"Maxwell-Gleichungen, Energiesatz und Lagrange-Dichte in der Kontinuumstheorie der Versetzungen, Acta Mech. **10** (1970), 59-66.

Maxwell's equations, the law of energy, and the Lagrangian density in the continuum theory of dislocations

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(Received on 21 June 1960)

Summary

The continuum theory of moving dislocations is mathematically analogous to MAXWELL's equations of electrodynamics. This analogy shows that the present linear theory of dislocations is incomplete and must be supplemented by constitutive equations between dynamical and kinematical quantities. MIE's generalized electrodynamics points the way to a Lagrangian density. Whereas, in the static case, the stress functions of the continuum are reaction forces with the task of preventing the motion of dislocations, they become impressed forces in the field of moving dislocations and are connected with the dislocation density by constitutive equations.

§ 1. Introduction. – At this point in time, the linear continuum theory of dislocations and internal stresses **[1]** consists of the system of three equations:

$$\varepsilon_{i\lambda\mu}\,\partial_\lambda\,\beta_{\mu k} = D_{ik}\,,\tag{1.1}$$

$$\partial_i v_k - \beta_{ik} = I_{ik} , \qquad (1.2)$$

$$\partial_i \sigma_{ik} - \rho \dot{v}_k = 0. \tag{1.3}$$

In this:

- β_{ik} Distortion tensor, whose symmetric part $\beta_{(ik)} = \varepsilon_{ik}$ is the deformation tensor
- v_k Material velocity vector
- ρ Mass density
- σ_{ik} Stress tensor
- *D*_{*ik*} Dislocation density tensor
- *I_{ik}* Dislocation current tensor

We call equations (1.1) and (1.2) the *kinematical equations*, while (1.3) are the *dynamical equations*.

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In our notations, x_1 , x_2 , x_3 are the Cartesian coordinates, ε_{ikl} is the unit tensor that is alternating in all indices, $\partial_i = \partial / \partial x_i$, and the dot over a quantity means its partial derivative with respect to time *t*.

HOOKE's law exists between stress and extension in an elastic body:

$$\sigma_{ik} = \lambda_{iklm} \, \mathcal{E}_{lm} \,. \tag{1.4}$$

H. GÜNTHER [1] has shown that the system of equations (1.1) to (1.4) can be integrated when one freely prescribes D_{ik} at one time-point and I_{ik} for all time.

§ 2. Maxwell's equations for the theory of dislocations. – If one ignores the index k in the basic equations (1.1), (1.2), and (1.3) then β_{ik} and v_k can be interpreted as the LORENTZ four-potential of an electromagnetic field $E_i \sim I_{ik}$, $B_i \sim D_{ik}$, while (1.3) seems to be the analogue of the equation of continuity for the charge density. That analogy with electrodynamics will become clearer when one eliminates the "potentials" β_{ik} and v_k from (1.1) and (1.2):

$$D_{ik} + \varepsilon_{i\alpha\beta} \partial_{\alpha} I_{\beta k} = 0, \quad \partial_i D_{ik} = 0.$$
(2.1), (2.2)

In these homogeneous "MAXWELL equations," (2.1) is the analogue of FARADAY's law of induction. Equation (2.2) contains the geometric statement that dislocation lines are always closed or that they can begin and end only on the outer surface of the body, and it is analogous to the non-existence of magnetic monopoles.

The inhomogeneous "MAXWELL equations" will appear when one fulfills:

$$\dot{\psi}_{ik} - \varepsilon_{i\alpha\beta} \,\partial_{\alpha} \,\varphi_{\beta k} = - \,\sigma_{ik} \,, \qquad \partial_i \,\psi_{ik} = - \,p_k \tag{2.3}, (2.4)$$

identically in the "impulse potentials" ψ_{ik} and the "stress potentials" φ_{ik} .

In the conventional notations of MAXWELL's theory, the analogy here reads:

Charge density	ρ ~ negative impulse	$\rho v_k = p_k$,
Current density	$s_i \sim \text{stress}$	$\sigma_{\!ik}$,
Charge potential	$D_i \sim \text{impulse potential}$	$oldsymbol{\psi}_{ik}$,
Current potential	$H_i \sim$ stress potential	$oldsymbol{arphi}_{ik}$.

