degree of $3p$ electron unpairing is roughly,

$$f_{3p}=A_\sigma/A_{3p}. \quad (27)$$

The atomic hyperfine constant A_{3p} in Eq. (26) has the expectation value,

$$A_{3p}=\tfrac{4}{5}\pi\mu_B\gamma_N\hbar\langle 1/r^3\rangle_{3p}=0.00488\text{ cm}^{-1}, \quad (28)$$

where the factor $\langle 1/r^3\rangle_{3p}$ is determined from the paper of Barnes and Smith.[37] The resultant fractional unpairing is, $f_{3p}=0.10$ which is approximately twice the value estimated by Shulman and Wyluda for f_{2p} in $CuF_2\cdot 2H_2O$. However, the estimate of f_{3p} for $CuCl_2\cdot 2H_2O$ may be sharply reduced by the contributions to A_σ of the Cl $2p$ electrons.

[37] R. G. Barnes and W. V. Smith, Phys. Rev. 93, 95 (1954).

ACKNOWLEDGMENT

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Influence of the Peierls Potentials on the Reversible Stress-Strain Relation for Dislocations

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The mechanical equation of state of kinked dislocations is considered. Contrary to dislocation strings, which follow under the assumption of constant line tension a linear stress-strain relation for stresses $\sigma/G<b/3L$ (L=line length, b=Burgers vector, G=shear modulus, σ=stress), one finds significant nonlinearities in the reversible stress-strain relation of kinked dislocations. The physical reason for the nonlinearities can be ascribed to the fact that, owing to the Peierls potentials, the energy of a dislocation increases in multiples of the double-kink energy $2W_k$ (W_k=kink energy). A linear range, which is confined to stresses $\sigma/G<(10^{-1}b/L)(\sin\varphi+5kT/Gb^3)$ (φ=angle against close-packed direction, T=temperature), is followed by a region with $\partial^2\epsilon/\partial\sigma^2<0$ (ϵ=strain). This region corresponds to the restricted motion of geometrical kinks. After passing through an inflection point, which is roughly determined by $\sigma/G=\alpha(b/L)(2W_k/Gb^3)$ (α=numerical factor between 1 and 2), a region with $\partial^2\epsilon/\partial\sigma^2>0$ follows. It is caused by double-kink generation. If the measuring time is too short for thermally activated double kink generation, the inflection point is determined by the stress which is required for stress-assisted thermally activated double kink generation. At $T=0$°K, the stress of the inflection point provides a measure for the Peierls stress. It is suggested that evidence for the Peierls potentials can be established through a verification of the nonlinear-stress-strain relation by the following experiments: (a) The restricted motion of geometric kinks should be detectable beyond the stress for activating Frank-Read sources as a *decrease* of the modulus defect with increasing stress amplitude. (b) The double-kink-generation peaks should, in *undeformed* material, rise out of the background in high-amplitude measurements. (c) The double-kink-generation peaks should be found in *undeformed* pure material by applying a static-bias stress. (d) In deformed material, high-amplitude oscillations should cause an increase of the peak height before the peak starts to shift to lower temperatures.

I. INTRODUCTION

This paper seeks to point out that the reversible stress-strain relation of bowing dislocation segments, as a direct consequence of the Peierls potentials, differs in a very characteristic manner from that of dislocation segments in a material with vanishing Peierls potentials. The Peierls potentials cause the stress-strain relation to become intrinsically nonlinear at relatively small stresses.[1] Consequently, the Peierls stress will be the source of amplitude-dependent internal friction and modulus defect.[1] A verification of the experimental consequences predicted by the particular stress-strain relation can be considered evidence for a finite Peierls stress and will also allow the Peierls stress to be measured directly.

Depending on the geometric kink density, one can divide the problem of deriving the equation of state of a kinked dislocation as follows: For low kink density (=low geometric kink density and not too high temperatures) the interaction of kinks can be ignored and the strain as a function of stress is determined by entropy changes of the kinks. The thermodynamic treatment follows closely the analogy to a one-dimensional gas. For high geometric kink density the change of the interaction of the kinks with stress dominates over entropy changes. Consequently, the stress-strain relation is determined by the interaction law of kinks. Between these two extremes extends a range in density for which the thermodynamic problem is very similar to that of real gases. A rigorous derivation of the stress-strain relation, including double-kink generation, is only possible for noninteracting kinks (Sec. II).

[1] G. Alefeld, J. Appl. Phys. 36, 2642 (1965).

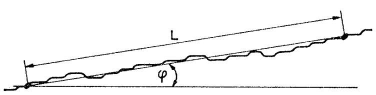

FIG. 1. A kinked dislocation line.

In Sec. III, we will derive the stress-strain relation for dislocations with high geometric kink density. We will first consider such low temperatures for which double-kink generation for the experimentally given time constant is possible only at high stresses. Subsequently we will include semiquantitatively double-kink generation. The discussion summarizes experimental consequences of the predicted nonlinear stress-strain relation.

II. NONINTERACTING KINKS

For low kink density, the restoring force of a dislocation is determined by the entropy of the kinks. In the following we will first determine the kink density in an external stress field σ by applying equilibrium thermodynamics. We will then calculate the strain resulting from sideward shifting of geometric and thermally created kinks. The resulting equation $\epsilon=\epsilon(\sigma,T)$ (ϵ=anelastic strain, T=temperature) is the stress-strain relation.

A. The Kink Density

Eshelby[2] and Seeger[3] suggested that the thermodynamics of double-kink generation can be treated similar to the pair production of electrons and positrons at high temperature.[4] We will apply the corresponding formalism to double-kink generation in an external stress field.

The condition for equilibrium between "positive kinks," "negative kinks," "phonons," and "dislocations," is given by

$$\mu^+ + \mu^- = \mu_d + \mu_{\rm ph}\,, \tag{1}$$

where μ^+=chemical potential of positive kinks, μ^-=chemical potential of negative kinks, μ_d=chemical potential of dislocation, and $\mu_{\rm ph}$=chemical potential of phonons. The chemical potential of the phonons is zero.[4] μ^+ and μ^- are functions of the kink density n^+ and n^-. (n^+=density of positive kinks, n^-=density of negative kinks.) For a positive kink, the potential energy in an external stress field σ is $E_{\rm pot}=ab\sigma x+\text{const}$; and for negative kinks, $E_{\rm pot}=-ab\sigma x+\text{const}$ (a=lattice constant, x=position of kinks, b=Burgers vector). Consequently, the condition for equilibrium is now given by[4]:

$$\mu^+ + ab\sigma x = C_1\,, \tag{2}$$

$$\mu^- - ab\sigma x = C_2\,. \tag{2'}$$

[2] J. D. Eshelby, Proc. Roy. Soc. (London) **A226**, 222 (1962).
[3] A. Seeger (private communication).
[4] L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon Press, Ltd., London, 1958).

