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Brief Notes

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LOGARITHMIC SCREW DISLOCATION

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Basing on linear elasticity, the displacement field $u_z = B\vartheta \ln r$ (in cylindrical coordinates r, ϑ, z) was derived. This displacement has a jump on the half-plane $\vartheta = 0$. Stresses orthogonal to this discontinuity plane are continuous.

Screw dislocation is probably the most commonly used model of a crystal imperfection. It is essential, that the displacement field of the dislocation is multivalued. It is discontinuous on a half-plane. Screw dislocation is a classical notion. Its motion was considered and the stresses and deformation were calculated both in the linear and nonlinear theory. Configurational forces in the linear theory and Newtonian forces in the nonlinear theory were calculated. Interaction with other defects, in particular with dislocation loops and point defects, were analysed.

Classical screw dislocation has the Burgers vector parallel to the z-axis. Denote its length by b. In cylindrical coordinate system $\theta^i = (r, \vartheta, z)$, the displacement field u^i and the stress field τ^{ij} are given by the expressions

$$u^1 = u^2 = 0, \qquad u^3 = b\vartheta, \tag{1}$$

$$\begin{aligned} \tau^{23} &= \tau^{32} = 2\mu b \frac{1}{r^2}, \\ \tau^{11} &= \tau^{22} = \tau^{33} = \tau^{12} = \tau^{21} = \tau^{13} = \tau^{31} = 0. \end{aligned} \tag{2}$$

In the Cartesian coordinate system (x, y, z) these fields are

$$u_x = u_y = 0, \qquad u_z = b \arctan\frac{y}{x}, \tag{3}$$

$$\begin{aligned} \tau_{zx} &= \tau_{xz} = 2\mu b \frac{-y}{x^2+y^2}, \qquad \tau_{zy} = \tau_{yz} = 2\mu b \frac{x}{x^2+y^2}, \\ \tau_{xx} &= \tau_{yy} = \tau_{zz} = \tau_{xy} = \tau_{yx} = 0. \end{aligned} \tag{4}$$

On the half-plane $\vartheta = 0$ the displacement u_z has a jump equal to $2\pi b$.

Consider the displacement field

$$u_x = u_y = 0, \qquad u_z = f(r)g(\vartheta), \tag{5}$$

where $f(r)$ and $g(\vartheta)$ are functions of one variable. Neither of them equals identically zero. We shall derive from (5) another dislocation field. The other dislocation has a jump of the displacement field on $\vartheta = 0$. It seems that the existence of the other dislocation was not noticted until now.

In the cylindrical coordinate system θ^i, the contravariant coordinates of the stress tensor corresponding to (5) are

$$\begin{aligned}\tau^{13} &= \tau^{31} = 2\mu\frac{df}{dr}g(\vartheta), \qquad \tau^{23} = \tau^{32} = 2\mu\frac{1}{r^2}f(r)\frac{dg(\vartheta)}{d\vartheta},\\ \tau^{11} &= \tau^{22} = \tau^{33} = \tau^{12} = \tau^{21} = 0.\end{aligned} \tag{6}$$

Two equilibrium equations are automatically satisfied, the third one leads to the differential equation

$$\left(\frac{d^2f(r)}{dr^2} + \frac{1}{r}\frac{df(r)}{dr}\right)g(\vartheta) + \frac{1}{r^2}f(r)\frac{d^2g(\vartheta)}{d\vartheta^2} = 0. \tag{7}$$

There exist two essentially different situations. If in Eq. (7) the derivative $d^2g(\vartheta)/d\vartheta^2$ is different from zero, then for each r and ϑ must be satisfied the relation

$$\frac{\dfrac{d^2f(r)}{dr^2} + \dfrac{1}{r}\dfrac{df(r)}{dr}}{\dfrac{1}{r^2}f(r)} = -\frac{\dfrac{d^2g(\vartheta)}{d\vartheta^2}}{g(\vartheta)}. \tag{8}$$

At the left-hand side there is a function of r alone, and at the right-hand side – a function of ϑ alone. Therefore each side must be equal to a constant that will be denoted by κ^2. Parameter κ is real or complex. It follows that the functions $f(r)$ and $g(\vartheta)$ are governed by the equations

$$\frac{d^2f(r)}{dr^2} + \frac{1}{r}\frac{df(r)}{dr} + \kappa^2\frac{1}{r^2}f(r) = 0, \qquad \frac{d^2g(\vartheta)}{d\vartheta^2}\kappa^2 g(\vartheta) = 0. \tag{9}$$

Solution of the second equation is the function

$$g(\vartheta) = A_1\exp(\kappa\vartheta) + A_2\exp(-\kappa\vartheta), \tag{10}$$

which for each ϑ is continuous. The conclusion is that the case when $d^2g(\vartheta)/d\vartheta^2$ is different from zero corresponds to a continuous displacement field, not a dislocation. Therefore further on we abandon this case.

