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NOTE

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It is well known that characteristics of plastic deformation of crystalline materials are closely related to that of inter-atomic forces of their composing atoms mainly through the structure and properties of dislocation.

The first step to reasonable atomic theory of dislocation had been started by Peierls(1) (1940), the theory succeeded in simplifying considerably the difficult problem of many body problem concerning the arrangement of atoms around a dislocation by introducing an approximation called as Peierls' approximation. The theory has been considered to be very promising and followed by some later investigators(2)(3)(4)(5), but the treatments were rather confined to some special cases where types of atomic forces were limited to some simpler ones.

The object of this study, therefore, is directed to extending the theory so as to be applicable for the crystals which have more general types of atomic forces.

Consider a straight dislocation (edge or screw) contained in an infinite crystal and placed along the axis z in the ship plane xz. And denote the Burgers' vector of the dislocation by $\boldsymbol{b}$, whose magnitude by b. In Peierls' approximation, the strained state of the crystal are approximated by an elastic continium excepting the central region contained between the two neighbouring atomic planes ($y=\pm b/2$), where the characteristics of atomic forces are taken into account. The condition of the equilibrium of the forces between the two atomic planes in consistent with the displacements of the atoms is expressed under the approximation by the Peierls' equation,

$$D\int_{-\infty}^{+\infty}\frac{du(x')}{dx'}\,\frac{1}{x'-x}\,dx' = \tau\,\{u(x)\}\,, \tag{1}$$

where u is the x compornent of the displacements of atoms situated at the points ($x=\pm nb$, $n=0,1,2,\cdots$, $y=b/2$), τ is the compornent of shear stress parallel to the direction x acting in the plane xz, and assumed to be determined as a function of u from the atomic forces, and $D=\pi G/2(1-\nu)$, G the rigidity modulus, ν the poisson's ratio when the dislocation is edge type and the elastic field is considered to be isotropic.

Then, taking into account that $\tau(x)$ and $\dfrac{du(x')}{dx'}$ in (1) are mutually Hibert transformations of each other, we propose now a solution for (1) in the form of series,

$$U=\left(\frac{2\pi u}{b}\right)=\sum_{l}\left[c_{l,0}\tan^{-1}\left(\frac{\zeta}{a_l}\right)+\sum_{i=1}^{\infty}c_{l,i}\,\frac{\zeta}{X_l^{\,i}}\right],$$

$$P=\left(\frac{2\pi\tau}{G}\right)=\sum_{l}\sum_{i=1}^{\infty}d_{l,i}\,\frac{\zeta}{X_l^{\,i}}\,,$$

$$\frac{dU}{d\zeta}=\sum_{l}\sum_{i=1}^{\infty} e_{l,i}\frac{1}{X_l^{i}} ,$$

$$X_l = a_l^2+\zeta^2,\quad \zeta=\frac{2(1-\nu)x}{b} , \tag{2}$$

where $d_{l,i}$, and $e_{l,i}$ are determined uniquely by $c_{l,i}$ while $c_{l,i}$, are determined so that the series (2) satisfy the boundary conditions $\left(\frac{b}{2}\frac{d\tau}{du}\right)_{x=\pm\infty}=G$ and $(u)_{x=\pm\infty}=\pm\frac{b}{4}$, and coincide with the given functional form of $\tau(u)$.

The energy of the dislocation generally varies periodically with the period b as the center of dislocation proceed along the x axis, consequently the total energy of the dislocation can be divided into the two parts, *i.e.* the average energy E_m and the periodic compornent E_p, from which Peierls stress τ_p is defined as

$$b\tau_p=\frac{d}{dx}E_p .$$

Then in our approximation E_m and τ_p can be expressed using (2) as,

$$E_m=\int_{-\infty}^{+\infty}\tau u\,dx+2\int_{-\infty}^{+\infty}\int_{x}^{\infty}\tau\frac{du}{dx'}\,dx'\,dx ,$$

$$\tau_p=\frac{4}{d}\sum_{S=1}^{\infty}\sin(2\pi s\alpha)\int_{-\infty}^{+\infty}\tau\frac{du}{d\zeta}\sin\left(\frac{2\pi s\zeta}{1-\nu}\right)d\zeta,\quad \alpha=\frac{x}{b} . \tag{3}$$

