Stress Distribution around a Screw Dislocation in a Thin Crystal

By

Minoru KAWAMOTO* and Toshinobu SHIBATA*

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This paper presents the result of calculations on the stress distribution around a screw dislocation in a thin foil-crystal calculated by use of the IBM digital computer. In an infinite medium, it is well known that a screw dislocation makes a stress field with one stress component $\tau_{\theta z}$, where z is the direction of the Burgers vector. In a thin foil-crystal, it was found that a screw dislocation makes a stress field with not only $\tau_{\theta z}$ which vanishes at free surface but $\tau_{r\theta}$ which concentrates at the surface.

1. Introduction

As the result of development of various measuring methods of the motion of dislocations, we need more knowledge of the precise stress fields around the dislocations. If the cylindrical coordinate system (r, θ, z) is taken and the z-axis is coincided with the direction of the Rurgers vector, in the infinite medium a screw dislocation makes a stress field having only one stress component[1]:

$$\tau_{\theta z} = -\frac{b\mu}{2\pi}\frac{1}{r}, \tag{1}$$

where b is the magnitude of the Burgers vector, μ the Lamé's constant, and r the position.

Many investigators have calculated the stress fields around the dislocations for the various situations. But most of them have been obtained under the assumption that the medium is infinite. As mentioned above, however, it is increased to use very thin foil, order of 10^{-4} mm or less than it, in order to observe the motion of dislocations.

This paper aimed to check whether the stress fields calculated under such assumption is applicable or not to the thin foiled medium. The calcu-

* Department of Mechanical Engineering

lation was made on a screw dislocation whose Burgers vector is perpendicular to the foil surface. Moreover, Mura's method[2] was used as the fundamental equations for this calculation.

2. Calculations

By using Mura's method and the tensor operation[3], the dislocation strain is given by

$$U_{m,n}(x) = \int_L \varepsilon_{njh} c_{ijks} G_{km,s}(x-x') b_i dL'_h \tag{2}$$

where,

- $U_m(x)$: the displacement at the point x in the m-direction,
- $U_{m,n}(x)$: the strain at point x obtained by differentiating the displacement $U_m(x)$ with respect to coordinate n,
- ε_{njh} : the permulation,
- c_{ijks} : the elastic constant of fourth rank tensor,
- $G_{km}(x-x')$: the Green's function which equals the displacement in the k-direction at point x caused by unit impulse force acting in m-direction at the point x',
- b_i : the i-component of Burgers vector b,
- dL'_h : h-component of the line element, and
- L : the dislocation loop.

On the other hand, the displacement (u, v, w) at the point (x, y, z) caused by the force (X_0, Y_0, Z_0) acted at the point (x', y', z') is given by[4]

$$(u, v, w) = \frac{\lambda+3\mu}{8\pi\mu(\lambda+2\mu)}\left(\frac{X_0}{\bar{r}}, \frac{Y_0}{\bar{r}}, \frac{Z_0}{\bar{r}}\right) + \frac{\lambda+\mu}{8\pi\mu(\lambda+2\mu)}\left(\frac{\bar{x}}{\bar{r}}, \frac{\bar{y}}{\bar{r}}, \frac{\bar{z}}{\bar{r}}\right)\frac{X_0\bar{x}+Y_0\bar{y}+Z_0\bar{z}}{\bar{r}^2} \tag{3}$$

or by using the index notation

$$U_m = \frac{a^2+c^2}{8\pi\mu a^2}\frac{X_{0m}}{\bar{r}} + \frac{a^2-c^2}{8\pi\mu a^2}\frac{\bar{x}_m}{\bar{r}}\frac{X_{0i}\bar{x}_i}{\bar{r}^2}, \tag{4}$$

where,

λ and μ : the Lamé's constants,

$\bar{r}^2 = (x-x')^2+(y-y')^2+(z-z')^2 = \bar{x}^2+\bar{y}^2+\bar{z}^2$,

$a^2 = (\lambda+2\mu)/\rho$,

$c^2 = \mu/\rho$, and

ρ : the density of the medium.

