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The force on a lattice defect in an elastic body

R.C. BATRA

Department of Engineering Mechanics, University of Missouri-Rolla, Rolla, MO 65401-0249, U.S.A.

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Abstract

It is shown that the force on a lattice defect in an elastic body is, like the force on a disclination in a nematic liquid crystal, a real force which, for equilibrium, must be balanced by an external force applied to the closed surface enclosing the defect.

Introduction

We refer to an imperfection such as an interstitial and impurity atom, vacant lattice site or a dislocation as a lattice defect. Nabarro [1] defines the force on a segment of a dislocation in an elastic solid so that the energy which could in principle be extracted by letting the segment undergo a small displacement is the scalar product of the force and the displacement. A force on a lattice defect, an inter-phase interface or a crack tip can be similarly defined. Mathematically, the force $\boldsymbol{F}$ on a defect presently located at the position $\boldsymbol{y}$ in an elastic body may be expressed as (Eshelby [2])

$$\boldsymbol{F} = -\frac{\partial}{\partial \boldsymbol{y}}(E_{\text{int}} + E_{\text{ext}}), \tag{1.1}$$

where E_{int} and E_{ext} equal, respectively, the strain energy of the body and the potential energy of surface tractions acting on its boundary. For a linear elastic body, the strain energy density at a screw or edge dislocation approaches infinity [3]. Similar behavior of the strain energy density may occur at a defect in a nonlinear elastic body. This necessitates the modification of equation (1.1) to the following equation

$$\boldsymbol{F} = -\lim_{\epsilon \to 0} \frac{\partial}{\partial \boldsymbol{y}}(E^*_{\text{int}} + E_{\text{ext}}). \tag{1.2}$$

E^*_{int} is the strain energy of the same elastic body except that it now has a hypothetical spherical hole (cylindrical tube in 2-dimensional problems) of radius ϵ centered at $\boldsymbol{y}$. In computing E^*_{int} the deformation field used is the same as that employed to find E_{int}.

Eshelby [2] showed that the force on a defect in an elastic body can be expressed as the integral of an elastic energy-momentum tensor over a surface embracing the defect. He calls this force a configurational force in order to distinguish it from an ordinary force which can be directly balanced by a weight or spring. In a rather recent paper, Eshelby [4] has proved that the energy-momentum tensor appropriate for finding the force on a disclination in a nematic liquid crystal is, to within an unimportant hydrostatic pressure, the same as the Ericksen stress tensor [5] which gives the traction that the fluid exerts on a surface element in it. This implies that the supposed configurational force on a disinclination in a nematic liquid crystal is in fact a real force exerted on the core of the disinclination by the surrounding medium. Here we show that the configurational force on a defect in a nonlinear elastic solid is also a true force exerted on the core of the defect by the surrounding medium. This force can be calculated either by integrating the surface tractions acting on the core of the defect or by integrating a quantity, that resembles the energy-momentum tensor of Eshelby, over a closed surface embracing the defect. In a way, we clarify the various terms to be used in Eshelby's energy-momentum tensor for the nonlinear elastic solid.

Preliminaries

We use a fixed set of rectangular Cartesian coordinate axes and denote the position of a material particle in the reference configuration by X^K ($K=1, 2, 3$) and the present position of the same material particle in the current configuration by x^i ($i=1, 2, 3$). Then

$$x^i = x^i(X^K) \tag{2.1}$$

or its inverse

$$X^K = X^K(x^i) \tag{2.2}$$

describes the deformation of the body. Here we assume that relations (2.1) and (2.2) are invertible except possibly in the neighborhood of a defect, if any, in the body. We use below

$$G_i^K = X^K{}_{,i} \equiv \frac{\partial X^K}{\partial x^i},$$

the inverse of the deformation gradient

$$F^i{}_K = \frac{\partial x^i}{\partial X^K}, \tag{2.4}$$

rather than $\boldsymbol{F}$ to describe the deformation in the neighborhood of a material point.