C_1 and C_2 are constants in regard to position x. Combining Eqs. (1), (2), and (2′), we find

$$C_1 + C_2 = \mu_d\,. \tag{3}$$

A second equation between C_1 and C_2 follows from the condition that the difference between the total number of positive and negative kinks must be equal to the number of geometric kinks[5] (see Fig. 1):

$$\int_0^{L\cos\varphi} [n^+(x) - n^-(x)]dx = N_0 = L\sin\varphi/a\,. \tag{4}$$

Eshelby[2] suggested, for the chemical potential of the kinks, the use of the chemical potential of a one-dimensional gas and the addition of the kink formation energy W_k.

$$\mu^+ = kT\ln[(N^+/L')(2\pi\hbar^2/M_kkT)^{\frac{1}{2}}] + W_k\,, \tag{5}$$

$$\mu^- = kT\ln[(N^-/L')(2\pi\hbar^2/M_kkT)^{\frac{1}{2}}] + W_k\,, \tag{5'}$$

where N^+ and N^-=number of positive and negative kinks, $L'=L\cos\varphi$, where L=line length, and φ=average angle against close-packed direction, M_k=kink mass, and $\hbar$=Planck's constant. Equations (5) and (5′) need some comments. Kinks do differ from a one-dimensional gas insofar as kinks cannot interchange their relative position. A certain kink has not the total length L available, but only the length between its neighbor kinks. The following partition function $Z(N,T,L)$

$$Z = \frac{(N^+ + N^-)!}{N^+!N^-!h^{(N^+ + N^-)}} \int_{p_1=-\infty}^{p_1=+\infty} \cdots \int_{x_1=0}^{x_1=x_2} \int_{x_2=0}^{x_2=x_3} \cdots \int_{x_N=0}^{L\cos\varphi} \times\exp\left(-\sum_{i=1}^{N^+ + N^-} \frac{p_i^2}{2M_k}\right) dp_1 \cdots dp_N dx_1 \cdots dx_N \tag{6}$$

takes into account, in the integration limits, that kinks cannot move past each other. An easy integration of Eq. (6) yields

$$Z = \frac{1}{N^+!N^-!}[(2\pi M_kkT/h^2)^{\frac{1}{2}}L]^{N^+ + N^-} \tag{6'}$$

which is the same result as one gets by integrating the partition function of the free one-dimensional gas

$$Z = \frac{1}{N^+!N^-!h^{(N^+ + N^-)}} \int_{p_1=-\infty}^{p_1=+\infty} \cdots \int_{x_1=0}^{L\cos\varphi} \cdots \int_{x_N=0}^{L\cos\varphi} \times\exp\left(-\sum_{i=1}^{N} \frac{p_i^2}{2M_k}\right) dp_1 \cdots dp_N dx_1 \cdots dx_N\,. \tag{7}$$

By applying standard thermodynamic relations to Eq. (6′), one arrives at Eqs. (5) and (5′).

[5] A. D. Brailsford, Phys. Rev. **122**, 778 (1961).

Undissociated screw dislocations can generate double kinks into several planes of the crystal. If there are no geometrical kinks, this multiplicity can be taken into account by a statistical weight factor g, which would appear in Eqs. (5) and (5′) in the denominator under the logarithm.

Finally, the chemical potential of the dislocation in which the kinks are formed has to be determined. Seeger and Schiller[6] calculated how the energy states $\hbar\omega_i$ of a dislocation with one kink differ from those without a kink. A dislocation with a kink loses one oscillatory degree of freedom of the kink. μ_d is given by twice the difference in free energy F between an unkinked dislocation and a kinked one, so that

$$\mu_d=2(F_1-F_2)=-2kT\ln(Z_1/Z_2). \qquad (8)$$

Z_1 and Z_2 are the partition functions of a dislocation without and with one kink. Z_1/Z_2 can be deducted from the result of Seeger and Schiller[6] as

$$Z_1/Z_2=kTa^2(E_LM)^{\frac{1}{2}}/W_k\pi^2\hbar, \qquad (9)$$

where E_L= line tension $\approx Gb^2/2$, and M= mass of dislocation per unit length $\approx\pi\rho b^2$ (ρ= density). We now use Eqs. (5) and (5′) in Eqs. (2) and (2′), respectively, and get the following result for the kink densities $n^+=N^+/L$ and $n^-=N^-/L$:

$$n^+(x)=\cos\varphi\left(\frac{M_kkT}{2\pi\hbar^2}\right)^{\frac{1}{2}}\exp\left(-\frac{W_k+ab\sigma x-C_1}{kT}\right)=n_0^+\exp\left(-\frac{ab\sigma x}{kT}\right), \qquad (10)$$

$$n^-(x)=\cos\varphi\left(\frac{M_kkT}{2\pi\hbar^2}\right)^{\frac{1}{2}}\exp\left(-\frac{W_k-ab\sigma x-C_2}{kT}\right)=n_0^-\exp\left(\frac{ab\sigma x}{kT}\right). \qquad (10')$$

In regard to their x dependence, Eqs. (10) and (10′) have the well-known form of the barometric height distribution.[5] The product of n_0^+ and n_0^- contains the sum C_1+C_2, which, owing to Eq. (3), can be replaced by μ_d.

Consequently,

$$n_0^+n_0^-=(\cos^2\varphi)(M_kkT/2\pi\hbar^2)\times\exp(-(2W_k-\mu_d)/kT). \qquad (11)$$

Using Eqs. (8) and (9), we get

$$n_0^+n_0^-=\cos^2\varphi\frac{M_kkT}{2\pi\hbar^2}\left(\frac{W_k\pi^2\hbar}{kTa^2(E_LM)^{1/2}}\right)^2\exp\left(-\frac{2W_k}{kT}\right)=\frac{A^2}{4a^2}\exp\left(-\frac{2W_k}{kT}\right). \qquad (11')$$

[6] A. Seeger and P. Schiller, Acta Met. **10**, 348 (1962).

