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On the stress field of a dislocation

By

GÜNTHER LEIBFRIED and KURT LÜCKE

(Communication from the Institut für theoretische Physik and the Institut für allgemeine Metallkunde, Göttingen)

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The stress field of a dislocation is described and compared by various methods. In the first section, a solution will be given by using the tools of pure elasticity theory, and in the second, a simplified derivation and extension of an argument by **Peierls** will be presented that considers the atomic structure approximately. It turns out that the two solutions agree in practice. Finally, those solutions will be compared to one that was given by **Taylor**.

1. – Introduction.

The foundations of the current conception of the mechanism of plastic deformation of crystals is based upon the picture of the formation and motion of dislocations. A dislocation is a characteristic perturbation of the crystal lattice ([1]). The arrangement of atoms in a dislocation for a primitive cubic lattice can be inferred from Fig. 1. One imagines that this arrangement is repeated in all parallel net-planes of the lattice. The characteristic of a dislocation is that above a certain plane – viz., the glide plane ($y = 0$, here) – a larger sequence of atoms is present than below it. Such an arrangement reacts to shear stresses with especial ease. One then describes the plastic deformation by the motion of dislocations in the crystal under the influence of shear stresses. The stress field and the actual atomic arrangement in a dislocation is then of interest in the name of a detailed representation and quantitative statements.

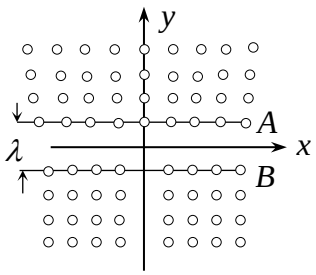

Fig.1. Atomic arrangement in a dislocation.

([1]) Here, we shall consider only the so-called "edge dislocations" that are explained in Fig. 1. As of recently, one also discusses a "screw dislocation" that **Burgers** discovered. However, we shall not go into the latter topic in what follows.

There are two approaches to solving that problem. First of all, one can treat that question with the methods of pure elasticity theory. The foundations for that can be inferred from the works of **Timpe** ([1]) and **Volterra** ([2]). **Taylor** ([3]), who was supported by the work of **Timpe**, gave a first solution for the stress field of a dislocation. However, in our opinion, it is not a good approximation. Later, **Köhler** ([4]) gave another solution without going into the details of what it was based upon. **Peierls** ([5]) gave a second way of arriving at a solution. He considered the atomic structure approximately. For both Ansätze, one assumes that the elastic properties are isotropic.

Here, we would first like to discuss the purely-elastic method in order to be able to compare it to **Taylor**'s solution. In essence, we will obtain **Köhler**'s result. We will then follow through the **Peierls** argument with a somewhat-simpler method in order to compare the solutions. It will show that they agree in practice.

2. – The planar state of dislocation.

We already explained above that in the description of a dislocation, one cares to assume that no displacement appears in the *z*-direction and that the displacement in the *x* and *y*-directions do not depend upon *z*. The *z*-axis is perpendicular to the *xy*-plane in Fig. 1 in the sense of a right-handed system. One will then have an especially-simple elastic problem, namely, the so-called planar state of dislocation ([6]). As a preliminary to the elastic calculations of the following section, we would now like to summarize the relations that are true for this simple case. If *u*, *v*, *w* are the displacements in the *x*, *y*, *z*-directions, resp., then:

$$u = u\,(x, y)\,, \quad v = v\,(x, y)\,, \quad w = 0\,.$$

If one considers that fact in the relations between stresses and displacements and lets p_{ik} ($i, k = x, y, z$) denote the components of the stress tensor then that will give:

$$p_{xz} = p_{yz} = 0\,, \quad p_{zz} = \sigma\,(p_{xx} + p_{yy})\,. \tag{1}$$

σ is **Poisson**'s constant ($0 < \sigma < 1/2$). The remaining stress components can be derived from a stress function $F\,(x, y)$, viz., the so-called **Airy** stress function, by differentiation:

$$p_{xx} = \frac{\partial^2 F}{\partial y^2}\,, \quad p_{yx} = -\frac{\partial^2 F}{\partial x\,\partial y}\,, \quad p_{yy} = \frac{\partial^2 F}{\partial x^2}\,. \tag{2}$$

([1]) **A. Timpe**, Diss. Göttingen, 1905.
([2]) **V. Volterra**, Ann. Ec. Norm. **24** (1907), pp. 401.
([3]) **G. I. Taylor**, Proc. Roy. Soc. London **145** (1934), pp. 362
([4]) **I. S. Köhler**, Phys. Rev. **60** (1941), pp. 397.
([5]) **R. Peierls**, Proc. phys. Soc. **52** (1940), pp. 34. The **Peierls** Ansatz is discussed thoroughly and explained by **F. R. N. Nabarro**, Proc. phys. Soc. **59** (1947), pp. 256.
([6]) One can find a thorough presentation in the any textbook on the theory of electricity, e.g., **Trefftz** in *Handbuch der Physik*, by **Geiger-Scheel**, Bd. VI.

