}),$$

$$\text{e)}\ \nu_{i,k,i} = 0$$

$$\text{f)}\ \nu_{ik,o} = \in_{irs} S_{sk,r}.$$

where $S_{ik} = \in_{irs} V_r^{(\nu)} \nu_{sk}$, $\alpha_{ij} = -\in_{irs} T^{rs}{}_j$, I_{ik} is torsion current, $V_r^{(\nu)}$ disclination velocity, v_k material velocity.

We remember to a possible interpretation of I, cf. [3]. If a disclination is varying its place, this in general is followed by a creation or annihilation of dislocations. This also can be followed by detailled consideration of the process of the motion of a disclination, cf. deWit [5]; geometry is only one way of getting the equations of moving disclinations.

2. Now, dislocations and disclinations create stress fields, and as a consequence of these fields they tend to leave its places. If you consider some source in its own field alone (as in electro dynamics was done e.g.by Abraham and Sommerfeld, [6]), you get as we will say the field theoretic dynamic equation for this source. As in electrodynamics for this you need the field and the force only. Now, from field equations you can get energy – impuls equation immediately by a suitable calculation or in general by Noethers theorem. Than the force on a source of the field is the consequence from the fact, that the generated field usually does not define an equilibrium state; that means energy – impuls conservation of the field is violated. Therefore the divergence of energy – impuls tensor of the field is not zero but defines the force density on the source. In analogy to Abraham–

Sommerfeld approach for electrons it is demanded that the whole source is in equilibrium again. That means, the total force on this source has to be zero, being an integral equation for the motion of the defect.

On this lines you can get for dislocations the Peach – Köhler – Kosevich force density

$$\widetilde{k}_i = 2(\sigma_{rs}\, T_i^{rs} + \frac{1}{2}\rho_o\, v_s\, J_{rs})$$

and as the consequence of the field theoretic dynamic equation

$$\widetilde{K}_i = \int k_i d\tau = 0 \qquad \text{(integration over the defect)}$$

you get vibrating dislocations (generalizing the string model), cf. Pegel (7), or in super sound region a differential equation for the motion of this specialized dislocation with the expression for mass and the Cerenkov damping force (8). As we have seen, the field equations for disclinations are known. Therefore it is only a matter of straight forward calculations according to the theory to get the general expression for the force in a medium with dislocations and disclinations. Refering to a linearized and isotrop medium with stresses and momentum stresses according to

II

a) $\sigma_{ij,i} - \rho_o \dot{v}_j = 0,$

b) $\mu_{ij,i} - \in_{jrs}\sigma_{rs} - \theta_{jk}\ddot{\varphi}_k = 0,$

where ρ_o is the density of the medium, σ_{ij} and μ_{ij} are the stresses and momentum stresses, φ_j angular velocity, θ_{jk} inertial tensor, and the material equations

III

a) $\sigma_{ik} = 2\mu\epsilon_{ik} + \lambda\delta_{ik}\epsilon,$

b) $\mu_{ik} = M\chi_{ik}$

hold. Than the force density reads as follows

$$k_j = \in_{jkl}(\sigma_{lm}\,\alpha_{km} + \sigma_{mk}\,(\chi_{ml} + \varphi_{lim}) + \mu_{lm}\,\nu_{km}) + \rho_o v_l J_{jl} - \\ - \theta_{lk}\dot{\varphi}_k\, S_{jl}\,. \qquad (2)$$

Here the term $\kappa_{em} + \varphi_{lim}$ is to be determined from

$$S_{ik} = \dot{\chi}_{ik} + \dot{\varphi}_{k,i}\,.$$

As we could point out, with suitable specifications and interpretations this force at first can be found in the papers of Kluge (9).

3. On the basis of

$$K_i = \int k_i \, d\zeta = 0 \tag{3}$$

we ask for the dynamical properties of a single wedge disclination in a two dimensional lattice. As is clear, an analogous dislocation would behave as a Newtonian material point, staying at rest or uniform motion, because this is the well known behaviour of a straight dislocation in a three dimensional lattice, if field theoretic forces are considered only. As we will see, the situation for disclinations is completely different from this, however.