A^2 is dimensionless and stands for

$$A^2=2\pi^3(\cos^2\varphi)(M_k/Ma)(W_k^2/kTE_La). \qquad (12)$$

With $M_k=Ma/10$, $W_k=0.1$ eV, $kT=10^{-2}$ eV, $E_La=6$ eV, $\cos\varphi=1$, one finds $A^2=1$.

We now apply the integration [Eq. (4)] to Eqs. (10) and (10′) to get a second relation between n_0^+ and n_0^-. The straightforward integration yields

$$n_0^+[1-\exp(-ab\sigma L\cos\varphi/kT)]+n_0^-[1-\exp(ab\sigma L\cos\varphi/kT)]=b\sigma L\sin\varphi/kT. \qquad (13)$$

We combine Eqs. (11′) and (13) and solve for n_0^+ and n_0^-:

$$n_0^+=\frac{1}{a}\frac{v\sigma}{2kT}\frac{\tan\varphi}{[1-\exp(-v\sigma/kT)]}\times\left\{\left[1+\frac{A^2\exp(-2W_k/kT)\sinh^2(v\sigma/2kT)}{(\tan^2\varphi)(v\sigma/2kT)^2}\right]^{\frac{1}{2}}+1\right\}, \qquad (14)$$

$$n_0^-=\frac{1}{a}\frac{v\sigma}{2kT}\frac{\tan\varphi}{[\exp(v\sigma/kT)-1]}\times\left\{\left[1+\frac{A^2\exp(-2W_k/kT)\sinh^2(v\sigma/2kT)}{(\tan^2\varphi)(v\sigma/2kT)^2}\right]^{\frac{1}{2}}-1\right\}, \qquad (15)$$

where

$$v=abL\cos\varphi. \qquad (16)$$

Equations (14) and (15) represent for $\sigma\to 0$ the kink density of the stress-free dislocation and approach the result of Eshelby,[2] except that in Eshelby's equation μ_d is ignored, so that A^2 has a different value. Furthermore, Brailsford,[5] starting from transport equations, has arrived at relations which show the same dependence on the stress σ. Yet Brailsford's result contains an unspecified function n_0p_0 which, as we have shown above, can be expressed in terms of kink formation energy W_k, temperature, and the factor A.

B. The Stress-Strain Relation

Starting from the kink densities found in Eqs. (10) and (10′), we will now calculate the anelastic strain ϵ, which results from sideward motion of geometrical or thermally created kinks.

The average shape of the kinked dislocation is given by the integral[5]

$$y(x)=a\int_0^x(n^+-n^-)dx. \qquad (17)$$

With Eqs. (10) and (10′) we get

$$y(x)=\cos\varphi aL(kT/v\sigma)\{n_0^+[1-\exp(-ab\sigma x/kT)]+n_0^-[1-\exp(ab\sigma x/kT)]\}. \qquad (18)$$

The anelastic strain, contributed by the line segment L, follows from[5]

$$\epsilon(\sigma)=(b\Lambda/L)\int_0^{L\cos\varphi}[y(x,\sigma)-y_0(x)]dx, \quad (19)$$

where $y_0(x)=x\tan\varphi$ represents the stress-free dislocation (Λ=dislocation density).

Integration of Eq. (19) yields

$$\epsilon=(b/L)(\cos\varphi kT/v\sigma)^2\Lambda L^2 a \times\{n_0^+[v\sigma/kT-(1-\exp\{-v\sigma/kT\})] +n_0^-[v\sigma/kT-(\exp\{v\sigma/kT\}-1)]\} -(\Omega b/2L)\tan\varphi(L\cos\varphi)^2. \quad (20)$$

We now have to replace n_0^+ and n_0^- by Eqs. (14) and (15) and find the following stress-strain relation:

$$\epsilon(\sigma,T)=\frac{b}{4L}\Lambda L^2\sin 2\varphi \times\left[1+\frac{A^2\exp(-2W_k/kT)\sinh^2(v\sigma/2kT)}{(\tan^2\varphi)(v\sigma/2kT)^2}\right]^{\frac{1}{2}} \times\left[\coth\frac{v\sigma}{2kT}-\frac{2kT}{v\sigma}\right]. \quad (21)$$

The last bracket is known as Langevin's function $L(x)$ and describes, in paramagnetism or paraelectricity, the orientation of dipoles in an electric or magnetic field. $L(x)$ is proportional to $x/3$ for small x and approaches 1 for large x. In our case of mechanical relaxation of kinks, the magnetic or electric dipole energy is replaced by the energy $v\sigma$ of a kink in a stress field σ. $L(x)$ in Eq. (21) describes the shifting of kinks, whereas the expression under the square root sign represents the double-kink generation.

Under the condition

$$A\exp(-W_k/kT)[(\sinh(v\sigma/2kT))/(v\sigma/2kT)]\ll\tan\varphi, \quad (22)$$

which is fulfilled for small stresses and low temperatures, double-kink generation can be ignored, and the stress-strain relation has the form

$$\epsilon=\frac{b}{4L}\Lambda L^2\sin 2\varphi \times\frac{\cosh(v\sigma/2kT)-(2kT/v\sigma)\sinh(v\sigma/2kT)}{\sinh(v\sigma/2kT)}. \quad (23)$$

For $\sigma=0$, condition (22) can be interpreted as stating that the number of thermal kinks must be small compared with the number of geometric kinks.

If, on the other hand, temperature or stress is high so that the following relation holds:

$$A\exp(-W_k/kT)[\sinh(v\sigma/2kT)]/v\sigma/2kT\gg\tan\varphi, \quad (24)$$

the stress-strain relation can be written as:

$$\epsilon=\frac{b}{2L}\Lambda L^2\cos^2\varphi A\exp(-W_k/kT) \times\frac{\cosh(v\sigma/2kT)-(2kT/v\sigma)\sinh(v\sigma/2kT)}{v\sigma/2kT}. \quad (25)$$

Both stress-strain relations [Eqs. (23) and (25)] become nonlinear at relatively small stresses. If we expand in terms of $v\sigma/2kT$, we get:

$$\epsilon=\frac{b}{24L}\frac{v\sigma}{kT}\Lambda L^2\sin 2\varphi\left[1-\frac{1}{60}\left(\frac{v\sigma}{kT}\right)^2+\cdots\right], \quad (23a)$$

and

$$\epsilon=\frac{b}{12L}\frac{v\sigma}{kT}\Lambda L^2\cos^2\varphi A\exp(-W_k/kT) \times\left[1+\frac{1}{40}\left(\frac{v\sigma}{kT}\right)^2+\cdots\right]. \quad (25a)$$