The stresses (1) and (2) will then be solutions of the elastic equations when the stress function satisfies the equation $\Delta\Delta F = 0$. The elastic state is described completely by the stress function. One obtains the stresses from it by differentiating and the displacements by integrating the stress-strain equations. The stress-strain equations themselves also assume a simpler form:

$$\left.\begin{aligned} 2G\frac{\partial u}{\partial x} &= (1-\sigma)p_{xx} - \sigma p_{yy}, \quad p_{xx} = \frac{2G}{1-2\sigma}\left\{(1-\sigma)\frac{\partial u}{\partial x} + \sigma\frac{\partial v}{\partial y}\right\}, \\ 2G\frac{\partial v}{\partial y} &= (1-\sigma)p_{yy} - \sigma p_{xx}, \quad p_{yy} = \frac{2G}{1-2\sigma}\left\{(1-\sigma)\frac{\partial v}{\partial y} + \sigma\frac{\partial u}{\partial z}\right\}, \\ G\left\{\frac{\partial u}{\partial x} + \sigma\frac{\partial v}{\partial y}\right\} &= p_{xy}\,. \end{aligned}\right\} \tag{3}$$

G is the shear modulus.

The assumptions that lead to the introduction of the planar state of dislocation represent an idealization. In general, from (1), p_{zz} is non-zero, which is also the case for the dislocation. If the body in question has a finite extent along the z-direction, and if it is bounded by planes perpendicular to the z-axis then one must apply corresponding normal forces to those boundary surface in order to maintain the planar state of dislocation. By contrast, if the outer surfaces are force-free, which one assumes for a dislocation in an ideal crystal, then that will require a deviation from the planar state. Qualitatively, nothing would change essentially. Quantitatively, one would expect percentage deviations with an order of magnitude σ^2 under the influence of lateral contraction.

3. – Treatment of a dislocation in the theory of elasticity.

Obviously, one can exhibit a dislocation, as in Fig. 2, in such a way that below the glide plane, one removes the series of atoms, which are suggested by filled circles, and then deforms the lattice in such a way that the neighboring series will once more take their normal lattice spacing at a sufficient distance.

If one imagines that a cylinder of radius a has been cut out from around the center of the dislocation and one neglects the influence of the interior then one will have the following problem in elasticity as a replacement for the dislocation. A plane-parallel disc of thickness λ is cut out of a hollow cylinder of radii a and b (Fig. 3). If one now bends the two boundary surfaces together in such a way that they make contact, and one attaches the contact surfaces together (say, by soldering) then one will get precisely the state that corresponds to a dislocation. That problem was first touched upon in the dissertation by **Timpe** ([1]). **Volterra** ([2]) gave a thorough discussion of it, with beautiful pictures of rubber cylinders that were deformed in that way. Here, we would like to give only the essential results.

([1]) **A. Timpe**, Diss. Göttingen, 1905.
([2]) **V. Volterra**, Ann. Ec. Norm. **24** (1907), pp. 401.

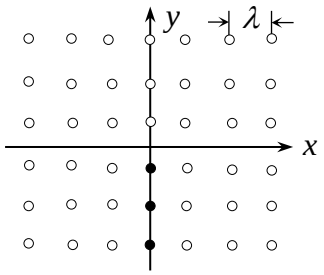

Fig.2. Creating a dislocation by removing a series of atoms.

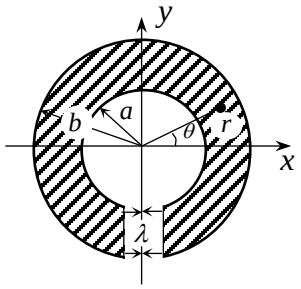

Fig. 3 Hollow cylinder with parallel gap.

The stress function:

$$F(x,y) = -\,A\,y\ln\sqrt{x^2+y^2} = -A\,r\ln r\cdot\sin\theta \tag{4.a}$$

corresponds to the stresses:

in rectangular coordinates	in polar coordinates
$p_{xx} = -\frac{A\,y}{r^2}\left\{1+\frac{2x^2}{r^2}\right\},$	$p_{rr} = -\frac{A}{r}\sin\theta,$
$p_{yy} = -\frac{A\,y}{r^2}\left\{1-\frac{2x^2}{r^2}\right\},$	$p_{\theta\theta} = -\frac{A}{r}\sin\theta,$
$p_{xy} = \frac{A\,x}{r^2}\left\{1-\frac{2x^2}{r^2}\right\},$	$p_{r\theta} = \frac{A}{r}\cos\theta,$

(4.b)

and the displacements:

$$u = \frac{A}{G}\left\{(1-\sigma)\left(\theta-\frac{\pi}{2}\right)+\frac{x\,y}{2r^2}\right\}, \qquad v = -\frac{A}{G}\left\{(1-\sigma)\left(\theta-\frac{\pi}{2}\right)+\frac{x\,y}{2r^2}\right\}. \tag{4.c}$$