Consider in turn the case when the derivative $d^2g(\vartheta)/d\vartheta^2$ equals zero. In accord with (6) there is

$$\frac{d^2 f(r)}{dr^2} + \frac{1}{r}\frac{df(r)}{dr} = 0, \qquad g(\vartheta) = B\vartheta + B_1, \tag{11}$$

where B and B_1 are constants. The constant B_1 does not have the expected physical meaning, since it changes the plane for which $\vartheta = 0$ and does not lead to discontinuity. Therefore we take $B_1 = 0$. The general solution of the differential equation $(11)_1$ is the function

$$f(r) = C_1 + C_2 \ln r, \tag{12}$$

where C_1 and C_2 are constants. The case $C_1 \neq 0$, $C_2 = 0$ describes the classical screw dislocation (1). Consider the other case $C_1 = 0$, $C_2 \neq 0$. It leads to the following expression for the components of the displacement vector in cylindrical coordinate system θ^i:

$$u^1 = u^2 = 0, \qquad u^3 = b\vartheta \ln r, \tag{13}$$

where B is a constant. This displacement field will be called the logarithmic screw dislocation. As it was proved above, there exist no other solutions of the form (5), which represents a discontinuous displacement. Obviously, any continuous solution of linear elasticity may be added to the field (13). Such added field does not change the discontinuities and the displacement jump.

The displacement field (13) may be expressed by the Cartesian coordinates x, y, z. There is

$$u_z = \frac{1}{2} B \log(x^2 + y^2) \arctan\frac{y}{x}, \qquad u_x = u_y = 0. \tag{14}$$

The deformation tensor is determined by the displacement gradient. We obtain

$$\begin{aligned}
\varepsilon_{xz} &= \varepsilon_{zx} = \frac{1}{2}\frac{\partial u_z}{\partial x} = \frac{1}{4} B \left(\frac{-y}{x^2+y^2} \log(x^2+y^2) + \frac{2x}{x^2+y^2} \arctan\frac{y}{x} \right), \\
\varepsilon_{yz} &= \varepsilon_{zy} = \frac{1}{2}\frac{\partial u_z}{\partial y} = \frac{1}{4} B \left(\frac{x}{x^2+y^2} \log(x^2+y^2) + \frac{2y}{x^2+y^2} \arctan\frac{y}{x} \right), \\
\varepsilon_{xx} &= \varepsilon_{yy} = \varepsilon_{zz} = \varepsilon_{xy} = \varepsilon_{yx} = 0.
\end{aligned} \tag{15}$$

The shearing stresses τ_{zx}, τ_{zy} are proportional to the deformations

$$\begin{aligned}
\tau_{xz} &= \tau_{zx} = \frac{1}{2} \mu B \left(\frac{-y}{x^2+y^2} \log(x^2+y^2) + \frac{2x}{x^2+y^2} \arctan\frac{y}{x} \right), \\
\tau_{yz} &= \tau_{zy} = \frac{1}{2} \mu B \left(\frac{x}{x^2+y^2} \log(x^2+y^2) + \frac{2y}{x^2+y^2} \arctan\frac{y}{x} \right) \\
\tau_{xx} &= \tau_{yy} = \tau_{zz} = \tau_{xy} = \tau_{yx} = 0,
\end{aligned} \tag{16}$$

where μ is the Lamé constant. It is easy to check that the stress (16) satisfies the equilibrium equations

$$\frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} = 0. \tag{17}$$

The displacement $u_z(x, y)$ given in (14) is a multi-valued function, since $\arctan y/x$ is such a function. In accord with (3), there is

$$\begin{aligned} u_z &= 0 && \text{for} \quad \vartheta = 0, \\ u_z &= 2\pi B \log r && \text{for} \quad \vartheta = 2\pi. \end{aligned} \tag{18}$$

The shearing stress τ_{zy} is a continuous function. On both sides of the half-plane $\vartheta = 0$ it has the same values

$$\tau_{zy} = 2\mu B \left(\frac{1}{x} - \log x \right). \tag{19}$$

In contrast to this, the stress τ_{zx} is a multivalued function

$$\begin{aligned} t_{zx} &= 0 && \text{for} \quad \vartheta = 0, \\ t_{zx} &= 2\pi\mu B \frac{1}{r} \ln r && \text{for} \quad \vartheta = 2\pi. \end{aligned} \tag{20}$$

Note that on the half-plane $\vartheta = 0$ both stresses and the displacement orthogonal to this half-plane are continuous.

Finally we give the expression for the energy density calculated for a unit volume. General expression for the energy density E is given by the formula

$$E = \frac{1}{2}(\tau_{zx}\varepsilon_{zx} + \tau_{zy}\varepsilon_{zy} + \tau_{xz}\varepsilon_{xz} + \tau_{yz}\varepsilon_{yz}), \tag{21}$$

which leads to the expression

$$E = 4\mu B \frac{1}{r^2} \left(\log r + 2\varphi^2 \right). \tag{22}$$

References

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