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*Abt. f. Metallphysik, II. Physikalisches Institut, Universität Köln,
Zülpicher Str. 77, D-5000 Köln 41, F.R.G.*

Résumé - Pour rendre compte des courbures de dislocations dans le silicium différentes estimations de la tension de ligne sont présentées et comparées aux résultats expérimentaux obtenus à faibles et fortes contraintes.

Abstract - Different approximations for the line tension of dislocation bends in silicon are discussed and compared with experimental results obtained for low stress and high stress deformation.

Introduction - In TEM-studies of deformed materials it is a widely used method to estimate the local stress acting on a dislocation from the measured radius of its curvature R. The static bow out of a dislocation between two obstacles is held in an equilibrium position by the driving force

$$F = \tau b \quad (1)$$

(τ = res. shear stress, b = Burgers vector of the perfect dislocation) and the backward directed force in the following text shortly called self force (S = line tension)

$$F = S/R \quad (2) \qquad \tau = S/(Rb) \quad (2a)$$

In silicon crystals deformed under high uniaxial stress the dislocations mainly are lying straight along the $\langle 110 \rangle$-directions with 60°-bends as transitions from one $\langle 110 \rangle$-Peierls trough to another one(Fig.1) /1/. This is also true for low stress deformed specimens if the dislocation density is low (A. Tönnessen, H. Gottschalk, and H. Alexander, to be published; Fig.3). On cooling the crystals with the load applied the dislocation motion is frozen in whereby the curvatures of the bends are maintained.

It is reasonable now to try to apply the concept of line tension to these dynamic bends as outlined for the static bow out. F. Louchet /2/ used this method to calculate the stress acting on dislocations in in-situ straining experiments in the HVEM.

A problem, however, lies in the arbitrariness of the line energy of a dislocation and therefore of the line tension which arises by the arbitrariness of the cut-off radii. To achieve a reasonable choice for the cut-off parameters different approaches to the line tension problem for this special case of 60°-bends are investigated and compared with experimental results in the low stress range. The best matching parameters are used to apply the method to isolated partial dislocations and to more complicated bend structures in the high stress range.

Experimental - Silicon crystals (FZ-Si, $9 \cdot 10^{12}$ cm^{-3} B) were deformed in uniaxial compression and cooled to room temperature with applied load.
Specimens Type A: Compression axis $\langle 213 \rangle$, τ = 30 MPa, T = 650°C, ε = 0.2%, 0.8% and 2.5%.
Specimens Type B: Compression axis $\langle 213 \rangle$, τ = 250 MPa, T =420°C, after predeformation τ = 30 MPa, T = 750°C, ε = 1.5%.
Specimens Type C: Compression axis $\langle 2,1,11 \rangle$, T = 420°C, after predeformation along $\langle 213 \rangle$, T = 750°C, ε = 1.5%.
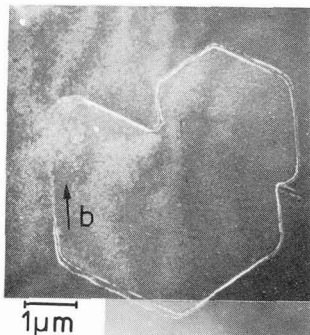
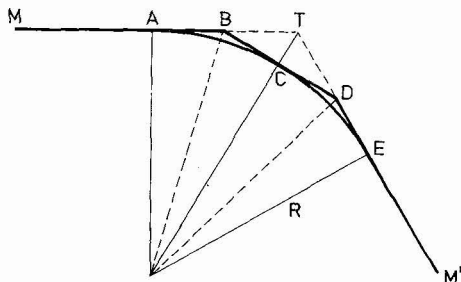Fig.1 - Dislocation loop in Si deformed
by high uniaxial stress along ⟨213⟩

Fig.2 - Geometrical approximation of a
60°-bend

Different types of bends - After low stress deformation the separation of the
partials d is small compared with the radius of curvature R. Therefore the
dislocations may be treated like perfect ones. For high stresses this condition is
not fulfilled and the actual situation of all partials in the bend has to be taken
into account.

In a hexagonal loop of a perfect dislocation two types of bends occur determined
by the character of the tangent at the apex (segment $\overline{BD}$, Fig.2):
1. the 30°-type (transition from a srew to a 60°-dislocation)
2. the 90°-type (transition from a (-60°)- to a(+60°)-dislocation).

In a dissociated dislocation loop for both the leading and the trailing partial
other two types of bends occur:
1. the 0°-type (transition from a (-30°)- to a (+30°)-partial)
2. the 60°-type (transition from a 30°- to a 90°-partial).

Three approaches to the line tension
1. A rough approximation of the line tension which is often given in the literature
is

$$S = Gb^2 \qquad (G = \text{shear modulus}) \qquad (3)$$

Here the variation of line energy with the character of the dislocation is not taken
into account. Since there is a clear evidence for an orientation dependence of the
line tension from the experimental results (Fig.3, different curvatures for
different types of bends) this approximation is not useful.