The arbitrary additive constants in the displacements are already available. One counts the angle θ from the negative *y*-axis from $-\pi/2$ to $3\pi/2$. If one now chooses $A = \frac{\lambda}{2\pi}\frac{G}{1-\sigma}$ then one will remark that one can describe the bending together of the cylinder in terms of those displacements. The left boundary ($\theta = 3\pi/2$) will be displaced by precisely $\lambda/2$ to the right along the *x*-direction, while the right boundary ($\theta = -\pi/2$) will be displaced by the same amount to the left when one neglects the terms in λ/a. Since the *y*-displacements are equal, the gap will close. That solution is still not complete, since boundaries *a*, *b* are not stress-free. One will get the complete solution from the stress function:

$$F = -\,y\left\{a\ln r+\frac{B}{2r^2}-\frac{C\,r^2}{2}\right\} = -\,\sin\theta\left\{A\,r\ln r+\frac{B}{2r}-\frac{C\,r^3}{2}\right\}, \tag{5.a}$$

with the stresses:

$$\left.\begin{aligned} p_{xx} &= -\frac{y}{r^2}\left\{A\left(1+\frac{2x^2}{r^2}\right)-\frac{B}{r^4}(3x^2-y^2)-3Cr^2\right\}, \quad p_{rr} = -\frac{\sin\theta}{r}\left(A-\frac{B}{r^2}-Cr^2\right), \\ p_{yy} &= -\frac{y}{r^2}\left\{A\left(1-\frac{2x^2}{r^2}\right)+\frac{B}{r^4}(3x^2-y^2)-Cr^2\right\}, \quad p_{\theta\theta} = -\frac{\sin\theta}{r}\left(A+\frac{B}{r^2}-3Cr^2\right), \\ p_{xy} &= \frac{x}{r^2}\left\{A\left(1-\frac{2x^2}{r^2}\right)-\frac{B}{r^4}(x^2-3y^2)-Cr^2\right\}, \quad p_{r\theta} = \frac{\cos\theta}{r}\left(A-\frac{B}{r^2}-Cr^2\right), \end{aligned}\right\} \tag{5.b}$$

and the displacements:

$$\left.\begin{aligned} u &= \frac{A}{G}\left\{(1-\sigma)\left(\theta-\frac{\pi}{2}\right)+\frac{xy}{2r^2}\right\}-\frac{Bxy}{2Gr^4}+\frac{Cxy}{2G}(3-4\sigma), \\ v &= \frac{-A}{2G}\left\{(1-2\sigma)\ln\frac{r}{a}+\frac{x^2}{r^2}\right\}-\frac{B}{4Gr^4}(y^2-x^2)+\frac{Cy^2(1-4\sigma)}{4G}-\frac{Cx^2(5-4\sigma)}{4G}. \end{aligned}\right\} \tag{5.c}$$

The constants *B*, *C* are calculated from the demand that the outer surface must be stress-free. Thus, the stress components p_{rr} and $p_{r\theta}$ must vanish for $r = a, b$. Two constants will suffice here for the four conditions, since p_{rr} and $p_{r\theta}$ exhibit the same radial dependency. *A* is established from the width of the gap. For *B*, *C*, one will get:

$$B = \frac{Aa^2b^2}{a^2+b^2}, \qquad C = \frac{A}{a^2+b^2}. \tag{5.d}$$

If one makes *b* then one can obviously drop *C* completely. That corresponds to a displacement in an infinitely-extended crystal. In that case, one will then have $B = A\cdot a^2$ and $C = 0$. The stresses and displacements can also be written in an especially-simple way then:

$$\left.\begin{aligned} p_{rr} &= -\frac{\lambda G}{2\pi(1-\sigma)}\frac{\sin\theta}{r^3}(r^2-a^2), \\ p_{\theta\theta} &= -\frac{\lambda G}{2\pi(1-\sigma)}\frac{\sin\theta}{r^3}(r^2+a^2), \\ p_{r\theta} &= \frac{\lambda G}{2\pi(1-\sigma)}\frac{\cos\theta}{r^3}(r^2-a^2), \end{aligned}\right\} \tag{6.a}$$

and ([1]):

([1]) For the sake of convenience, the free additive constant $\frac{\lambda}{4\pi(1-\sigma)}$ is added to (5.c) for *v* here.

$$\left.\begin{aligned} u &= \frac{\lambda}{2\pi}\left(\theta-\frac{\pi}{2}\right)+\frac{\lambda}{2\pi(1-\sigma)}\cdot\frac{x\,y}{2r^4}(r^2-a^2), \\ v &= -\frac{\lambda(1-2\sigma)}{4\pi(1-\sigma)}\ln\frac{r}{a}+\frac{\lambda}{4\pi(1-\sigma)}\cdot\frac{(r^2-a^2)(y^2-x^2)}{2r^4}. \end{aligned}\right\} \tag{6.b}$$

The displacements are brought into the simplest form possible in (6.b). On the interior boundary, one has only the displacement in the *x*-direction that is proportional to θ.