One test for the correctness of this association is to calculate the analogues of the LORENTZ force density f_k and the power density λ :

$$f_k = \rho E_k + \varepsilon_{klm} \, s_l \, B_m \,, \tag{2.5}$$

$$\lambda = s_i E_i , \qquad (2.6)$$

which are:

$$F_k = -\rho v_i I_{ik} + \mathcal{E}_{klm} \sigma_{li} D_{mi} , \qquad (2.7)$$

$$\Lambda = \sigma_{ik} I_{ik} , \qquad (2.8)$$

resp.

The expression ε_{klm} σ_{li} D_{mi} is the well-known PEACH-KOEHLER force density, which originates in the dislocation density in the stress field [2]. The first sum on the right in (2.7) was found by KOSEVICH [3]. He interpreted it as the force density that originates in the dislocation current density I_{ik} in the velocity field.

We will encounter the expression (2.8) once more when we present the law of energy. It is the power density that is transferred from the field of the moving dislocations to the "matter" [4].

However, this impressive analogy will collapse when we consider the constitutive equations (viz., material law) in both theories. An analogue to HOOKE's law (1.4) does not exist in MAXWELL's theory. The four-vector of the LORENTZ potential is only a computational convenience. Things are different in the theory of dislocations:

 β_{ik} and v_k in (1.1) and (1.2) are well-defined quantities that are coupled to σ_{ik} and p_k by constitutive equations. In MAXWELL's theory of macroscopic electrodynamical phenomena, it is known that constitutive laws exist between D_i and E_i , on the one hand, and H_i and B_i , on the other. If we were to try to draw an analogy to the theory of dislocations here then the impulse and stress potentials ψ_{ik} , φ_{ik} , which have been only computational conveniences, up to now, would have to be coupled with the dislocation current density I_{ik} and the dislocation density D_{ik} by constitutive laws. Here, a fundamental deficiency in our dislocation theory becomes clear, namely, that the dislocation current density I_{ik} (a measure of the number of dislocations that enter into a volume element per second) must be given for all times if the system of equations (1.1) to (1.4) is to be integrable. However, from whence does once gather that knowledge? Here, we have only one-half of the theory before us. The analogy points to the way that one must extend the theory to moving dislocations.

§ 3. The law of energy. – We shall first summarize the equations of the theory of dislocations that include differentiations with respect to time:

$$-\dot{p}_{k}+\partial_{i}\sigma_{ik}=0, \qquad (3.1)$$

$$\dot{D}_{ik} + \mathcal{E}_{i\alpha\beta} \,\partial_{\alpha} \,I_{\beta k} = 0, \tag{3.2}$$

$$-\dot{\beta}_{ik} + \partial_i v_k = I_{ik}, \qquad (3.3)$$

$$\dot{\psi}_{ik} - \varepsilon_{i\alpha\beta} \,\partial_{\alpha} \,\varphi_{\beta k} = - \,\sigma_{ik} \,. \tag{3.4}$$

Now if (as we presume) all quantities that enter into these equations by way of their spatial derivatives (hence, v_k , σ_{ik} , φ_{ik} , I_{ik}) are coupled to those quantities that appear in time derivatives (namely, p_k , β_{ik} , D_{ik} , ψ_{ik}) by constitutive equations then a closed system of equations must arise (say, for p_k , β_{ik} , D_{ik} , ψ_{ik}) in which those quantities are coupled to each other by way of their temporal and spatial derivatives and that is integrable with the prescribed initial conditions. Now, it follows from (3.2) that:

$$\frac{\partial}{\partial t}(\partial_i D_{ik}) = 0, \qquad (3.5)$$

and from (3.2) and (3.3) that:

$$\frac{\partial}{\partial t} \left(D_{ik} - \varepsilon_{i\lambda\mu} \,\partial_\lambda \,\varphi_{\mu k} \right) = 0, \tag{3.6}$$

and from (3.1) and (3.4):

$$\frac{\partial}{\partial t}(\partial_i \,\psi_{ik} + p_k) = 0. \tag{3.7}$$

However, those are, in essence, the remaining equations of the theory of dislocations. It one demands that they should be valid at a certain time-point then they will be valid for all times on the basis of the integrable system of equations (3.1) to (3.4).

All of this consists of only suspicions to begin with. However, MIE's generalized electrodynamics [5], namely, "Die Grundlagen einer Theorie der Materie," points the way to the constitutive equations that we are still missing. We shall follow the clear and concise presentation of that theory by H, WEYL [6].