Let the body occupy a 3-dimensional, bounded and smooth region Ω in the present configuration, and let $W(\boldsymbol{G}(\boldsymbol{x}), \boldsymbol{X}(\boldsymbol{x}))$ denote the strain energy density per unit present volume of the material point $\boldsymbol{X}$ currently situated at the place $\boldsymbol{x}$. We note that for a body that is homogeneous in the reference configuration, W will, in general, depend upon $\boldsymbol{X}$. We assume that W is smooth enough so that the various operations indicated below are meaningful. Loosely speaking, $W \in C^2(\cdot, \cdot)$ will suffice. Equations governing the deformations of the body are (e.g., see Ericksen [6])

$$\left(\frac{\partial W}{\partial G_i^K}\right)_{,i} \quad \frac{\partial W}{\partial X^K} = 0 \quad \text{in } \Omega,$$

$$t_{ij} n_j = f_i \qquad \text{on } \partial_1\Omega, \tag{2.6}$$

$$x_i = \bar{x}_i \qquad \text{on } \partial_2\Omega = \partial\Omega - \partial_1\Omega, \tag{2.7}$$

where

$$t_{ij} \equiv W\delta_{ij} - \frac{\partial W}{\partial G_i^K} G^K{}_j$$

is the Cauchy stress tensor, f_i is the surface traction per unit present area acting on the part $\partial_1\Omega$ of the boundary $\partial\Omega$ of the body, n_i is the outward unit normal on the boundary $\partial\Omega$, δ_{ij} is the Kronecker delta, $\bar{x}_i$ is a prescribed function of X^K on $\partial_2\Omega$, and the usual summation convention on repeated indices is used. Since $\det[G_i^K]$ is assumed to be nonzero, eqn. (2.5) is equivalent to $t_{ij,j} = 0$. We refer the reader to Ericksen's elegant paper [6] for the derivation of eqns. (2.5) and (2.6), their relation to other forms of balance laws, and some other interesting topics in elastostatics.

Now let us assume that an elastic body occupying the region Ω in the present configuration and subjected to surface tractions f_i on the part $\partial_1\Omega$ of the boundary and prescribed current position vectors $\bar{x}_i$ on the part $\partial_2\Omega$ of the boundary has only one defect at a point y in the interior of Ω. Furthermore, let V denote the spherical region of radius ϵ centered at y, and let

$$E = \int_{\Omega - V} W \, \mathrm{d}v + E_{\text{ext}}, \tag{2.9}$$

where E_{ext} is the potential energy of surface tractions f_i on $\partial_1\Omega$. Since f_i depends upon the deformation of $\partial_1\Omega$, E_{ext} is to be computed by integrating the expression

$$\mathrm{d}E_{\text{ext}} = -\int_{\partial_1\Omega} f_i \, \mathrm{d}x_i \, \mathrm{d}s.$$

The deformation field (2.1) or (2.2) and hence the value of E will depend upon, among other factors, the position y of the defect. Eqns. (2.5) and (2.6) will hold everywhere in $\Omega - V$. For a straight line defect such as an edge or a screw dislocation through y, we take for V a cylindrical region of radius ϵ with its axis coinciding with the line defect. Henceforth, this modification of V to the cylindrical region for a line defect will be implied without expressly stating so.

In the following we assume that $|\Delta \boldsymbol{X}|$, $|\Delta \boldsymbol{x}|$ and $|\Delta \boldsymbol{G}|$ are of the order of $|\Delta \boldsymbol{y}|$ where $|\cdot|$ signifies the magnitude of the enclosed quantity. For example, $|\Delta \boldsymbol{y}| = (\Delta y_i \, \Delta y_i)^{1/2}$.

Our main result is the following

THEOREM: *Let $\Sigma \subset \Omega$ be a closed surface enclosing the defect. Then the force F_i on it is given by*

$$F_i = \int_\Sigma \left(W\delta_{ij} - \frac{\partial W}{\partial G_i^K} G_j^K \right) n_j \, \mathrm{d}s = \int_\Sigma t_{ij} n^j \, \mathrm{d}s, \tag{2.10}$$

where $\boldsymbol{n}$ is the outward unit normal to Σ.

Proof of the Theorem.

Let the defect undergo a virtual infinitesimal displacement Δy. Because of this, the deformation field in Ω and the current shape of the body will change. We denote by

Ω^* the region occupied by the body after the defect has moved to $y + \Delta y$, V^* the spherical region of radius ϵ centered at $y + \Delta y$. Then

$$E^* = \int_{\Omega^* - V^*} W\left(G_i^K + \Delta G_i^K,\ X^K + \Delta X^K\right) \,\mathrm{d}v + E^*_{\text{ext}}. \qquad (\quad$$

The change in E because of the displacement Δy of the defect can be written as

$$\Delta E = \int_{\partial\Omega} W(G,\ X)\ \Delta x^i n_i \,\mathrm{d}s - \int_{\partial V} W(G,\ X)\ \Delta y^i n_i \,\mathrm{d}s$$

$$+ \int_{\Omega - V} \left[W(G + \Delta G,\ X + \Delta X) - W(G,\ X)\right] \mathrm{d}v - \int_{\partial_1\Omega} f_i\ \Delta x^i \,\mathrm{d}s. \qquad (3.2)$$