One can also interpret the same stress state in a different way. Namely, if one counts the angle θ from the positive *x*-axis from 0 to 2π and adds the constant λ / 4 to *u* then one will get the following picture (Fig. 4): Immediately above the positive *x*-axis, one has no displacement on the inner boundary, while immediately below it, one has a displacement by λ to the right. Nothing changes in regard to the stresses as a result of that consideration. One can also exhibit the same stress state as follows then: If one cuts out a hollow cylinder along the position *x*-axis, then displaces the upper part through the segment λ to the right with respect to the upper part of the cut, and fixes that state by soldering then one will likewise get the stress state (5.b) with the same constants *A*, *B*, *C*. **Taylor** ([1]) had interpreted a dislocation elastically in that way.

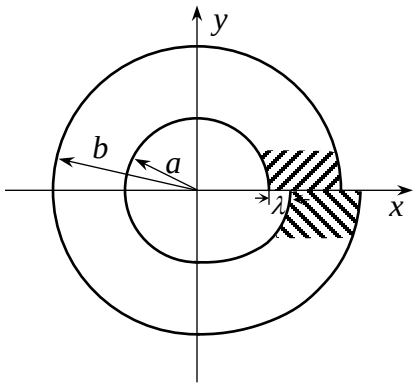

Figure 4. **Taylor**'s definition of a dislocation.

One will then get an expression for the elastic energy *E* per unit length that is stored in the cylinder that is bent together:

$$E = \frac{G\lambda^2}{4\pi(1-\sigma)}\left\{\ln\frac{b}{a}-\frac{b^2-a^2}{b^2+a^2}\right\} \tag{7}$$

that diverges logarithmically with *b*.

The total energy in a cylinder of length *l* is then $E \cdot l$. If the linear dimensions *l* and *b* are large compared to the width of the gap then one can replace *a* with a value of order of magnitude λ in order to determine the energy of a dislocation approximately and neglect the second term in (7), which refers to the influence of the p_{zz} boundary stresses, as well as that of the atoms inside of *a*. In that way, one will get the total energy *U* as:

$$U = \frac{G\cdot l\,\lambda^2}{4\pi(1-\sigma)}\ln\frac{b}{\lambda}\ .$$

Along with the linear dimensions of the piece of the crystal considered, *U* depends upon only the gap-width and increases quadratically with increasing gap-width in practice.

([1]) **G. I. Taylor**, Proc. Roy. Soc. London **145** (1934), pp. 362.

If one regards the formation of dislocations as definitive for plastic deformation then, on energetic grounds, one will have a strong argument for the observed preference for the most densely-populated lattice line as the glide direction. One has no reference point for the choice of glide plane. In fact, preferring the most densely-populated lattice line over all other glide directions is indeed much more canonical than the corresponding choice of glide planes. Even when new glide systems are created at higher temperatures, that will normally manifest themselves in changes of the glide planes, but not the glide directions. In the special case of α-iron, a well-defined glide direction probably exists, namely, [111] (and likewise the most densely-populated lattice line), but there is in no way a preferred glide plane ([1]).

The elastic model that is considered here differs from an actual dislocation, above all, by the fact that there is no intrinsic cylindrical surface for a dislocation that is stress-free. In reality, one would have a complicated stress distribution on such an excised surface that one would have to infer from a more-precise atomic theory. However, one can neglect that influence at a great distance from the center of the dislocation, just as one can drop the term in a^2 there, since it drops off with a higher power of distance. Thus, at a great distance from the center, the elastic state of a dislocation will be described eq. (4) alone. **Köhler** ([2]) had also employed those formulas. One can initially make no statement about the domain of validity for the elastic calculations. One can probably assume that formulas (4) are a useful approximation at, say, ten lattice separations from the center of the dislocation. The atomistic considerations that we will go into in the following section will show us that the elasticity-theoretic results are useful in a much-broader context than one is inclined to assume.

4. – The Peierls argument.

One best recognizes that the assumptions of the theory of elasticity will be altered for strong distortions, not just quantitatively, but also qualitatively, in the homogeneous shearing of a primitive cubic lattice. In the elastic domain, one has:

$$p_{xy} = G\frac{u_A - u_B}{\lambda}, \tag{8}$$

when u_A and u_B are the displacements of two neighboring atomic planes (Fig. 5). For large shears:

$$p_{xy} = \frac{G}{2\pi}\sin\frac{2\pi}{\lambda}(u_A - u_B) \tag{8.a}$$

will be a useful approximation. Atomic positions for which the nonlinear domain of the sine law is applicable occur in the neighborhood of the center of a dislocation, and above all, in the transition to the glide planes. Now, the idea of **Peierls** consists of treating the parts of the crystal

([1]) **E. Schmidt** and **W. Boas**, *Kristallplastizität*, Berlin, 1935, pp. 90.
([2]) **I. S. Köhler**, Phys. Rev. **60** (1941), pp. 397.

above and below the glide plane separately by pure elasticity theory, while one assumes that the transition to the glide plane obeys the sine law. One can do that when the dislocation is sufficiently extended that only small distortions can arise inside of each half-crystal. It turns out that this assumption is not fulfilled especially well.