MIE postulated that the energy is localizable in space and time in such a way that a law of energy of the form:

$$\frac{\partial W}{\partial t} + \partial_i \Sigma_i = 0 \tag{3.8}$$

would exist, where W is the energy density and Σ_i is the energy current vector.

In order to get such an equation in our theory if dislocations, we first multiply eq. (3.1) by v_k and eq. (3.3) by σ_{ik} and add them:

$$-v_k \dot{p}_k - \sigma_{ik} \dot{\beta}_{ik} + \partial_i (v_k \sigma_{ik}) = \sigma_{ik} I_{ik}.$$
(3.9)

For later purposes, we define the analogue to POYNTING's law of electrodynamics by multiplying (3.2) by φ_{ik} and (3.4) by I_{ik} and then adding. After an intermediate calculation, we will get:

$$\varphi_{ik}D_{ik} + I_{ik}\dot{\psi}_{ik} + \partial_i \left(v_k \,\sigma_{ik}\right) = - \,\sigma_{ik} \,I_{ik} \,. \tag{3.10}$$

On the right-hand side of both equations (3.9) and (3.10), we again recognize the power density (2.8). In (3.10), it was inferred from the "dislocation field," and in (3.9), it was supplied by the "matter field", or conversely.

We must now call upon an intermediate consideration in regard to the symmetry of our tensors. The symmetry of the stress tensor $\sigma_{ik} = \sigma_{ki}$ requires that the impulse potential ψ_{ik} in (2.3) and (2.4) must also be a symmetric tensor. Furthermore, the symmetry of σ_{ik} has the consequence that the asymmetric stress potential $\varphi_{\beta k}$ in (2.3) must be replaced with:

$$\varphi_{\beta k} = \varepsilon_{k\lambda\mu} \,\partial_\lambda \,F_{\beta\mu} \,, \tag{3.11}$$

so with the BELTRAMI stress function $F_{\beta\mu} = F_{\mu\beta}$. If we indicate the symmetric part of a tensor by parentheses, as usual, then equation (3.9) will imply that:

$$- v_k \dot{p}_k - \sigma_{ik} \dot{\varepsilon}_{ik} + \partial_i (v_k \sigma_{ik}) = \sigma_{ik} I_{(ik)}, \qquad (3.12)$$

and (3.10), with (3.11), will imply that:

$$\varepsilon_{k\lambda\mu}\dot{D}_{ik}\partial_{\lambda}F_{i\mu}+I_{(ik)}\dot{\psi}_{ik}+\partial_{i}\left(\varepsilon_{irs}I_{rk}\varepsilon_{k\lambda\mu}\partial_{\lambda}F_{s\mu}\right)=-\sigma_{ik}I_{(ik)}.$$
(3.13)

Now, one has:

$$\varepsilon_{k\lambda\mu}\dot{D}_{ik}\partial_{\lambda}F_{i\mu} = \partial_{i}(\varepsilon_{i\mu k}F_{\lambda\mu}\dot{D}_{\lambda k}) + F_{ik}\varepsilon_{k\lambda\mu}\partial_{\lambda}\dot{D}_{ik}. \qquad (3.14)$$

Due to the symmetry of F_{ik} , the second summand on the right here can be written as:

$$F_{ik} \frac{1}{2} \Big(\varepsilon_{k\lambda\mu} \partial_{\lambda} \dot{D}_{i\mu} + \varepsilon_{i\lambda\mu} \partial_{\lambda} \dot{D}_{k\mu} \Big) = F_{ik} \dot{\eta}_{ik}, \qquad (3.15)$$

in which we have introduced KRÖNER's incompatibility tensor [7]:

$$\eta_{ik} = \frac{1}{2} \Big(\varepsilon_{k\lambda\mu} \partial_{\lambda} \dot{D}_{i\mu} + \varepsilon_{i\lambda\mu} \partial_{\lambda} \dot{D}_{k\mu} \Big).$$
(3.16)

Due to (1.1), one will have:

$$\eta_{ik} = \varepsilon_{i\alpha\beta} \varepsilon_{k\lambda\mu} \partial_{\alpha} \partial_{\lambda} \beta_{(\beta\mu)} = \varepsilon_{i\alpha\beta} \varepsilon_{k\lambda\mu} \partial_{\alpha} \partial_{\lambda} \varepsilon_{\beta\mu} . \qquad (3.17)$$