So both stress-strain relations become nonlinear for

$$v\sigma>2kT. \quad (26)$$

The essential difference lies in the sign of the nonlinearity. In the first relation [Eq. (23)], the strain increases slower than proportional to the stress, as one expects, due to the restricted motion of geometric kinks. In the second relation [Eq. (25)], the strain increases faster than proportional to the stress because double-kink generation supplies more kinks with increasing stress. Consequently, the complete stress-strain relation, Eq. (21), generally has first an exhaustion region, in which $\partial^2\epsilon/\partial\sigma^2<0$. At a certain stress level, which is determined by condition (24), double-kink generation becomes significant, the sign of $\partial^2\epsilon/\partial\sigma^2$ becomes positive, and, as shown in Fig. 2, the strain increases exponentially with stress, as

$$\epsilon=(b/2L)(kT/v\sigma)\Lambda L^2 A \times\exp[(-2W_k+|v\sigma|)/2kT]. \quad (25b)$$

The exhaustion region disappears at temperatures for which condition (24) is already fulfilled for zero stress. We realize that the exhaustion region extends to the larger stresses, the larger $\tan\varphi$, which means the higher the geometric kink density.

We will now determine the limitation of the above treatment. Clearly, the exponential increase of strain with stress demonstrated in Eq. (25b) cannot continue, and at a certain kink density the interaction of kinks must modify the stress-strain relation.

The interaction energy between two kinks has been determined by several authors as[2,6–8]:

$$U=\pm(Gb^2a^2\beta/8\pi d), \quad (27)$$

[7] F. Kroupa and L. M. Brown, Phil. Mag. **6**, 1267 (1961).
[8] A. D. Brailsford, Phys. Rev. **128**, 1033 (1962).

where d = distance between the kinks, $\beta=[(1+\nu)\cos^2\Phi+(1-2\nu)\sin^2\Phi]/(1-\nu)$, ν = Poisson ratio, and Φ = angle between Burgers vector and close-packed direction.

Our treatment is not applicable for kink densities for which the kinks have an average potential energy which is comparable with kT, so we must require[4,9]

$$(Gb^2a^2\beta n)/(4\pi kT)<1 \quad \text{with} \quad n=n^+ \text{ or } n^-. \tag{28}$$

Without external stresses, n equals $\sin\varphi/a$, so that

$$(Gb^2a\beta/4\pi)\sin\varphi<kT. \tag{29}$$

With $kT=10^{-2}$ eV, $Gb^2a\beta=3$ eV, one finds $\varphi<0.04$.

Condition (29) thus establishes an upper limit for the angles φ, for which the stress-strain relation of Eq. (21) can be applied.

Under stress, the highest kink density, consisting of positive kinks, accumulates at $x=0$.

Using Eq. (14) in condition (28), we get with $v\sigma>kT$ and for small angles φ

$$(Gb^2a\beta/8\pi kT)A\exp[(-2W_k+v\sigma)/2kT]<1, \tag{30}$$

or

$$v\sigma<2W_k-2kT\ln(Gb^2a\beta A/8\pi kT). \tag{30'}$$

This relation is of interest insofar as Paré[10] suggests the relation

$$v\sigma_i\geq 2W_k \quad (\sigma_i=\text{internal stress}) \tag{31}$$

as a necessary condition for the existence of a double-kink generation peak in cold-worked materials. Comparing conditions (31) and (30), we realize that the condition (31) for the existence of a peak necessarily implies that the kinks interact with each other. Consequently, interaction of kinks cannot be ignored in determining the peak height, as well as the activation energy for the double-kink generation peak.

Another quantity of interest is the total number of kinks as a function of stress. Integrating Eqs. (10) and (10′) yields the result

$$N^{\pm}=\frac{L}{2a}\sin\varphi\left\{\left[1+\frac{A^2\exp(-2W_k/kT)}{\tan^2\varphi}\times\frac{\sinh^2(v\sigma/2kT)}{(v\sigma/2kT)^2}\right]^{\frac{1}{2}}\pm1\right\}. \tag{32}$$

We realize that the total number of kinks is an even function of stress, as it must be for symmetry reasons. So for small oscillating stresses, the total number of kinks of each sign does not change; only their relative positions to each other change.

[9] For a more refined criterion, involving the gradient of the potential energy, see Ref. 11.

[10] V. K. Paré, J. Appl. Phys. 32, 332 (1961), and thesis, Cornell University, Ithaca, New York 1958 (unpublished).

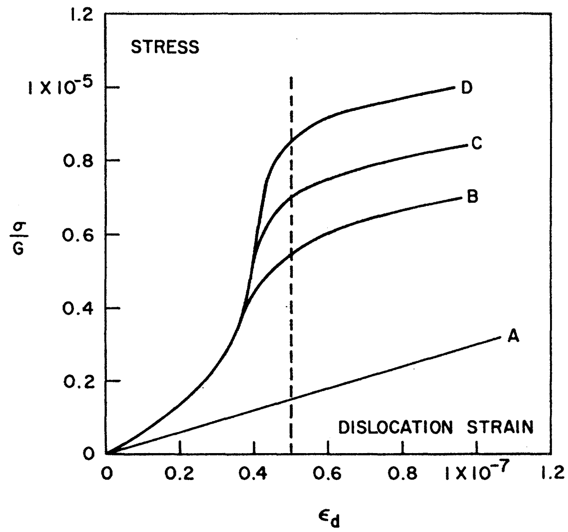

FIG. 2. Stress-strain relation for a dislocation string (A) and for a kinked dislocation with low kink density (B, C, D) [Eq. (21)]. The parameters used are: $\Lambda L^2=10^{-1}$, $E_L=Gb^2/4$, $Gb^2a=660kT$, $A^2=5$, $L=3\times10^3b$, $W_k=10kT$ (curve B), $11.5kT$ (curve C), $13kT$ (curve D). The dashed line represents the total strain which can be achieved without double kink generation.

III. INTERACTING KINKS

A. Temperature $T=0$°K

We will now determine the distribution of interacting kinks under external stress, taking into account only nearest-neighbor interaction. In a preceding paper,[11] it has been shown that the results following from nearest-neighbor interaction of the kinks represent fairly well the results for long-range interaction, if one increases the effective line tension $E_L=Gb^2\beta/4\pi$ of the kink chain, as determined in nearest-neighbor interaction, by a factor $\ln N$, where N is the number of kinks in the line segment.