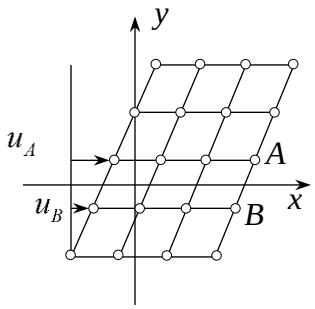

Figure 5. Homogeneous shear

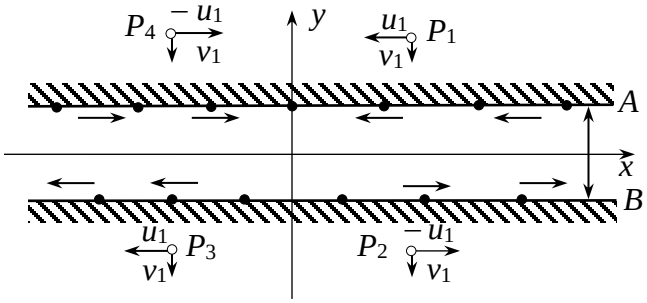

Figure 6. Symmetry relationships in the **Peierls** Ansatz.

The two half-crystals are bounded by the planes *A* and *B*, as in Fig. 6 ([1]). We next imagine that the interaction between the two halves is turned off and each half is deformed by itself by forces that are applied to the outer surfaces *A*, *B* in a manner that would correspond to the actual dislocation. The forces of interaction must now compensate the forces on the surfaces precisely in order for the crystal to be in equilibrium.

One can now formulate the **Peierls** assumptions as follows: A transfer of purely-tangential forces exists between the planes *A*, *B*. Those forces will be described by the sine law (8.a).

The tangential forces that are applied to *A*, *B* while turning off the interaction then have opposite signs, and they will change signs at the *y*-axis on symmetry grounds, moreover. They are suggested by arrows in Fig. 6. Four points P_1, …, P_4 are plotted in that figure that emerge from each other under reflection in the *x* and *y*-axis. One can adjust the displacements to the symmetries of the outer surface forces. Since the outer surface forces will not change under a rotation by 180° around the *y*-axis, and the sign will invert under a corresponding rotation around the *x*-axis, one can assume that the displacements exhibit the same behavior. Therefore, if the displacements are known at P_1 then one can get the displacements at the other points P_2, P_3, P_4 by considerations that purely relate to symmetry. For the displacements, one then has:

$$\left.\begin{aligned} u(x,y) &= -u(x,-y) = -u(-x,y), \\ v(x,y) &= v(x,-y) = v(-x,y), \end{aligned}\right\} \tag{9.a}$$

and one has, correspondingly, for the stresses:

$$p_{yy}(x,y) = -p_{yy}(x,-y) = p_{yy}(-x,y)\,. \tag{9.b}$$

In particular, one will then have:

([1]) The rest positions of the atoms in *A* are displaced with respect to the ones in Fig. 5 by $\lambda / 2$, on symmetry grounds. The null positions of the atoms are suggested in Fig. 6. That change requires a change of sign in (8.a).

$$u_A = - u_B \ . \tag{9.c}$$

In addition, one sees that the assumption of the adjustment of pure tangential forces between *A*, *B* is fulfilled quite well. When the elastic equations are valid throughout, from (9.b), one would have $p_{yy} = 0$ for $y = 0$. The normal forces in the glide plane would vanish then. Indeed, one can infer the same thing from the elasticity-theoretic treatment of bent cylinders. Certainly, the normal forces at the neighboring planes *A*, *B* can also be neglected as small, with the exception of perhaps the center of the dislocation, where the atoms are furthest from their normal equilibrium positions.

If one imagines that the shear stresses $p_{xy}^{A}(x)$ are given at *A* then one can determine the displacements $u_A(x)$ from them with the help of the theory of elasticity. However, due to (8.a) and (9.c), the shear stress is coupled with the displacement u_A directly, in addition ([1]):

$$p_{xy}^{A}(x) = - \frac{G}{2\pi} \sin \frac{4\pi}{\lambda} u_A(x) \ .$$

From that coupling, **Peierls** obtained an integral equation for u_A in the following form:

$$\int_{-\infty}^{+\infty} \frac{1}{x - x'} \frac{du_A(x')}{dx'} dx' = \frac{1-\sigma}{2} \sin \frac{4\pi}{\lambda} u_A(x) \ . \tag{10.a}$$

The solution that corresponds to a dislocation is:

$$u_A(x) = - \frac{\lambda}{2\pi} \arctan \frac{x}{\lambda} \, 2(1-\sigma) \ , \tag{10.b}$$

as one can see by substitution. The integral in (10.a) is understood to mean the **Cauchy** principal value. Eq. (10) was given by **Peierls** ([2]) and **Nabarro** ([2]). **Nabarro** has explained the **Peierls** calculation and carried it further. However, the derivation of (10.a) is somewhat awkward. We would like to carry out the derivation of the equation here by a simpler method.