Here and below the unit normal on ∂V points into $\Omega - V$ whereas n on $\partial\Omega$ points out into the exterior of Ω. Since X^K are co-ordinates of a material point in the reference configuration,

$$\Delta X^K + G_i^K\ \Delta x^i = 0. \qquad (3.3)$$

To the first order in $|\Delta X|$ or $|\Delta x|$, the third term on the right-hand side of (3.2) may be simplified as follows.

$$\int_{\Omega - V} \left[W(G + \Delta G,\ X + \Delta X) - W(G,\ X)\right] \mathrm{d}v$$

$$= \int_{\Omega - V} \left[\frac{\partial W}{\partial G_i^K} \Delta G_i^K + \frac{\partial W}{\partial X^K} \Delta X^K\right] \mathrm{d}v$$

$$= -\int_{\Omega - V} \left[\frac{\partial W}{\partial G_i^K} \left(G_j^K\ \Delta x^j\right)_{,i} + \frac{\partial W}{\partial X^K} G^K_{,j}\ \Delta x^j\right] \mathrm{d}v$$

$$= -\int_{\partial_1\Omega} \frac{\partial W}{\partial G_i^K} G_j^K\ \Delta x^j n_i \,\mathrm{d}s + \int_{\partial V} \frac{\partial W}{\partial G_i^K} G_j^K\ \Delta y^j n_i \,\mathrm{d}s$$

$$- \int_{\Omega - V} \left(\frac{\partial W}{\partial X^K} - \left(\frac{\partial W}{\partial G_i^K}\right)_{,i}\right) G_j^K\ \Delta x^j \,\mathrm{d}v.$$

In deriving (3.6) from (3.5)we have integrated by parts, used the divergence theorem, and have set $\Delta x^i = \Delta y^i$ on ∂V. The various terms in the integrands of (3.6) are evaluated at $(G_i^K,\ X^K)$. Note that the integrand of the third integral on the right-hand side of (3.6) is zero because of (2.5). Substitution from (3.6) into (3.2) gives

$$\Delta E = \int_{\partial_1\Omega} \left[\left(W\delta_{ij} - \frac{\partial W}{\partial G_i^K} G_j^K\right) n_i - f_j\right] \Delta x^j \,\mathrm{d}s - \int_{\partial V} \left(W\delta_{ij} - \frac{\partial W}{\partial G_i^K} G_j^K\right) \Delta y^i n_j \,\mathrm{d}s,$$

where W and $\dfrac{\partial W}{\partial G}$ are evaluated at $(G,\ X)$. Because the boundary condition (2.6) is satisfied, the first integral on the right-hand side of (3.7) vanishes. Since, to the first order in $|\Delta y|$,

$$\Delta E = \frac{\partial E}{\partial y^i} \Delta y^i,$$

therefore, from (3.7)

$$\frac{\partial E}{\partial y_i} = -\int_{\partial V}\left(W\delta_{ij} - \frac{\partial W}{\partial G_i^K} G_j^K\right) n_j \, \mathrm{d}s = -\int_{\partial V} t_{ij} n_j \, \mathrm{d}s. \tag{3.8}$$

Let Σ be any closed surface (or a cylindrical tube) enclosing V and hence the defect. Since there is no other defect in the body, various fields such as t_{ij} are smooth in the region enclosed between Σ and ∂V. If there were other defects present in Ω, we would need to choose Σ so that it surrounds V and has no defect other than the one included in V. Thus the integration in (3.8) may be performed over Σ rather than ∂V. Hence

$$\frac{\partial E}{\partial y_i} = -\int_{\Sigma} t_{ij} n_j \, \mathrm{d}s.$$

Recalling (1.2), taking the limit of both sides as $\epsilon \to 0$, and noting that the right-hand side is independent of ϵ gives (2.10).

Remarks

Eqn. (2.10) gives the present force on a defect and since it is obtained by integrating the surface tractions over a closed surface embracing the defect, it equals the force exerted on the closed surface by the surrounding medium. This closed surface can be taken to be the core of the defect. Our result (2.10) agrees with Eshelby's [4] for the force on a disclination in a nematic liquid crystal.

In a recent paper Nabarro [7] has given an outline of the calculations which confirm the view that there is a real mechanical force between an edge dislocation and a line of misfitting solute atoms lying parallel to its own plane, and in the conventional extra half plane.

Expressions like $(2.10)_1$ have been used by Rice [8] and others to find the force on the tip of a crack. Rice's path independent integral corresponds to the component of Eshelby's energy-momentum tensor in the direction of the crack. It seems that one ought to be able to use eqn. (2.10) to find the present force on a crack tip even though we have not explored this in any detail.

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