The potential energy of the kink i in the stress field of its neighbor kinks and the external stress σ is given, according to Eq. (27), by

$$U_i=(Gb^2a^2\beta/8\pi)\times(1/(x_i-x_{i-1})+1/(x_{i+1}-x_i))-ab\sigma x_i, \tag{33}$$

x_i = position of the kink i.

The force is consequently

$$K_i=(Gb^2a^2\beta/8\pi)[(x_i-x_{i-1})^{-2}-(x_{i+1}-x_i)^{-2}]+ab\sigma. \tag{34}$$

If we abbreviate $d_i=x_i-x_{i-1}$, we can write the equations $K_i=0$ as[12]

$$d_i^{-2}-d_{i+1}^{-2}=-\alpha 4N/L^2 \quad i=1\cdots N+1. \tag{35}$$

where α is dimensionless and is given by

$$\alpha=\tfrac{1}{2}(4\pi\sigma L^2/Gab\beta N)=\tfrac{1}{2}(\sigma/G)(L/b\sin\varphi)Gb^2/E_L. \tag{36}$$

[11] G. Alefeld, J. Appl. Phys. 36, 2633 (1965).

[12] This set of equations has already been derived by W. Lems, Physica 30, 1617 (1964).

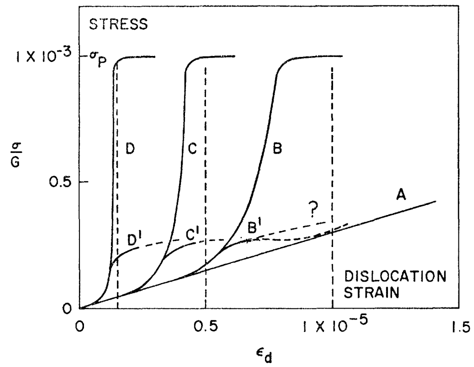

FIG. 3. Stress-strain relation for a dislocation string (A) and for a kinked dislocation with large kink density at $T=0$ (B, C, D) [Eqs. (49) and (50)] and for temperatures above the double-kink generation peak (B', C', D'). The parameters used are: $\Lambda L^2=10^{-1}$, $E^-=Gb^2/4$, $(b/L)\sin\varphi=2\times10^{-4}$ (curve B), 10^{-4} (curve C), 3×10^{-5} (curve D). $\sigma_P=10^{-3}$ G. (It is assumed that the line tension E_L of the string is the same as that of the kink chain.)

The sum of the distances d_i must add up to L. This gives the condition

$$\sum_1^{N+1} d_i=L. \quad (37)$$

By adding Eqs. (35) from 1 to i, one can express all distances d_i as a function of d_1.

$$d_i^{-2}=(i-1)4N\alpha/L^2+d_1^{-2}$$

or

$$d_i=d_1[1+4N(i-1)\alpha(d_1/L)^2]^{-\frac{1}{2}}. \quad (38)$$

The distance d_1 must be determined as follows:

$$(d_1/L)\sum_{i=1}^{N+1}[1+4N(i-1)\alpha(d_1/L)^2]^{-\frac{1}{2}}=1. \quad (39)$$

This equation gives the distance d_1 as a function of stress σ. The other distances can then be determined by means of Eq. (38).

For small stresses, the summation of Eq. (39) can be replaced by an integration, with the result that

$$[1+4N^2\alpha(d_1/L)^2]^{\frac{1}{2}}-1=2N\alpha d_1/L. \quad (40)$$

Solving for d_1 yields

$$d_1=(L/N)/(1-\alpha). \quad (41)$$

Clearly this result does not hold for $\alpha=1$. For large stresses, or $\alpha>1$, one can find another solution of Eq. (39) as follows: Except for $i=1$, we can ignore 1 compared with $4N(i-1)\alpha(d_1/L)^2$, so that the summation has the form

$$(d_1/L)\left[1+\sum_1^N(4i\alpha N)^{-\frac{1}{2}}L/d_1\right]=1. \quad (42)$$

The sum over $i^{-\frac{1}{2}}$ is to a good approximation, given by

$$\sum_i^N i^{-\frac{1}{2}}=2N^{\frac{1}{2}}-\tfrac{3}{2}.$$

Solving for d_1 yields

$$d_1=L[1-\alpha^{-\frac{1}{2}}(1-3N^{-\frac{1}{2}}/4)]. \quad (43)$$

For $\alpha=1$, the distance d_1 as determined by Eq. (43) is given by $d_1=(L/N)3N^{\frac{1}{2}}/4$. This means that d_1 has increased by a factor $N^{\frac{1}{2}}$ compared with the equilibrium value. The distance d_1 increases continuously with stress. Half of the other distances $d_i(1<i<N/2)$ first increase with stress, reach a maximum, and then decrease to zero. The distances d_i with $i>N/2$ decrease already for small stresses.

With the solutions [Eqs. (41) and (43)] for d_1, we now determine the stress-strain curve for the stress regions $\alpha<1$ and $\alpha>1$.

Lems[12] has shown that the strain ϵ is given by

$$\epsilon=(\Lambda ab/L)\sum_i^N[d_i(N+1-i)-id_0]$$

d_0 stands for L/N. (44)

Inserting Eq. (38) into Eq. (44) yields

$$\epsilon=\Lambda ab\frac{d_1}{L}\left\{\sum_{i=1}^N\frac{N-(i-1)}{[1+4N(i-1)\alpha(d_1/L)^2]^{\frac{1}{2}}}-d_0\sum_{i=1}^N i\right\}. \quad (45)$$

For $N>1$, the individual sums in Eq. (45) can be replaced as follows:

$$\sum_{i=1}^N i=N^2/2 \quad (46)$$

$$N\sum_{i=1}^N[1+4N(i-1)\alpha(d_1/L)^2]^{-\frac{1}{2}}=NL/d_1$$

[See Eq. (39)]. (47)

The third sum can be evaluated for $\alpha<1$ or $\alpha>1$ by employing the same methods which were used above to determine d_1.

$$\sum_{i=1}^N\frac{(i-1)}{[1+4N(i-1)\alpha(d_1/L)^2]^{\frac{1}{2}}}$$
$$=(1/12N^2\alpha^2)(L/d_1)^4\{1-[1+4N^2\alpha(d_1/L)^2]^{\frac{1}{2}}$$
$$\times[1-2N^2\alpha(d_1/L)^2]\} \quad \text{for} \quad \alpha<1,$$
$$=\tfrac{1}{3}(N/\alpha^{\frac{1}{2}})(L/d_1) \quad \text{for} \quad \alpha>1. \quad (48)$$