For that, we require the solution for a "planar" isolated force. If the force *K* per unit length is applied to the entire *z*-axis, and if only the half-space $y > 0$ is filled with matter (Fig. 7) then the problem can be solved by the stress function:

$$F = - \frac{K}{\pi} y \theta \ , \tag{11.a}$$

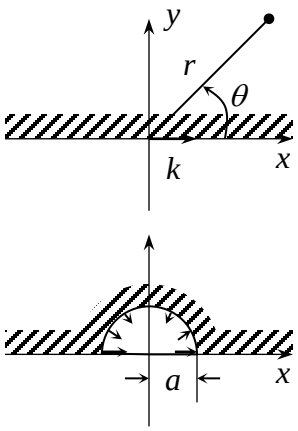

Figure 7. The definition of a planar isolated force.

([1]) See the remark on pp. 8.

([2]) **R. Peierls**, Proc. Phys. Soc. **52** (1940), pp. 34. The **Peierls** Ansatz is discussed thoroughly and explained by **F. R. N. Nabarro**, Proc. phys. Soc. **59** (1947), pp. 256.

with the stresses:

$$\left.\begin{aligned} p_{xx} &= -\frac{2K}{\pi}\frac{x^3}{r^4}, \qquad p_{rr} = -\frac{2K}{\pi}\frac{\cos\theta}{r}, \\ p_{yy} &= -\frac{2K}{\pi}\frac{x\,y^2}{r^4}, \quad p_{\theta\theta} = 0, \\ p_{xx} &= -\frac{2K}{\pi}\frac{y\,x^2}{r^4}, \quad p_{r\theta} = 0, \end{aligned}\right\} \tag{11.b}$$

and the displacements:

$$u = -\frac{K}{2G\pi}\left\{(1-\sigma)\ln\frac{r^2}{a^2}+\frac{y^2}{r^2}\right\}, \qquad v = -\frac{K}{2G\pi}\left\{(1-2\sigma)\,\theta-\frac{x\,y}{r^2}\right\}. \tag{11.c}$$

One makes the meaning of formulas (11) clear most simply by cutting out a half-cylinder of radius a (a can be arbitrarily small) around the z-axis and then discussing the stresses and displacements (Fig. 7). Surface forces appear only at the walls of the half-cylinder. If K is positive then one will have normal forces on the lateral surface, as is suggested by arrows in Fig. 7. Upon integrating the forces over a lateral surface of length c, one will get a force of magnitude $K\,c$ in the x-direction as the resultant force.

If the point of application of the isolated force does not lie at $x = 0$, but $x = \xi$, then one needs only to replace x with the quantity $x - \xi$ everywhere in (11). If the outer surface stresses $p_{xy}(\xi)$ are given for $y = 0$ then every interval $d\xi$ will correspond to an isolated force $-p_{xy}(\xi)\,d\xi$. If one then replaces K with $-p_{xy}(\xi)\,d\xi$ and x with $x - \xi$ in eq. (11) then upon integrating over ξ, one will get the corresponding quantities for the given outer surface forces. The displacement $u_A(x)$ of the outer surface:

$$u_A(x) = \frac{(1-\sigma)}{G\pi}\int_{-\infty}^{+\infty} p_{xy}(\xi)\,\tfrac{1}{2}\ln(x-\xi)^2\,d\xi\,. \tag{12}$$

That equation is equivalent to (10.a), and one can rewrite one as the other directly ([1]). It will likewise be solved by (10.b) then. With the solution (10.b) for u_A, the outer surface stresses will then be known, as well, and they are given by:

([1]) If one forms the **Peierls** expression with (13):

$$\int_{-\infty}^{+\infty}\frac{du_A(x')}{dx'}\cdot\frac{dx'}{x-x'}$$

then one will get:

$$\int_{-\infty}^{+\infty}\frac{du_A}{dx'}\cdot\frac{dx'}{x-x'} = -\frac{(1-\sigma)}{2\pi^2}\int\int_{-\infty}^{+\infty}\frac{\sin\left\{\frac{4\pi}{\lambda}u_A(\xi)\right\}}{(x-x')(x'-\xi)}\,d\xi\,dx'\,.$$

$$p_{xy}^{A}(\xi) = \frac{G\beta}{\pi}\frac{\xi}{\xi^2+\beta^2} \qquad \text{with} \quad \beta = \frac{\lambda}{2(1-\sigma)}. \tag{14}$$

Upon integrating ([1]) eq. (11), one will get from (14) the stress function, stresses, and dislocations for the entire upper half-plane. Evaluating it will yield the stress function:

$$F = -\frac{G\beta}{\pi}\, y\, \tfrac{1}{2}\ln\{x^2+(y+\beta)^2\} \tag{15}$$

and the displacements:

$$\left.\begin{aligned} u &= \frac{\beta(1-\sigma)}{\pi}\left\{\arctan\frac{y+\beta}{x}-\frac{\pi}{2}\right\}+\frac{\beta}{2\pi}\frac{x\,y}{x^2+(y+\beta)^2}, \\ v &= -\frac{\beta(1-2\sigma)}{2\pi}\frac{1}{2}\ln\frac{x^2+(y+\beta)^2}{\beta^2}+\frac{\beta}{2\pi}\frac{y(y+\beta)}{x^2+(y+\beta)^2}. \end{aligned}\right\} \tag{16}$$

If one would like to compare those quantities with the ones from the purely-elastic theory then one would have to replace y with the quantity $y - \lambda / 2$ everywhere. That is because eqs. (11) all refer to the plane A, which lies $\lambda / 2$ above the glide plane, but not to the glide plane. If the glide

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All integrals are understood to mean **Cauchy** principal values. Now, one can prove, under very general assumptions on a function $f(\xi)$, that:

$$\int\!\!\int_{-\infty}^{+\infty} \frac{f(\xi)}{(x-x')(x'-\xi)}\,dx'\,d\xi = -\pi^2 f(x).$$

That will imply the asserted equivalence.