We now use (2.1), (3.14), and (3.15), in order to put (3.13) into the form:

$$F_{ik} \dot{\eta}_{ik} + I_{(ik)} \dot{\psi}_{ik} + \partial_i \varepsilon_{irs} \varepsilon_{k\lambda\mu} (I_{rk} \partial_\lambda F_{\mu s} - F_{rk} \partial_\lambda I_{\mu s}) = -\varepsilon_{ik} I_{(ik)}.$$
(3.18)

We shall now show that the symmetric parts $I_{(rk)}$ and $I_{(\mu s)}$ of I_{rk} and $I_{\mu s}$, resp., can also be substituted in the third summand on the left. Performing the differentiation implies:

$$\varepsilon_{irs} \varepsilon_{k\lambda\mu} \left(\partial_i F_{rk} \partial_\lambda I_{\mu s} - \partial_i I_{rk} \partial_\lambda F_{\mu s} + F_{rk} \partial_i \partial_\lambda I_{\mu s} - I_{rk} \partial_i \partial_\lambda F_{\mu s} \right)$$

= $\varepsilon_{irs} \varepsilon_{k\lambda\mu} \left(F_{rk} \partial_i \partial_\lambda I_{(\mu s)} - I_{(rk)} \partial_i \partial_\lambda F_{\mu s} \right),$ (3.19)

when one permutes the dummy indices in the first term suitably. With that, it has been shown that the law of energy includes only the symmetric parts of all tensors that occur. The parentheses in the indices shall now be dropped.

We add (3.12) and (3.18), and a comparison with (3.8) will yield:

$$\Sigma_{i} = v_{k} \, \sigma_{ik} + \varepsilon_{irs} \, \varepsilon_{k\lambda\mu} \, (F_{rk} \, \partial_{\lambda} \, I_{(\mu \, s)} - I_{(rk)} \, \partial_{\lambda} \, F_{\mu \, s}) \tag{3.20}$$

for the energy current, and furthermore that:

$$\frac{\partial W}{\partial t} = -v_k \dot{p}_k - \sigma_{ik} \dot{\varepsilon}_{ik} + F_{ik} \dot{\eta}_{ik} + I_{ik} \dot{\psi}_{ik} . \qquad (3.21)$$

§ 4. Lagrangian density and constitutive equations. – In order to bring a certain degree of order to matters here, we set:

$$W = -p_k v_k + \psi_{ik} I_{ik} - L, (4.1)$$

and with (3.21), we will get:

$$\frac{\partial L}{\partial t} = -p_k \dot{v}_k + \sigma_{ik} \dot{\mathcal{E}}_{ik} - F_{ik} \dot{\eta}_{ik} + \psi_{ik} \dot{I}_{ik} . \qquad (4.2)$$

All kinematical quantities appear in (4.2) as temporal derivatives.

Now, since an energy density W [or, from (4.1), a Lagrangian density L] should exist, according to (4.2), one would need to have:

$$\frac{\partial L}{\partial v_k} = -p_k , \quad \frac{\partial L}{\partial \varepsilon_{ik}} = \sigma_{ik} , \quad \frac{\partial L}{\partial \eta_{ik}} = -F_{ik} , \quad \frac{\partial L}{\partial I_{ik}} = \psi_{ik} .$$
(4.3)

Hence, *L* will have the form:

$$L = L(v_k, \mathcal{E}_{ik}, \eta_{ik}, I_{ik}), \qquad (4.4)$$

and (4.3) will be the constitutive equations.

HAMILTON's principle reads:

$$\delta \int L \, dx_1 \, dx_2 \, dx_3 \, dt = \int \delta L \, dx_1 \, dx_2 \, dx_3 \, dt = 0, \tag{4.5}$$

with

$$\delta L = -p_k \,\,\delta v_k + \,\sigma_{ik} \,\,\delta \varepsilon_{ik} - F_{ik} \,\,\delta \eta_{ik} + \,\psi_{ik} \,\,\delta I_{ik} \,\,. \tag{4.6}$$