As an example, consider the particular case of (2),

$$U=(1-\varepsilon)\tan^{-1}\frac{\zeta}{a_1}+\varepsilon\tan^{-1}\frac{\zeta}{a_2}+K\frac{\zeta}{a_3^2+\zeta^2} ,$$

$$P=(1-\varepsilon)\frac{2\zeta}{a_1^2+\zeta^2}+\varepsilon\frac{2\zeta}{a_2^2+\zeta^2}+K\frac{4a_3\zeta}{(a_3^2+\zeta^2)^2} ,\quad K=(1-\varepsilon)a_1+\varepsilon a_2-1. \tag{4}$$

In this case, E_m and τ_p are calculated as

$$\left(\frac{8\pi^2(1-\nu)}{Gb^2}E_m\right)=2\pi\left[\left\{\log\frac{e(1-\nu)x}{b}\right\}_{x\to\infty}-\frac{1}{2}\log(a_1a_2)-\frac{1}{2}(1-2\varepsilon)\log\left(\frac{a_1}{a_2}\right)-\varepsilon(1-\varepsilon)\log\frac{(a_1+a_2)^2}{4a_1a_2}\right.$$

$$\left.+2\left\{\frac{(1-\varepsilon)}{a_1+a_3}+\frac{\varepsilon}{a_2+a_3}\right\}K+\frac{K^2}{4a_3^2}\right] ,$$

$$\left(\frac{\pi^2}{G}\tau_p\right)=2\pi\sum_{S=1}^{\infty}\sin(2\pi s\alpha)\left[e^{-\frac{\pi Sa_1}{1-\nu}}\left\{\frac{(1-\varepsilon)^2\pi s}{2(1-\nu)}+\frac{\varepsilon(1-\varepsilon)}{a_2-a_1}+\frac{(1-\varepsilon)K}{(a_3-a_1)^2}\right\}\right.$$

$$+e^{-\frac{\pi Sa_2}{1-\nu}}\left\{\frac{\varepsilon^2\pi s}{2(1-\nu)}+\frac{\varepsilon(1-\varepsilon)}{a_1-a_2}+\frac{\varepsilon K}{(a_3-a_2)^2}\right\}$$

$$\left.+Ke^{-\frac{\pi Sa_3}{1-\nu}}\left\{-\frac{(1-\varepsilon)}{(a_3-a_1)^2}-\frac{\varepsilon}{(a_3-a_2)^2}-\left(\frac{(1-\varepsilon)}{a_3-a_1}+\frac{\varepsilon}{a_3-a_2}\right)\frac{\pi s}{1-\nu}+\frac{K}{12}\frac{\pi^3s^3}{(1-\nu)^3}\right\}\right] . \tag{5}$$

Since the solution contains the parameters, a_1, a_2 and a_3, it can represent rather wide range of functional form of $\tau(u)$. And we can easily see that the contribution of the term containing the smallest a_l in (4), which correspond to a peak near $u=0$ in the curve of $\tau(u)$, predominates in the Peierls stress (5).

The solution of the form (2) is considered to be particularly suitable for unextended dislocation such as contained in body centered cubic crystals and ionic crystals. On the other hand, for extended dislocation such as contained in face centered cubic crystals, we may adopt the type of solution constructed combining the two sets of solutions of the type (2) corresponding to the two partial dislocations situated at $\zeta=\pm\eta$,

$$U_{\text{ext}}=\frac{1}{2}\{U(\zeta-\eta)+U(\zeta+\eta)\},$$
$$P_{\text{ext}}=\frac{1}{2}\{P(\zeta-\eta)+P(\zeta+\eta)\}. \tag{6}$$