Using the above sums [Eqs. (46)–(48)] in Eq. (45) and replacing d_1 by Eq. (41) and Eq. (43), respectively, yields for the strain ϵ contributed by the dislocation segment of the length L and with N kinks:

$$\epsilon=(\Lambda abN/b)\alpha=(\Lambda L^2/12)(Gb^2/E_L)(\sigma/G) \quad \alpha<1, \quad (49)$$

and

$$\epsilon=\frac{\Lambda abN}{2}(1-\tfrac{2}{3}\alpha^{-\frac{1}{2}})$$

$$=\frac{\Lambda Lb}{2}\sin\varphi\left[1-\frac{2}{3}\left(\frac{2b\sin\varphi}{L}\frac{G}{\sigma}\frac{E_L}{Gb^2}\right)^{\frac{1}{2}}\right]\quad \alpha>1. \qquad (50)$$

We realize that both ϵ and $d\epsilon/d\alpha$ fit together continuously at $\alpha=1$.

In Fig. 3, we have plotted the stress-strain relation [Eqs. (49) and (50)] for different geometric kink density. At $\sigma=\sigma_P$, double-kink generation will set in even at zero temperature. Consequently, the stress-strain relation has a sharp strain increase at $\sigma=\sigma_P$. This takeoff will then allow the Peierls stress to be experimentally measured directly. It is interesting to note that the measurement of the complete stress-strain relation allows one to determine ΛL^2 as well as ΛLb, so that dislocation density as well as line length can be estimated. Yet it should be emphasized that Eq. (50) gives only the general form of the stress-strain relation in the region of restricted geometric kink motion. The numerical accuracy suffers from the extension of the interaction law, Eq. (27), to small distances d. We furthermore have ignored the fact that the crystallographic direction against which the kinks are pressed has an angle smaller than 90° to the dislocation line.

B. Finite Temperature

At finite temperature the sharp strain increase (Fig. 3) will be shifted to lower stresses. One expects that it disappears at the double-kink generation peak. This argument is based on rate considerations. We are assuming that the stress-strain relation is measured within a certain time or at a certain frequency which can be related to the relaxation time of the double-kink generation peak. Yet we found in Sec. II that independent of rate considerations the stress-strain relation of noninteracting kinks is modified for reasons which follow from purely thermodynamic equilibrium considerations. We will now show that the stress-strain relation of interacting kinks will also be different from that of a string, even if we measure at temperatures which are above the double-kink generation peak. In Sec. III A we showed that the deviation from a linear stress-strain relation occurred at $\alpha\geq 1$ or

$$\sigma/G\geq 2(b/L)\sin\varphi(E_L/Gb^2). \qquad (51)$$

We now have to estimate for interacting kinks the stress at which significant double-kink generation compensates for the exhaustion of geometric kink motion. This estimate will be based on the condition that the free energy of the dislocations with a new double kink is smaller than that of dislocations without a new double kink. The newly created kinks pile up behind the existing kinks. If the double kink is stable, then the dislocation has continued to bow by the distance a, which is measured perpendicular to the close-packed direction. Consequently, the area gained due to the formation of a double kink is approximately $A\approx aL/2$. The work done by the external stress is correspondingly $ab\sigma L/2$. Simultaneously, the interaction energy of the kinks increases by a certain amount ΔU, which depends on the detailed configuration of the already existing kinks.

The condition for creation of double kinks can consequently be written as

$$2W_k-ab\sigma L/2+\Delta U-T\Delta S\leq 0. \qquad (52)$$

ΔS is the entropy difference between the states with and without a new double kink. It will be of the order or several k, so that $T\Delta S$ approaches $2W_k$ only at temperatures which are large compared with the temperature of the double-kink generation peak. ΔU can in general be assumed to be positive. (It could be negative, for example, when one of the newly created kinks moves to the pinning point and decreases its potential energy in the field of the geometric kinks of the next line segment more than the energy increases due to the piling up of the existing kinks by the other newly created kink.)

We now write Eq. (52) as follows:

$$\sigma/G>(2b/L)(2W_k+\Delta U-T\Delta S)/Gb^2a \qquad (52')$$

and compare the stress with that of Eq. (51). We thus find that for a certain range in angles φ, namely,

$$\sin\varphi<(2W_k+\Delta U-T\Delta S)/E_La, \qquad (53)$$

the stress for creation of stable double kinks is larger than the stress [Eq. (51)] at which the exhaustion region starts out. Consequently, for these dislocations the linear stress-strain region is followed by a region in which $\partial^2\epsilon/\partial\sigma^2<0$ (Fig. 3). The subsequent inflection point is roughly determined by Eq. (52′). The existence of an exhaustion region in the stress-strain law even above the double-kink generation peak is a consequence of the fact that the free energy of a line segment increases in multiples of $2W_k$. Only for dislocations with many geometric kinks is the stress needed to reach the exhaustion region large enough for creation of new double kinks. With $2W_k\approx 1$ eV (tungsten) and $E_La=5$ eV, we find for $2W_k/E_La\approx 0.2$. Since ΔU will increase this value and $T\Delta S$ is significant only at high temperatures, we find that a large part of all dislocations do have an inflection point in their stress-strain relation (Fig. 3) which disappears only at high temperatures if ΔS is positive. Equation (52′) indicates, furthermore, that the smaller the line length L, the larger the stress needed for significant double-kink generation.

The details of the stress-strain relation after passing the inflection points depend on the interaction law of the kinks and how the compressed kinks finally lose their individuality. Since double kinks exist in sufficient

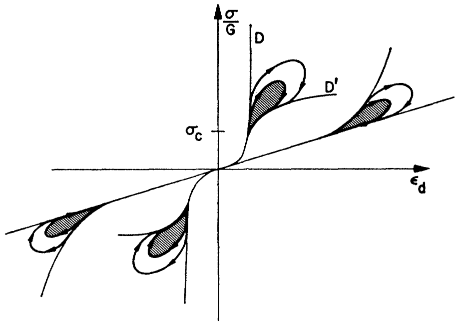

FIG. 4. Amplitude-dependent hysteresis loops caused by double kink generation. The stress-strain curves D (for temperatures below the double kink generation peak) and D' (above peak) are taken from Fig. 3. For $\sigma < \sigma_C$ only a vanishingly small loop exists. The two concentric loops correspond to different maximum oscillation amplitudes, whereas the two different stress-strain relations correspond to different geometric kink density. $\sigma_c/G = \alpha(b/L)(2W_k/Gb^2a)$.

amount, the stress-strain relation will not differ appreciably from that of a string in a Peierls-stress-free material. But it may be possible that a second inflection point exists before the kinked dislocation follows a string-like stress-strain relation.

