THE MIGRATION ENERGY FOR DISLOCATION KINK

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Abstract—*The kink migration energy is evaluated by modifying the line tension model of dislocations. A sinusoidal variation of Pierels pontential is used for dislocations, which gives a neglible migration energy for kink motions for typical metals. This confirms the general expectation that kinks can move freely along dislocation lines with no necessity of activation.*

1. INTRODUCTION

Dislocation motions in crystals can be made much more easily if kinks are formed on it. The continuous kink motion along a dislocation line will finally result the dislocation jumping one Burgers-vector distance. Hewever, due to the discrete lattice structure of solids the kink also migrates in a periodic potential. This is analogous to a dislocation moving in its Pierels potential. Kinks are thus sometimes referred as second-order dislocations. Although the precise calulation has not yet been made, it is generally expected that a kink migrates on a much smaller energy barrier than a dislocation does[1]. In this paper we introduce a simple model of kink to calculate its migration energy analytically. We use elastic line tension model of dislocation to fine the shape of a kink and when it is moving the kink is assumed to maintain its shape unchanged. By then introducing the discrete structure on the dislocation line the kink energy can be evaluated by this model.

2. THE MODEL

Our model is shown in Fig. 1. We can see a dislocation line is straddled on two Pierels troughs and a kink is formed at $x=0$. The Pierels dotential $w(y)$ is assumed sinusoidal variation along slip direction y[5]. That is

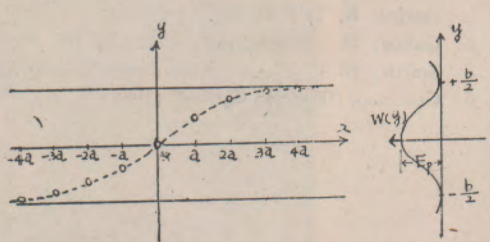

Fig. 1.

$$w(y)=\frac{E_p}{2}\left(1+\cos\frac{2\pi y}{b}\right) \tag{1}$$

here E_p is the dislocation Pierels energy and b its Burgers vector. If there is no external stress on the dislocation the equilibrium line shape can be solved by the equation[2]

$$w_o\frac{\partial^2 y}{\partial x^2}=\frac{\partial w(y)}{\partial y} \tag{2}$$

together with boundary conditions $x\to\infty$, $\frac{dy}{dx}\to 0$, $y\to\pm\frac{b}{2}$ and $x\to 0$, $y\to 0$. w_o is the line tension or the line energy of the dislocation.

Equation (2) can be solved easily for the Pierels potential of eqn. (1). the soluation

is $$y=f(x)=\frac{b}{2\pi}\left[4\tan^{-1}\exp\left(-\frac{\pi}{b}\ \frac{2E_p}{w_0}x\right)-\pi\right] \quad (3)$$

for the kink at position $x=0$. By our assumption that the kink does not change its shape when it is moving the shape of the kink at position $x_0=a\alpha$ is described by

$$y=f(x+a\alpha) \quad (4)$$

To obtain the kink migration energy we must introduce the discrete structure of the lattice. We set atomic planes perpendicular to porential troughs at $x=0$, $\pm a$, $\pm 2a,\ldots\ldots,\pm na,\ldots\ldots$, a is the lattice parameter. The energy of the dislocation is assumed to concentrate on these positions. Since kink shape does not change with position the only contribution to the kink migration energy is from the Pierels energy of each atomic plane, that is the sum

$$E_k=\sum_{n=-\infty}^{+\infty} w(y_n)$$

$$=\sum_{n=-\infty}^{+\infty}\frac{E_p}{2}\left[1+\cos\left\{4+an^{-1}\exp\left(-\frac{\pi}{b}\sqrt{\frac{2E_p}{W_0}}(n+\alpha)a-\pi\right\}\right)\right]$$

Which can be simplified to

$$E_k=E_pa\sum_{n=-\infty}^{+\infty}\operatorname{sech}^2[\beta a(n+\alpha)] \quad (5)$$

here $\beta=\sqrt{\frac{2E_0}{w_0}}\cdot\frac{\pi}{b}=\frac{a\pi}{bd}$ is a measure of the kink width d. The smaller the β, the wider the kink.

In order to get what we want, the sum must be transformed into a periodic function of α. This can be done by the following procedures.