([1]) Evaluating the terms that do not include $\ln r$ or θ results immediately from the residue theorem of the theory of functions. In the integrals that do contain $\ln r$ and θ, one must replace the limits with $\pm M$ and define the integral by the limit as M goes to ∞. One can then, e.g., calculate the quantity:

$$f(x,y) = \int_{-\infty}^{+\infty} \frac{\xi}{\xi^2+\beta^2}\ln\{(x-\xi)^2+y^2\}\,d\xi$$

in that way.

$f(x, y = 0)$ is known here from (10.b), and $\partial f / \partial y$ can be evaluated from the residue theorem. One gets:

$$\frac{\partial f}{\partial y} = \frac{\pi x}{x^2+(y+\beta)^2}.$$

One then has:

$$f(x,y) = f(x,0)+\int_0^y \frac{\partial f}{\partial y}\,dy = -\pi\arctan\frac{x}{y+\beta}.$$

There are terms that remain constant under the integral over θ that include the upper limit. However, those constant terms do not need to be considered in either the stress function of the displacements. Moreover, one can also convince oneself that they describe the desired state immediately from the integrated formulas.

plane is $y = 0$, once more as in the purely-elastic calculations, then from (15) and (16), one will have:

$$F = -\frac{G\lambda}{2\pi(1-\sigma)}\left(y-\frac{\lambda}{2}\right)\cdot\frac{1}{2}\cdot\ln\left\{x^2+\left(y+\frac{\sigma\lambda}{2(1-\sigma)}\right)^2\right\}, \tag{15.a}$$

$$\left.\begin{aligned} u &= \frac{\lambda}{2\pi}\left\{\arctan\frac{y+\frac{\sigma\lambda}{2(1-\sigma)}}{x}-\frac{\pi}{2}\right\}+\frac{\lambda}{4\pi(1-\sigma)}\cdot\frac{x\left(y-\frac{\lambda}{2}\right)}{x^2+\left(y+\frac{\sigma\lambda}{2(1-\sigma)}\right)^2} \\ &= -\frac{\lambda}{2\pi}\arctan\frac{x}{y+\frac{\sigma\lambda}{2(1-\sigma)}}+\frac{\lambda}{4\pi(1-\sigma)}\cdot\frac{x\left(y-\frac{\lambda}{2}\right)}{x^2+\left(y+\frac{\sigma\lambda}{2(1-\sigma)}\right)^2}, \\ v &= -\frac{\lambda(1-2\sigma)}{4\pi(1-\sigma)}\cdot\frac{1}{2}\ln\frac{x^2+\left(y+\frac{\sigma\lambda}{2(1-\sigma)}\right)^2}{\left(\frac{\lambda}{2(1-\sigma)}\right)^2}+\frac{\lambda}{4\pi(1-\sigma)}\cdot\frac{\left(y-\frac{\lambda}{2}\right)\left(y+\frac{\sigma\lambda}{2(1-\sigma)}\right)}{x^2+\left(y+\frac{\sigma\lambda}{2(1-\sigma)}\right)^2}. \end{aligned}\right\} \tag{16.a}$$

A comparison with the elasticity formulas (5) and (6) shows a far-reaching agreement when one drops the a^2 from the elasticity (in addition to the term that is logarithmic in v, and in which one can replace, say, a with $\lambda / 2$). Since the **Peierls** assumptions are not fulfilled at the center of the dislocation, in any case, it would only make sense to compare the solutions at some lattice separations. However, neither the term in $\lambda / 2$ nor the quantity $\frac{\sigma\lambda}{2(1-\sigma)}$ will have any noticeable influence there. Therefore, for all applications that are not concerned with the center of the dislocation directly, one can just as well employ the one-term stress function (4.a), e.g., for all problems that are concerned with the interactions of two dislocations.

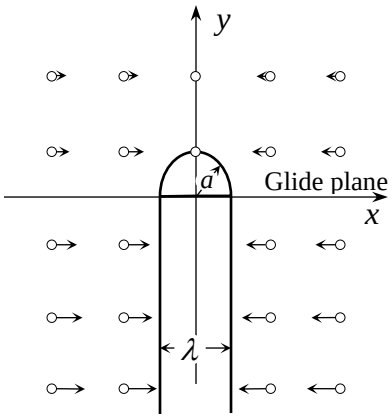

Figure 8. u-displacements for the elasticity solution with $a = \lambda / 2$.