In this case the stacking fault energy γ of the extended dislocation can be represented by the potential energy at $\zeta=0$,

$$\gamma=2\int_0^\infty \tau\frac{du}{d\zeta}d\zeta\ . \tag{7}$$

For instance if we take the case $a_1=a_2=a_3=a$ in (2),

$$U=\tan^{-1}\xi+\frac{(a-1)}{a}\frac{\xi}{1+\xi^2},$$
$$P=\frac{2}{a}\frac{\xi}{1+\xi^2}+\frac{2(a-1)}{a^2}\frac{2\xi}{(1+\xi^2)^2},$$
$$\xi=\frac{\zeta}{a}, \tag{8}$$

we have the expressions for E_m, τ_p and γ as follows;

$$\left(\frac{8\pi^2(1-\nu)}{Gb^2}E_m\right)=2\pi\Big[\Big\{\log\frac{(1-\nu)x}{ab}\Big\}_{x\to\infty}-\frac{1}{4}\log\Big\{1+\Big(\frac{\eta}{a}\Big)^2\Big\}$$
$$+\Big\{\frac{(a-1)}{2a}(2a^2+\eta^2)+\frac{1}{4}(a-1)^2\Big\}\frac{1}{a^2+\eta^2}+\Big\{a^4+\Big(2a^2-\frac{a}{2}+\frac{1}{2}\Big)\eta^2+\eta^4\Big\}\frac{1}{(a^2+\eta^2)^2}\Big],$$

$$\left(\frac{\pi^2\tau_p}{G}\right)=\pi\sum_{S=1}^{\infty}\sin(2\pi s\alpha)\,e^{-\frac{\pi Sa}{1-\nu}}\Big[$$
$$\cos\Big(\frac{\pi s\eta}{1-\nu}\Big)\times\frac{1}{2}\Big(\frac{\pi s}{1-\nu}\Big)\Big\{1+\Big(\frac{\pi s}{1-\nu}\Big)(a-1)+\frac{1}{6}\Big(\frac{\pi s}{1-\nu}\Big)^2(a-1)^2-\frac{(a-1)}{2\eta^2}\Big\}$$
$$+\sin\Big(\frac{\pi s\eta}{1-\nu}\Big)\times\frac{(a-1)}{4\eta^3}\Big\{(a-3)+\Big(\frac{\pi s}{1-\nu}+\frac{1}{a-1}\Big)2\eta^2+\frac{2a^2(a^2+2\eta^2)}{(a^2+\eta^2)^4}\Big\}\Big],$$

$$\left(\frac{2\pi^2\gamma}{Gb}\right)=\frac{1}{4}\Big[\Big\{\frac{2}{\eta}+\frac{(a-1)^2}{\eta^3}-\frac{2(a-1)\eta}{(a^2+\eta^2)^2}\Big\}\tan^{-1}\frac{\eta}{a}-\frac{(a-1)^2}{a}\frac{1}{\eta}$$
$$+\frac{3a^2-2a+1}{a(a^2+\eta^2)}+\frac{2a(a^2-1)}{(a^2+\eta^2)^2}+\frac{8a^3(a-1)^2}{3(a^2+\eta^2)^3}\Big]. \tag{9}$$

On this example we can see that the magnitude of Peierls stress $(\tau_p)_{\max}$ oscillates with the period nearly equal to $b/2$ as η increases. Numerical examples and detailed examinations of the solutions (2) and (6) together with the calculations of $\tau(u)$ for particular atomic forces and the examinations of the method of approximation itself will be discussed in succeeding papers.

Lastly it may be noted that the method of approximation can also be applied for the analyses of nucleation of crack,[6] dislocation or stacking fault and structure of phase boundary.[7]

References

(1) R. E. Peierls: Proc. Phys. Soc. (London), 52 (1940) 34.
(2) F. R. N. Nabarro: Proc. Phys Soc. (London), 59 (1947) 256.
(3) A. J. Foreman, M. A. Jaswon and J. K. Wood: Proc. Phys. Soc. (London), 64 (1951) 156.
(4) H. B. Huntington: Proc. Phys. Soc. (London), 68 (1955) 1043.
(5) A. Seeger: Handbuch der Physik, VII-1 (1955, Springer, Berlin) 383.
(6) K. Kitajima: Bull. Res. Inst. Applied Mechanics, Kyushu Univ., No. 19 (1962) 1.
(7) J. H. Van der Merwe; J. Appl. Phys., 34 (1963) 117.

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