At first we satisfy I b), c), e), f) by

$$\begin{aligned}
\nu_{33} &= \Omega \underset{\alpha}{\delta}(y)\, \underset{\alpha}{\delta}[x - s(t)], \\
V_r^{(\nu)} &= \delta_r^1 \, \dot{s}(t), \\
\alpha_{32} &= -\Omega \underset{\alpha}{\delta}(y)(\underset{\alpha}{\theta}[x - s(t)] - \theta(x)), \\
S_{23} &= -\Omega \underset{\alpha}{\delta}(y)\, \underset{\alpha}{\delta}[x - s(t)] \cdot \dot{s}(t), \\
J_{ik} &= 0, \\
\chi_{23} + \varphi_{3,2} &= \Omega \underset{\alpha}{\delta}(y)\, \underset{\alpha}{\theta}[x - s(t)], \quad \text{(the other components vanish)}
\end{aligned} \tag{4}$$

where

$$\underset{\alpha}{\delta}(x)\, \underset{\alpha}{\delta}(y) = \frac{1}{4\pi^2} \int e^{-\alpha\sqrt{k^2 + \chi^2}} \, e^{i(ky + \chi x)} \, dk d\chi,$$

$$\underset{\alpha}{\theta}(x)\, \underset{\alpha}{\delta}(y) = -\frac{i}{4\pi^2} \int \frac{e^{-\alpha\sqrt{k^2 + \chi^2}}}{\chi} \, e^{i(ky + \chi x)} \, dk d\chi,$$

α being a parameter defining the size of the disclination. We now assume, the inertial term being of the form $\theta_{i\rho} = \rho_o r_o^2 \delta_{ik}$ and the terms resulting from momentum stresses shall be small compared with the terms from force stresses, i.e.

$$\mu_{ij} \ll \sigma_{ij}, \qquad r_o^2, M \ll \lambda, \mu .$$

Expanding strain in a power series of M and restricting to first order terms in M

$$\epsilon_{ij} = \underset{o}{\epsilon}_{ij} + M \underset{r}{\epsilon}_{ij},$$

it can be followed from field equations I, II, III and (3) that:

A) The field $\underset{o}{\epsilon}_{ij}$ is statically, tending to the solution of Anthony (2) for $\alpha \to 0$ (for the exact formulas see [4]).

B) $\underset{1}{\epsilon}_{ij}$ is of the form

$$\underset{1}{\epsilon}_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$$

C) A non vanishing force K_i only results from $\underset{1}{\epsilon}_{ij}$. The only component different from zero reads

$$\underset{1}{K}_1 = 2\mu\Omega \iint u_{1,1} \underset{\alpha}{\delta}(y)\, \underset{\alpha}{\theta}(x)\, dxdy + M\Omega \iint \alpha_{32}\, \underset{\alpha}{\delta}(y)\, \underset{\alpha}{\delta}[x - s(t)]\, dxdy \qquad (5)$$

where u_1 is to be determined from field equation I, II, III. Assuming a constant position $s(t) = s_o$ of the disclination, after some calculations we get

$$\underset{1}{K}_1^{(S_o)} = -\frac{M\Omega^2}{4\pi\alpha} \frac{s_o}{\sqrt{s_o^2 + 4\alpha^2}} \frac{\sqrt{s_o^2 + 4\alpha^2} - 2\alpha}{\sqrt{s_o^2 + 4\alpha^2} + 2\alpha} \qquad (6)$$

with the limits

$$\underset{1}{K}_1^{(s_o)} \xrightarrow[s_o \gg \alpha]{} -\frac{M\Omega^2}{4\pi\alpha} \operatorname{sign}(s_o), \qquad (7)$$

$$\underset{1}{K}_1^{(s_o)} \xrightarrow[s_o \ll \alpha]{} -\frac{M\Omega^2}{16\pi\alpha} \left(\frac{s_o}{2\alpha}\right)^3. \qquad (8)$$

That means, the disclination is bound to the equilibrium position $s_o = 0$. For small s_o there is acting a restoring force $\sim s_o^3$, and for big s_o the restoring force will be constant.