By the idendity

$$\operatorname{sech}^2 x=4\int\frac{t\cdot\cos(2xt)}{\sinh(\pi t)}dt$$

equ. (5) can be written as

$$E_k=4E_pa\lim_{N\to\infty}\sum_{n=-N}^{+N}\int_0^\infty\frac{t\cdot\cos[2t\beta a(n+\alpha)]}{\sinh(\pi t)}dt$$

$$=4E_pa\lim_{N\to\infty}\int_0^\infty\frac{t}{\sinh(\pi t)}dt\sum_{n=-N}^{+N}\cos[2t\beta a(n+\alpha)]$$

$$=4E_pa\lim_{N\to\infty}\int_0^\infty\frac{t\cdot\cos(2t\beta a)}{\sinh(\pi t)}\cdot\frac{\sin[t\beta a(2N+1)]}{\sin(t\beta a)}dt \quad (6)$$

We have changed the sequence of summation and integratin in the second step and used the equality

$$\sum_{n=-N}^{+N}\cos[2t\beta a(n+\alpha)]=\cos(2t\beta a)\cdot\frac{\sin[t\beta a(2N+1)]}{\sin(t\beta a)}$$

in the last step. From Direchlet's second integral[3]

$$\lim_{N\to\infty}\int_0^b \frac{\sin(2N+1)x}{\sin x}f(x)dx=\frac{\pi}{2}f(o) \quad o<b<\pi$$

or its extension

$$\lim_{N\to\infty}\int_0^\infty \frac{\sin(2N+1)x}{\sin x}f(x)dx=\frac{\pi}{2}\sum_{n=0}^{\infty}f(n\pi) \tag{7}$$

we finally arrive, by comparing eqn. (6) and eqn. (7), the expression of the kink energy

$$E_k=\frac{2E_p}{\beta}\sum_{n=-\infty}^{+\infty}\frac{n\pi^2/\beta a}{\sinh(n\pi^2/\beta a)}\cos(2\pi n\alpha) \tag{8}$$

New we have obtained another sum form of E_k. However, each term in the sum is a periodic function of α, so the sum is also a periodic function of α with a periodicity a along Pierels valley.

3. RESULT AND CONCLUSION

For typical materials $E_p/W_0\cong 10^{-3}$. If we set the Burgers vector $b=a$, then $a\cong \frac{a\pi}{b}\sqrt{\frac{1}{500}}\cong 0.14$. This corresponds to a kink width of about $20\,a$. Thus the kink energy $E_k\cong(2E_p/\beta[1+70/\sinh 70)\cos(2\pi\alpha)+(140/\sinh 140)\cos(4\pi\alpha)+...\cong(2E_p/\beta)[1+(70/\sinh 70)\cos(2\pi\alpha)]$. Only the first two terms need to be retained for good approximation. Hence we can safely say for typical materials

$$E_k\cong\frac{2E_p}{\beta}\left[1+\frac{\pi^2/\beta a}{\sinh(\pi^2/\beta a)}\cos(2\pi nx/a)\right] \tag{9}$$

The vibrational amplitude of the harmonic term corresponds to the kink migration energy E_{km}, that is

$$E_{km}=\frac{4E_p}{\beta}\cdot\frac{\pi^2/\beta a}{\sinh(\pi^2/\beta a)} \tag{10}$$

Again this is very small. It is only about 10^{-40} of the Pierels energy E_p for the last example. The discrete lattice strutcure introduces only small ripples on the kink motion path. We have also used a double-parabolic Pierels potential for the dislocation[6] and find that the kink migration energy increses to a value

$$E_{km}=E_p a.\ \mathrm{ctnh}\,(\beta a/2) \tag{11}$$

which is about $0.07\,E_p a$ for the same example, an order smaller than the Pierels energy.

All we have derived thus consists with the general expectation that kink migration energy is quite small. For a typical Pierels energy of $10^{-4}\,ev$, for the first sinusoidal potential model E_{mk} is essentially zero, for the parabolic model $E_{mk}\cong .7\times 10^{-5}\,ev$ which is equivalent to the thermal energy of $0.35°k$ and snould not be obse-rvable by experiments at room temperature. Thus a kink, once formed, is free to move with no activation requirement, if it is not met by other defects.

The precise numerical calculation is not obtained here because a Pierels potential form has to be assumed. For narrow kink the model loses its sense since local atomic arrangements become complicated and the energy can not be conside.ed to concentrate on points as we have done. However, it is still good for order estimations. The effectiveness of this modified line tension model to evaluate kink migration energy is similar to the elasticty theory to evaluate the dislocation Pierels energy[4,5].

REFERENCES

1. J.P. Hithe and J. Lothe, "Theory of Dislocation," McGraw-Hill, Inc. 1968.
2. W.T. Read, "Dislocations in Crystals," McGraw-Hill, New York' 1953, p. 53.
3. Bromwich "Infinite Series,s" 2nd edition, 1926, p. 494.
4. R.E. Peierl, Proc. Phys. Soc., 52, 23, 2940.
5. F.R. N. Nabarro, Proc. Phys. Soc., 9, 256, 1947.
6. V. Celli, M. Kabler, T. Ninomiya and R. Thomson, Phys. Rev. 131, 1, 1960.