Now the Green's function G_{km} is given as a function of position x only, because the dislocation in the consideration is stationary, so that, using U_m in Eq. (4) or (3), G_{km} becomes

$$G_{km}(x-x') = \frac{a^2+c^2}{8\pi\mu a^2}\frac{\delta_{km}}{\bar{r}} + \frac{a^2-c^2}{8\pi\mu a^2}\frac{\bar{x}_k\bar{x}_m}{\bar{r}^3}. \quad (5)$$

Eq. (5) means the displacement in the k-direction caused by a unit force in the m-direction: the forces X_0, Y_0, Z_0 in Eq. (3) are taken as unity. Now, the elastic constant c_{ijks} is written with the Lamé's constants λ and μ as

$$c_{ijks} = \mu(\delta_{ik}\delta_{js}+\delta_{is}\delta_{jk})+\lambda\delta_{ij}\delta_{ks}. \quad (6)$$

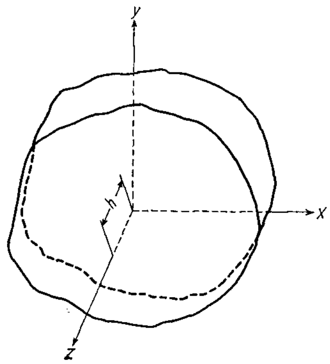

Fig. 1. The coordinate system.

In the expression (6), the medium is assumed to be isotropic and continuous.

Now let the thickness of the foil-crystal be h as shown in Fig. 1. Suppose that the Burgers vector of a screw dislocation is taken for the positive z-axis and it lies on the z-axis. Then the following are specified:

$$\left.\begin{aligned} dL'_h &= dz', \qquad h=3 \\ b_i &= b_3, \qquad i=3 \\ \bar{r}^2 &= \bar{x}^2+\bar{y}^2+\bar{z}^2, \\ \bar{x} &= x, \quad \bar{y}=y, \quad \bar{z}=z-z' \end{aligned}\right\} \quad (7)$$

Therefore, the differential form of Eq. (2) becomes, using the relations (7),

$$\begin{aligned} dU_{m,n} &= \varepsilon_{njh}c_{ijks}G_{km,s}(x-x')b_i dL'_h \\ &= \varepsilon_{nj3}c_{3jks}G_{km,s}(x-x')b_3 dz' \\ &= (\varepsilon_{n13}c_{31ks}+\varepsilon_{n23}c_{32ks})G_{km,s}b_3 dz'. \end{aligned} \quad (8)$$

Using the relation (6), the each component of $dU_{m,n}$ becomes

$$\left.\begin{aligned} dU_{m,1} &= \mu(G_{3m,2}+G_{2m,3})b_3 dz', \\ dU_{m,2} &= -\mu(G_{3m,1}+G_{1m,3})b_3 dz', \\ dU_{m,3} &= 0. \end{aligned}\right\} \quad (9)$$

Then the equality

$$\int_{-\infty}^{\infty} G_{km,3}b_3 dz' = \int_{-\infty}^{\infty}\frac{db_3}{dz'}G_{km}dz'$$

will lead the expression (9) into

$$\left.\begin{aligned}
dU_{1,1} &= \mu\left(G_{31,2}b_3 + G_{21}\frac{db_3}{dz'}\right)dz', \\
dU_{2,1} &= \mu\left(G_{32,2}b_3 + G_{22}\frac{db_3}{dz'}\right)dz', \\
dU_{3,1} &= \mu\left(G_{33,2}b_3 + G_{23}\frac{db_3}{dz'}\right)dz', \\
dU_{1,2} &= -\mu\left(G_{31,1}b_3 + G_{31}\frac{db_3}{dz'}\right)dz', \\
dU_{2,2} &= -\mu\left(G_{32,1}b_3 + G_{13}\frac{db_3}{dz'}\right)dz', \\
dU_{3,2} &= -\mu\left(G_{33,1}b_3 + G_{13}\frac{db_3}{dz'}\right)dz', \\
dU_{1,3} &= dU_{2,3} = dU_{3,3} = 0.
\end{aligned}\right\} \tag{10}$$

For the convenience of the calculations, let

$$\left.\begin{aligned}
D_1 &= \frac{\lambda+3\mu}{8\pi\mu(\lambda+2\mu)} = \frac{a^2+c^2}{8\pi\mu a^2}, \\
D_2 &= \frac{\lambda+\mu}{8\pi\mu(\lambda+2\mu)} = \frac{a^2+c^2}{8\pi\mu a^2}, \\
r^2 &= x^2+y^2.
\end{aligned}\right\} \tag{11}$$

Then Eq. (5) is rewritten as

$$G_{km} = D_1\delta_{km}/\bar{r} + D_2\bar{x}_k\bar{x}_m/\bar{r}^3. \tag{12}$$

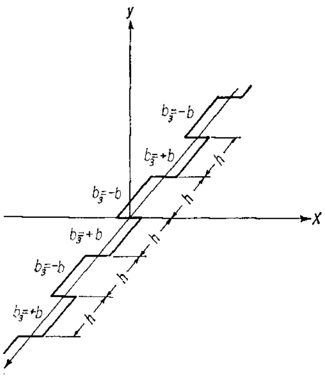

Fig. 2. Distribution of dislocations.