If the motion of disclination $s = s(t)$ is not prescribed arbitrarily, this function $s(t)$ is determined by the field theoretic dynamic equation (3). Omitting the calculations again, we get a non linear integral equation for $s(t)$

$$\underset{1}{K}_1^{(d)} \equiv \frac{M\Omega^2}{4\pi\alpha} \frac{s(t)}{\sqrt{s(t^2) + 4\alpha^2}} - \frac{M\Omega^2}{2\pi^2} C_T \int_{-\infty}^{t} dt' \int_{0}^{\infty} d\rho \int_{0}^{2\pi} d\psi\, e^{-2\alpha\rho} \rho \sin[\rho C_T(t-t')]$$

$$\sin[\rho \cos\psi\, s(t')] \frac{\sin^2\psi}{\cos\psi} = 0, \qquad (9)$$

where c_T is the velocity of transversal sound waves.

In order to discuss physical contents of (9) we expand (9) in a power series of $s/2\alpha$ (being small by definition). Denoting $\sigma = s/2\alpha$, $\omega_o = C_T/2\alpha$, we get, restricting to third order terms in σ

$$\sigma(t) - \frac{1}{2}\sigma^3(t) + \int_0^{\infty} [2\sigma(t - \frac{\zeta}{\omega_o}) \frac{\zeta^3 - 3\zeta}{(1+\zeta^2)^3} +$$

$$\sigma^3(t - \frac{\zeta}{\omega_o}) \frac{\zeta^5 - 10\zeta^3 + 5\zeta}{(1+\zeta^2)^5}]\, d\zeta = 0, \quad (\sigma \ll 1) \quad (10)$$

Taking into consideration first order terms only, there is a formal solution

$$\sigma = a + bt. \tag{11}$$

However, (11) soon comes into contradiction to the supposition $\sigma \ll 1$ and than restoring forces according to (6) appear. Further, if we ask for periodic solutions than the point $s_o = 0$ has to be a symmetry point for the function s(t). Therefore with the initial condition s(0) = 0, only solutions of the kind s(t) = –s(-t) shuolc to be expected, that is

$$\sigma (t) = - \sigma (- t). \tag{12}$$

Any periodic solution than would allow an expansion

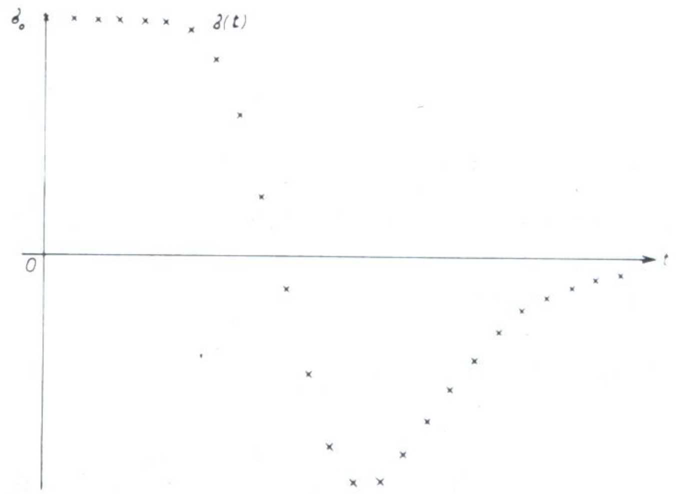
$$\sigma (t) = \sum_{n=1}^{\infty} a_n \sin (n\omega t) \tag{13}$$

Nevertheless, it can be shown by the power series expansion of (9) up to any fixed order in σ, that equation (9) for $\sigma(t)$ according to (13) allways demands

$$a_n = 0 \quad \forall_n : \sigma \equiv 0. \tag{14}$$

That means, any reasonable periodic solution of (9) does not exist.

Therefore, if we ask for the motions of disclinations only due to self forces, than only damped oscillations are to be expected. In order to get such solutions the numerical approach to solve (10) seems to be reasonable. The calculations are not finished as yet. A priliminary result is given by the figure below



(For this disclination we have supposed, that it is turned out by any external force up to $\sigma(t) = \sigma_o$, $t < 0$, but for $t > 0$ only self forces are acting).

LITERATURE

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Резюме

Дисклинации расматриваются в модели сплошней среди. Исследуется при помощи интегрального уравнения, следующего из закона сохранения энергии импульса теории поля, движение дисклинаций под действием собственных сил. В результате получается, что дисклинации связанны с положением равновесия с характеристической возвращающей млой. Дисклинации не могут совершить периодические собственные колебания, возможы только затукающие колебания.

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