It initially seems very remarkable that the elasticity solution exhibits such a good agreement with the atomic Ansatz. However, one must consider that for the case of small radii (compared to the gap width), it by no means describes the problem of the bent-together cylinder anymore. In fact, the gap is closed only at distances that are large compared to the gap width. Therefore, one can still regard the elasticity solution itself as a useful approximation when one sets the internal radius equal to, say, $\lambda / 2$ (Fig. 8). That will also immediately give the possibility of obtaining more detailed information about the arrangement of the atoms in a dislocation. One can employ the elasticity

solution for a radius a with the same order of magnitude as the lattice constant as an initial solution and then consider the atomic forces on the atoms, which lie on the boundary (interior, resp.) of the cylinder of radius a. In that way, it will also be possible to consider the crystalline structure, which certainly plays a role at the center of the dislocation. That possibility shall be pursued in a later work.

With such an Ansatz, one would be able to determine precisely the influence of the atomic arrangement at the center of the structure and the length of a dislocation. That is because neither the **Peierls** solution nor the elasticity-theoretic one allows one to expect that they will give the displacements at the center correctly, because all assumptions are fulfilled to the least extent at precisely that location. On the one hand, the type of lattice is significant there. Furthermore, the vanishing of the normal stress is questionable there. In addition, the calculation with continuous displacements is no longer permissible. However, the structure of the center is definitive for the dynamics of a dislocation.

5. – Taylor's solution.

In conclusion, we would like to discuss the meaning of the stress state that **Taylor** ([1]) gave. The stresses that were given by **Taylor** are:

$$p_{rr} = \frac{G\lambda}{\pi}\frac{\sin\theta}{r}, \qquad p_{\theta\theta} = -\frac{G\lambda}{\pi}\frac{\sin\theta}{r}, \qquad p_{r\theta} = \frac{G\lambda}{\pi}\frac{\cos\theta}{r}.$$

It is derived from the stress function:

$$F = -\frac{G\lambda}{\pi}\{y\ln r + x\theta\},$$

and the displacements are:

$$u = \frac{\lambda}{2\pi}\theta, \qquad v = \frac{\lambda}{2\pi}\ln r.$$

The shifts here likewise exhibit the properties that are necessary for the description of the bent-together cylinder. In essence, what we have here is a superposition of (4) and an isolated material force that is applied to the origin in the $-y$-direction with a magnitude of $2G\lambda$, as we can also see by a comparison with (11).

Now, what is the difference between the quantities that were given here and our solution (5)? The solutions (5) describe the bent-together cylinder under the influence of p_{zz} boundary stresses, which we assume do not influence the result essentially. The cylinder jackets a, b are stress-free. **Taylor**'s solution once more describes the bent-together cylinder, except that here the boundary stresses have a different distribution. p_{zz} is zero here, so one must keep the stresses that were given above in equilibrium on the cylinder jackets a, b, which do not have to be in equilibrium on *one of*

([1]) **G. I. Taylor**, Proc. Roy. Soc. London **145** (1934), pp. 362.

them. One can add a further divergenceless solution [e.g., the term in eq. (5) that is affected with *B*] in order to make p_{rr} *or* $p_{r\theta}$ vanish on the internal boundary (but not both of them, as **Taylor** stated, as a result of a sign error).

In order to compare the two stress fields, we give them in Cartesian coordinates:

According to **Taylor**	According to (4)
$p_{xx} = -\frac{G\lambda}{\pi}\cdot\frac{y}{r^2},$	$p_{xx} = -\frac{G\lambda}{2\pi(1-\sigma)}\cdot\frac{y}{r^2}\cdot\left\{\frac{y^2+3x^2}{r^2}\right\},$
$p_{yy} = \frac{G\lambda}{\pi}\cdot\frac{y}{r^2},$	$p_{yy} = -\frac{G\lambda}{2\pi(1-\sigma)}\cdot\frac{y}{r^2}\cdot\left\{\frac{y^2-x^2}{r^2}\right\},$
$p_{xy} = \frac{G\lambda}{\pi}\cdot\frac{x}{r^2},$	$p_{xy} = \frac{G\lambda}{2\pi(1-\sigma)}\cdot\frac{x}{r^2}\cdot\left\{\frac{x^2-y^2}{r^2}\right\}.$

The differences are significant in a theory of solidification or a theory of the diffusion of foreign atoms into a deformed crystal, as was recently give by, e.g., **Cottrell** ([1]).

The question is now: “Which of the two approximate solutions should one prefer?” We believe that the solution (5) must be given priority, since the consideration of the p_{zz} boundary stresses would not affect the result essentially. In addition, the **Taylor** solution does not at all describe an important property of dislocations. It is divergenceless (due to the fact that $p_{rr} + p_{\theta\theta} = 0$), so neither dilatations nor compressions occur in the lattice. On the other hand, it is intuitively clear that dislocation that is treated here must compress the lattice above the glide plane and dilate the lattice below it.

We would like to thank Herren Prof. **G. Masing** and **R. Becker** for some stimulating discussions.

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([1]) **A. H. Cottrell**, *Report of a Conference on the Strength of Solids*, Bristol, 1948.