The above equations were led for arbitrary screw dislocation directed positive z-axis in infinite medium. As we are, now, interested in the stress distribution in the thin foil, thickness h, let us assume an infinite medium as shown in Fig. 2, and calculate the stress field in one part of thickness h in this medium with the help of the principle of mirror reflection. That is, the positive and negative screw dislocations are put in order infinitely with distance h as shown in the figure. In the other words, the Burgers vector of these dislocations is represented by

$$b_3 = b_3(z') = (-1)^n b, \tag{13}$$

where

$$n = [z'/h]. \tag{14}$$

The parenthesis in Eq. (14) notes the Gauss' integer notation.

Substituting Eqs. (12), and (13) into Eq. (10) and integrating it from $-\infty$ to $+\infty$ with respect to z' gives us the following results:

$$\left.\begin{aligned}
U_{1,1} &= 4b\mu D_2 xy \sum_{n=-\infty}^{\infty} \frac{(-1)^n}{h^3\{(r/h)^2+(z/h-n)^2\}^{3/2}} \\
&= 2b\mu D_2 \frac{\sin 2\theta}{r}(r/h)^3 \sum_{n=-\infty}^{\infty} \frac{(-1)^n}{\{(r/h)^2+(z/h-n)^2\}^{3/2}}, \\
U_{2,2} &= -U_{1,1}, \\
U_{1,2}+U_{2,1} &= -2\cot 2\theta\, U_{1,1}, \\
U_{3,1} &= b\mu(D_1+D_2)\frac{\sin\theta}{r} \sum_{n=-\infty}^{\infty} (-1)^n \Big[\frac{z/h-\overline{n+1}}{\{(r/h)^2+(z/h-\overline{n+1})^2\}^{1/2}} \\
&\quad -\frac{z/h-n}{\{(r/h)^2+(z/h-n)^2\}^{1/2}}\Big] \\
&\quad -2b\mu D_2 \frac{r}{h}\sin\theta \sum_{n=-\infty}^{\infty} (-1)^n \Big[\frac{z/h-\overline{n+1}}{\{(r/h)^2+(z/h-\overline{n+1})^2\}^{3/2}} \\
&\quad -\frac{z/h-n}{\{(r/h)^2+(z/h-n)^2\}^{3/2}}\Big], \\
U_{3,2} &= -\cos\theta\, U_{3,1},
\end{aligned}\right\} \tag{15}$$

where we used the change of coordinate systems from the Cartesian one (x, y, z) to the cylindrical one (r, θ, z):

$$\begin{aligned}
r^2 &= z^2+y^2, \quad \text{or} \\
x &= r\cos\theta, y = r\sin\theta, \quad \text{and} \\
z &= z.
\end{aligned}$$

Now the dislocation stress σ_{pq} in the Cartesion coordinate system can be obtained by multiplying Eq. (2) by the elastic constants c_{pqmn}. The components of the strain tensor are given by Eqs. (15), so we can easily calculate the stress tensor in the Cartesian coordinate system. From those stress tensor, the stress field in the cylindrical coordinate system can be, also, easily transformed, and the results of these are:

$$\begin{aligned}
\sigma_{rr} &= \sigma_{xx}\cos^2\theta+\sigma_{yy}\sin^2\theta+2\tau_{xy}\cos\theta\sin\theta = 0, \\
\sigma_{\theta\theta} &= 0, \\
\sigma_{zz} &= 0, \\
\tau_{r\theta} &= -4b\mu^2 D_2 \frac{1}{r}(r/h)^3 \sum_{n=-\infty}^{\infty} \frac{(-1)^n}{\{(r/h)^2+(z/h-n)^2\}^{3/2}} \\
\tau_{\theta z} &= b\mu^2(D_1+D_2)\frac{1}{r} \sum_{n=-\infty}^{\infty} (-1)^2 \Big[\frac{Z/h-\overline{n+1}}{\{(r/h)^2+(z/h-\overline{n+1})^2\}^{1/2}} \\
&\quad -\frac{z/h-n}{\{(r/h)^2+(z/h-n)^2\}^{1/2}}\Big]
\end{aligned} \tag{16}$$

$$-2b\mu^2 D_2 \sum_{n=-\infty}^{\infty} (-1)^n \left[\frac{z/h-\overline{n+1}}{\{(r/h)^2+(z/h-\overline{n+1})^2\}^{3/2}} - \frac{z/h-n}{\{(r/h)^2+(z/h-n)^2\}^{3/2}} \right]. \tag{17}$$

3. Results

For the screw dislocation in a thin foil-crystal, two components $\tau_{r\theta}$ and $\tau_{\theta z}$ remain and the other components vanish. And it is clear that from Eqs. (16) and (17) $\tau_{\theta z}$ vanishes at the surfaces, $z=0$ and $z=h$, and $\tau_{r\theta}$ vanishes at the $z=h/2$.