IV. DISCUSSION

We have shown that the reversible stress-strain relation of kinked dislocation segments differs significantly from that of a dislocation in a material with vanishing Peierls stress. The physical reason can be found in the fact that due to the Peierls potentials the free energy of the dislocations increases only in multiples of the double-kink energy $2W_k$. From this follow two consequences: (a) If the measuring time is short compared with the time constant for double-kink creation, one can at high stresses (static or oscillatory) exhaust the possible dislocation motion, which results from shifting of geometric kinks. This argument is based on rate considerations and is consequently limited to temperatures below the double-kink generation peak. (b) Independent of this rate argument, we have shown that one can deduce from purely thermodynamic equilibrium considerations that the stress-strain relation for a large part of the dislocation spectrum (spectrum in angles against close-packed direction) has after a linear region a section in which the strain increase per unit stress becomes smaller with increasing stress–i.e., $\partial^2\epsilon/\partial\sigma^2 < 0$. This region exists independently, regardless of whether the entropy or the interaction determines the linear region. It is the result of the restricted motion of geometric kinks. When the stress is high enough for significant double-kink generation, the stress-strain relation passes through an inflection point. There may be a second inflection point before the stress-strain relation approaches that of a string.

We will now state experimental consequences resulting from the particular shape of the reversible stress-strain relation of kinked dislocations:

(1) The restricted motion of geometric kinks between $T = 0°K$ and the double-kink generation peak can be experimentally detected as a *decrease* of the modulus defect at high amplitudes. At $T \approx 0°K$, the modulus defect increases sharply only when $\sigma = \sigma_P$. If σ_P is larger than the stress required to activate Frank-Reed sources, such a decrease followed by a sharp increase of the strain cannot be explained in terms of the string model. Because of thermal activation at higher temperatures, the increase at large amplitudes will occur at correspondingly lower stresses. One will have to be prepared for the observation that the decrease of the modulus defect is also being preceded by an increase which is due to breakaway from pinning points or to motion of dislocations over internal stress ranges.

(2) It has been shown that the stress-strain relation is also nonlinear above the double-kink generation peak (see Fig. 3). These nonlinearities will manifest themselves mainly as an increase of modulus defect and of kilo- or megacycle damping when the stress amplitude reaches the stress of Eq. (31) or Eq. (52'). Careful measurements may detect small decreases of both quantities before they start to rise.

(3) If it is assumed that the sideward motion of existing kinks is a process which at low temperatures occurs rapidly compared with kink creation, the relaxation strength Δ_M of the double-kink generation peak is determined by the difference of the strain per stress increment which can be achieved with or without double-kink generation. Since at small stresses bowing is achieved by sideward shifting of existing kinks only, the relaxation strength is thus zero. Paré[10] suggested that internal stresses σ_i [Eq. (31)] induced by cold working increases the relaxation strength to an observable value.[13] Only for a bowed dislocation segment does the strain increase due to a small stress increment depend on whether or not double kinks are being created. Yet it has been observed by Chambers[14] that in pure bcc metals certain peaks which appear after cold working the material can also be observed in *undeformed material* by high-amplitude oscillations. Our result about the stress-strain relation of kinked dislocations shows that this observation provides evidence for an interpretation of these peaks in terms of the double-kink generation mechanism. Using the stress-strain curves of Fig. 3, Fig. 4 indicates how an absorption peak which had vanishing relaxation strength at small amplitudes rises with rising oscillation amplitude. The criterion for the peak appearance is given by Eq. (31) or Eq. (52'), in which σ/G now means the maximum oscillation amplitude. It should be pointed out that there is only small

[13] See also A. D. Brailsford, Phys. Rev. **137**, A1562 (1965).
[14] R. H. Chambers, in *Physical Acoustics*, edited by W. P. Mason, Vol. III-A (to be published).

hope for measuring the hysteresis loops of Fig. 4 directly. The required stress amplitudes σ_c simultaneously make the background of internal friction, which is probably caused by the motion of dislocations over internal stress hills, rise to such high values that the loops of Fig. 4 appear only as a distortion of the total hysteresis loop. Nevertheless, an internal friction peak will be detectable above a high but structureless background.

There is an additional requirement which must be fulfilled in order for a well-defined peak to grow out of the background by high-amplitude oscillation: the double-kink generation energy should not change significantly at the required amplitudes of oscillation. If we require that the activation energy for double-kink generation change less than $2kT$ at the stress given by Eq. (31), we get the following condition for the activation volume v_P for double-kink generation:

$$v_P\sigma < 2kT \tag{54}$$

or

$$v_P < (kT/W_k)abL. \tag{54'}$$

With $kT \approx 10^{-1}W_k$, we find that it must be smaller than one-tenth of the activation volume for double-kink recombination. This condition seems at first glance to be trivial, but it is important for the following reason: Paré[10] has shown that the contribution to internal friction from dislocations which are not exposed to the required internal stresses [Eq. (31)] are vanishingly small peaks, which are located at lower temperatures than the observed peak. If the activation volume for kink creation were as large as that for kink annihilation ($\approx abL$), then these little peaks would be shifted by high-amplitude oscillation individually to even lower temperature and would decrease even more in height. Only if the activation volume for forward motion of the dislocation is very small compared with that for backward motion will these peaks increase in height, be shifted to higher temperature, and accumulate at one common temperature.[15] This asymmetry in regard to the stress dependence of the activation energy for forward and backward motion is, in contrast to other relaxation mechanisms, characteristic of the double-kink generation and annihilation mechanism.[16]

In deformed material one expects to see the existing double-kink generation peaks grow with increasing oscillation amplitude[17] because at high amplitudes the absorption of dislocations is added which did not have the required internal stress to contribute at small amplitudes.

If the two activation volumes are strongly different (as is the case for bcc metals, and also for fcc metals if the line length is large), then one will find experimentally first a peak rise, before the peak shifts to lower temperatures. Whether this peak shift is experimentally observable, and how large and broad the peak is for $\sigma = \sigma_P$, depends on what mechanism determines the macroscopic flow.