In general, the kinematical quantities v_k , ε_{ik} , η_{ik} , I_{ik} cannot be varied independently of each other, since from (3.17), one will have:

$$\delta \eta_{ik} = \varepsilon_{i\alpha\beta} \, \varepsilon_{k\lambda\mu} \, \partial_{\alpha} \, \partial_{\lambda} \, \delta \varepsilon_{\beta\lambda}, \qquad (4.7)$$

and from (1.2):

$$\delta I_{ik} = \frac{1}{2} \left(\partial_i \, \delta v_k + \partial_k \, \delta v_i \right) - \frac{\partial}{\partial t} \, \delta \mathcal{E}_{ik} \,. \tag{4.8}$$

Only v_k and ε_{ik} are free to be varied in (4.4), (4.5), (4.6). The field equations that HAMILTON's principle (4.5) will lead to can already be inferred from (4.6) with no knowledge of the constitutive equations (4.3). The variation δv_k yields:

$$p_k + \partial_i \,\psi_{ik} = 0, \tag{4.9}$$

and the variation $\delta \epsilon_{ik}$ yields:

$$\sigma_{\beta\mu} - \varepsilon_{i\alpha\beta} \,\varepsilon_{k\lambda\mu} \,\partial_{\alpha} \,\partial_{\lambda} \,F_{ik} + \dot{\psi}_{\beta\mu} = 0. \tag{4.10}$$

However, those are the dynamical equations of the theory of dislocations.

If we once more start from (3.21) and introduce the dual Lagrangian density L^* by way of:

$$W = -\sigma_{ik} \varepsilon_{ik} + F_{ik} \eta_{ik} - L^*$$
(4.11)

then we will have:

$$\frac{\partial L^*}{\partial t} = v_k \dot{p}_k - \varepsilon_{ik} \dot{\sigma}_{ik} + \eta_{ik} \dot{F}_{ik} - I_{ik} \dot{\psi}_{ik} . \qquad (4.12)$$

The variations δp_k and $\delta \sigma_{ik}$ in δL^* are once more coupled with $\delta \psi_{ik}$ and δF_{ik} by:

$$\delta p_k = -\partial_i \, \delta \psi_{ik} \tag{4.13}$$

and

$$\delta \sigma_{ik} = \varepsilon_{i\alpha\beta} \, \varepsilon_{k\lambda\mu} \, \partial_{\alpha} \, \partial_{\lambda} \, \delta F_{\beta\mu} - \frac{\partial}{\partial t} \, \delta \psi_{ik} \,, \qquad (4.14)$$

such that the variation $\delta \psi_{ik}$ will imply that:

$$\frac{1}{2} \left(\partial_i v_k + \partial_k v_i \right) - \dot{\mathcal{E}}_{ik} - I_{ik} = 0, \tag{4.15}$$

and the variation δF_{ik} will imply that:

$$\eta_{ik} - \varepsilon_{i\alpha\beta} \varepsilon_{k\lambda\mu} \partial_{\alpha} \partial_{\lambda} \varepsilon_{\beta\mu} = 0.$$
(4.16)

However, those are the kinematical equations for the theory of dislocations, and generally in symmetric form. Our theory then dispenses with a whole series of facts that would follow from the starting equations (1.1) and (1.2). The data that is not utilized here first becomes meaningful in the context of a COSSERAT continuum with compatible curvatures [9].

§ 5. Outlook. – Both of the variational problems with the Lagrangian densities L and L^* confirm that the postulate of the law of energy (3.8) leads to a "complete" and closed theory of dislocations. Whether that theory is in a position to describe, say, the mechanics of an elastic-plastic crystal, depends upon the choice of constitutive equations (4.3). If certain statements can also be made about the constitutive equations *a priori* then their ultimate form must be supported by experiments. We can emphasize that an essential result of this new theory of dislocations is that constitutive equations must exist between impulse potentials and stress potentials, on the one hand, and dislocation densities and dislocation current densities, on the other. In the statics of a continuum with dislocations, the stress potentials degenerate into stress functions that can often be quite useful in calculations, but mainly expendable. In the sense of Lagrangian system mechanics (as HEUN and HAMEL [8] have envisioned it), the stress functions in the static case are "reaction forces" that prevent the dislocations are put into motion that the stress functions will become stress potentials and "impressed forces" whose physical

origins are expressed in the constitutive equations. That suggests a comparison with the forces of static and kinetic friction.

The next problem will now be the computational investigation of the consequences of making the simplest assumption about the constitutive equations.

I would like to thank by colleague J. BAUMGARTE for stimulating discussions.

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