Since the medium is, as assumed before, isotropic, if we substitute D_1, D_2 in Eq. (11) into Eqs. (16) and (17) and represent the Lamé's constant λ with μ (also the Lamé's constant and equals the transverse elastic constant) and the Poisson's ratio ν, these two stress components $\tau_{r\theta}$ and $\tau_{\theta z}$ become the functions of b, μ, and ν, also the position.

Figs. 3 and 4 are the examples of stress distributions calculated with the IBM digital computor. The Poisson's ratio ν was taken as 0.3 and the thickness of the foil 30 times of the Burgers vector b. The stresses are shown in the equi-stress diagrams. Fig. 3 shows the equi-stress for $\tau_{r\theta}$, and Fig. 4 for $\tau_{\theta z}$. In both figures the absciassa is r-axis and the unit of it is the Burgers vector b, and the vertical axis is z-axis, unit of it the thickness of the foil $30b$. Also, the unit of the stress is $b\mu/2\pi$.

Now, the stress for the infinite medium has only one component $\tau_{\theta z}$, and its magnitude given by Eq. (1) is drawn in Fig. 4 by the broken line. For the thin foil the stress component $\tau_{r\theta}$ occurs due to the free surface perpen-

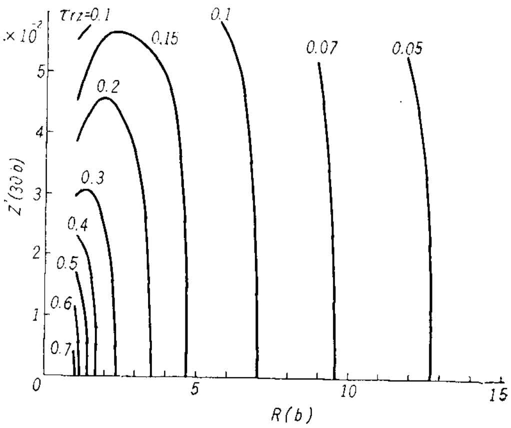

Fig. 3. The equi-stress diagrams of $\tau_{r\theta}$.

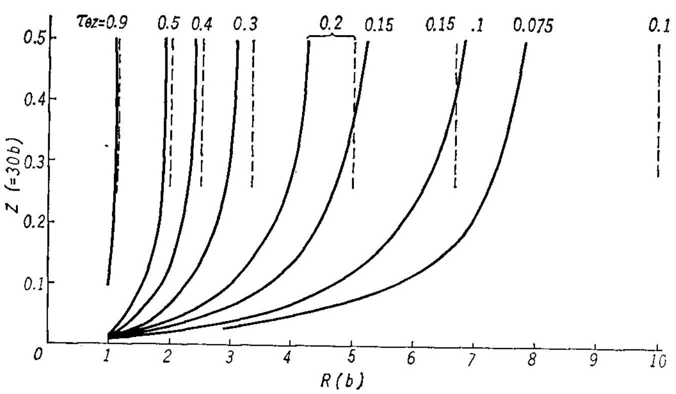

Fig. 4. The equi-stress diagrams of $\tau_{\theta z}$.

dicular th the Burgers vector, but this stress concentrate at the surface as seen in Fig. 3, and vanishes rapidly to the interior of the foil. Next, the stress component $\tau_{\theta z}$ is, as stated previouly, zero at the surface, and at the center of the thickness it approaches to the value given by Eq. (1). But always it is smaller than the value given by Eq. (1). When the thickness h is $30b$ as in this example, the stress $\tau_{\theta z}$ at the center of the thickness is small compared with the value shown by the broken line, but if h becomes about 1000 b, at the middle part of the foil the stress $\tau_{\theta z}$ is entirely nearly equal to the value for the infinite medium. And the thickness of the surface layer where the stress is very different from the value given by Eq. (1) becomes negligibly thin compared with the total thickness of the foil.

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