(4) Another experimental possibility to verify the nonlinear stress-strain relation of kinked dislocations is as follows: A static external bias stress should, *in undeformed pure material*, cause the appearance of an absorption peak as measured at low-amplitude oscillations. The high purity is required to rule out an explanation of the increase of the relaxation strength by unpinning. The methods of high-amplitude oscillations or a static bias stress applied to undeformed material are clearly more selective in an effort to identify the absorption mechanism of these peaks, than the hitherto standard method of introducing dislocation-dislocation interaction by cold working.

(5) Figure 3 shows that for $\sigma = \sigma_P$ a "flow stress" is reached. This flow stress can be the flow stress for long-range flow (for example, bcc structures at low temperatures) or also the flow stress for short-range flow (fcc structures in which the cutting of dislocations is rate determining for long-range flow). This "micro" or "macro" flow stress at $T \approx 0°K$ should be observable in both cases and is a measure for the Peierls stress σ_P. The flow at $\sigma \approx \sigma_P$ cannot be expected to be as sharp as drawn in Fig. 3. Stress concentrations near the pile-ups of geometric kinks add to the external stress. Thus, locally along the same line, the Peierls stress is reached before the external stress σ_a equals σ_P. This stress concentration can be interpreted as an increase in the activation volume over that for double-kink creation on a straight line. The microflow or macroflow stress at $T=0$ thus gives only a lowest value for the Peierls stress σ_P. This statement is important if one calculates a Peierls stress from the measured double-kink generation energy and compares this stress with the flow stress at $T=0$. It may be the answer to why the macroflow stress in fcc metals at $T=0$ is smaller than the calculated Peierls stress. The microflow stress has not yet been measured in these materials. It should be pointed out that even in fcc metals which have very high perfection[18] and purity the velocity with which dislocations move at low temperatures is determined by the double-kink generation mechanism. In Al, for example, a double-kink generation energy of 0.26 eV has been found.[19] On the other hand, Nunes *et al.*[20] have

[15] This statement can be proven rigorously for an asymmetric double-well potential, which Paré (Ref. 10) used as a model for the double-kink generation mechanism (to be published).

[16] Another consequence of this asymmetry in activation volume for forward and backward motion of a kinked dislocation is the following: When an originally bowed dislocation has been oscillated at high amplitudes, it will not stay as bowed after stopping the oscillation if the temperature is below the double-kink generation peak. The dislocation loses some or all of its double kinks without being able to create them at the given stress and temperature. One thus builds up internal stresses which relax with the time constant of the double-kink creation peak.

[17] V. K. Paré (Ref. 10) observed for the Bordini peak in cold-worked copper a small increase in peak height with increasing amplitude.

[18] F. Young, J. Appl. Phys. **32**, 1815 (1961).

[19] J. L. Routbort, thesis, Cornell University, Ithaca, New York 1965 (unpublished).

[20] A. C. Nunes, Jr., A. Rosen, and J. E. Dorn, Trans. ASM **58**, 38 (1965).

determined the activation energy for flow as 0.22 eV and interpreted the mechanism as cutting of dislocations. Already Lothe and Hirth[21] have suggested that the rate for low-temperature creep in Al may be determined by the double-kink generation mechanism.

(6) Throughout this paper we have considered the consequence of the existence of only one Peierls stress. Experiments on bcc metals[14] suggest that these materials have more than one Peierls stress, either due to different dislocation types[22] (screws, edges) or due to different crystallographic directions. If more than one Peierls stress exists, then, for example, the stress-strain relation at liquid-He temperature in Fig. 3 should show steps at the different Peierls stresses. Also, the stress-strain relation at higher temperature will have more fine structure owing to the different components.

(7) The width of the double-kink generation peak has been the subject of extensive discussion.[5,10,13] The multiplicity of Peierls potentials[22] is one reason. We will now consider the question of whether one can expect a unique activation energy at all, even if there is only one Peierls potential. It appears as if the requirement of dislocation-dislocation interaction for the existence of a peak necessarily implies a certain spectrum in activation energies. For dislocations with high kink density the double kinks are created in an environment in which they interact with already existing kinks. Let us assume that a line of length L is bowed by internal stresses to half the Frank-Read radius. If one approximates the kinked dislocation line by a circle, one easily shows that the new kinks are created at distance d from the next existing kinks which is smaller than $\sqrt{(La)}$. From Eq. (27) one finds, with $Gb^2a=5$ eV, $\beta=2$, $L=10^3a$, an interaction energy of 0.025 eV, which is 25% of the average double-kink generation in copper. With $Gb^2a=25$ eV (tungsten), ΔU is 0.13 eV. The stress required to bow a line of the length of 10^3a to half its Frank-Read radius is of the order of 3×10^{-4} G, which can easily be expected in deformed metals.

For dislocations with low kink density, the activation energy for double-kink creation can be lowered by the required internal stress,[10] as the following calculation shows: A rough estimate for the activation volume for double-kink creation v_P follows from the condition that the activation energy U is zero for $\sigma=\sigma_P$. So

$$v_P\sigma_P\approx U. \qquad (55)$$

An internal stress σ_i of the size given by Eq. (31) lowers the activation energy U by $\Delta U=v_P\sigma_i$. The relative change in energy can thus be written as

$$(\Delta U/U)=(b/L)(2W_k/Gab^2)(G/\sigma_P). \qquad (56)$$

With $2W_k/Gab^2=1/50$ and $\sigma_P/G=10^{-4}$ (fcc metals) and $L=10^3b$, one finds a 20% lower activation energy. Thus one can hardly expect that a double-kink creation peak has the width of a single relaxation peak. Its shape depends on the type of deformation which determines the arrangement and length of the contributing dislocations as well as the size of the internal stresses.

(8) Finally, it should be mentioned that the stress-strain relation of bowing dislocation segments determines the stress dependence of the activation energy for other dislocation rate processes, as, for example, cutting of dislocations or breakaway from pinning points.[23] In general, one can predict that the activation volume which is determined by kinked dislocation segments is smaller than that of string segments. We thus find that the Peierls potentials also determine details of rate processes other than double-kink generation.

[21] J. Lothe and J. P. Hirth, Phys. Rev. **115**, 543 (1959).
[22] D. O. Thompson and D. K. Holmes, J. Appl. Phys. **30**, 525 (1959).
[23] R. H. Chambers, Appl. Phys. Letters **2**, 165 (1963).