2. The orientation dependent line tension approximation first given by de Wit and
Koehler /3/ and discussed by Hirth and Lothe /4/ for a bow out of length L is given
in the form (ν = Poisson's ratio)

$$S = W_S/L + \frac{\partial^2}{\partial \beta^2}(W_S/L) = \frac{Gb^2}{4\pi(1-\nu)} ((1+\nu)\cos^2\beta + (1-2\nu)\sin^2\beta) \ln(L/e\rho) \qquad (4)$$

$$\ln e = 1; \qquad S = (Gb^2/4\pi)K'\ln(L/e\rho) \qquad (4a)$$

with the energy of a dislocation segment of length L

$$W_S = (Gb^2/4\pi)(\cos^2\beta + \sin^2\beta/(1-\nu)) L \ln(L/e\rho) \qquad (5)$$

Considering the dislocation bend the parameter L is not clearly defined. β is the
angle between dislocation line and Burgers vector and ρ is a suitable cut-off para-
meter which Hirth and Lothe assume to be b/8 /5/. Hirth and Lothe chose ρ so small
to include the dislocation core energy. In the literature some similar relations are
presented varing in the logarithmic term. In most cases the cut-off radius is
chosen larger. Weertman and Weertman /6/ in a simpler approximation not taking into
account the orientation dependence of line tension use ln(R/5b). When the length L
is identified with the segment $\overline{BD}$ in Fig.2 the comparison of both parameters yields:

$$L = \overline{BD} = R/(2\text{tg}15°) = 2R/(2+\sqrt{3}) \qquad (6)$$

$$L/(e\rho) = R/(1.866e\rho) = R/(5.07\rho) = R/(5b); \qquad \rho \approx b \qquad (6a)$$

It is shown later that the experimental results for ρ = b are in satisfying

agreement with this calculation, if the applied stress is low and therefore the radii of curvature are large. That confirms that the properties of the bend are determined by the character of the dislocation segment $\overline{BD}$ (Fig.2) in the apex of the bend. Another simple choice for L is L = R; its effect is described later.

3. When using the orientation dependent line tension eq.(4) the actual arrangement of dislocation segments outside the bend is not considered. The forces of the straight segments adjacent to the bend, however, acting on the dislocation at the apex are parts of the self force.

To improve the calculation of the line tension for an application to dislocations at high stress a method described by Hirth and Lothe /4/ is applied to the approximated bend according to Fig.2. The curved dislocation segment ACE, 60°-sector of a circle with radius R is approximated by the straight segments $\overline{AB}$, $\overline{BD}$, and $\overline{DE}$. The energy of an arbitrary segmented dislocation arrangement considered by the authors is composed of the self energies W_{Si} and the interaction energies W_{ij} of all segments

$$W = \sum W_{Si} + \sum_{i<j} W_{ij}$$

For a dislocation bend part of a large loop (diameter D ≫ R) the line tension results to

$$S = {}_m \lim_{\to \infty} (\partial W / \partial l) \big/ {}_m = \text{const.} \qquad (7)$$

$m = \overline{MT} = \overline{M'T}$ (Fig.2); for dl, the differential change of the dislocation length l, one finds (see Fig.2)

$$dl = dL(1-2/\sqrt{3})$$

For the four bend types in consideration the results are (ν (Si) = 0.217), setting:

$$p = 4/(2 + \sqrt{3}) \qquad q = 2(1 - \nu)(\sqrt{3} - 2) \qquad E = (Gb^2/4\pi)$$

1. 0°-type
$$S = (E/q)((q - \nu) \ln (L/\varrho) + (4 - 3\nu) \ln p) \qquad (8)$$
$$S(Si) = E K \ln (R/2.687\varrho); \quad K = 1.517 \qquad (9)$$

2. 30°-type
$$S = (E/2q)((4\sqrt{3} - 8 - \nu(3\sqrt{3} - 5)) \ln (L/\varrho) + (8 - 5\nu) \ln p) \qquad (10)$$
$$S(Si) = E K \ln (R/2.869\varrho); \quad K = 1.328 \qquad (11)$$

3. 60°-type
$$S = (E/2q)((4\sqrt{3} - 8 - \nu(\sqrt{3} - 3)) \ln (L/\varrho) + (8 - 3\nu) \ln p) \qquad (12)$$
$$S(Si) = E K \ln (R/3.538\varrho); \quad K = 0.949 \qquad (13)$$

4. 90°-type
$$S = (E/q)(2(\sqrt{3} - 2) + \nu) \ln (L/\varrho) + (4 - \nu) \ln p) \qquad (14)$$
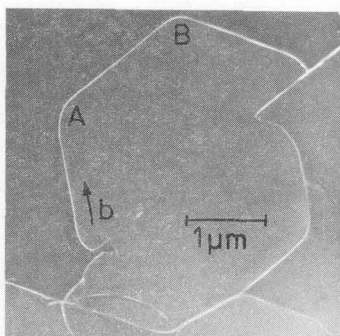$$S(Si) = E K \ln (R/4.247\varrho); \quad K = 0.760 \qquad (15)$$

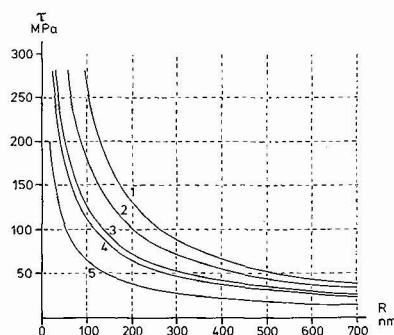Fig.3 - Dislocation loop in a specimen with low stress applied (30 MPa) bend A: 30°-type; bend B: 90°-type

Fig.4 - Calculated stress vs radius of curvature R. Lines 2 to 4:30°-type bends Line 5: 90°-type bends (eq.(15),ϱ =b) Line 1: both types (eq.(3)); 2: eq.(11) ϱ =b/8; 3: eq.(11) ϱ =b; 4: eq. (4) ϱ =b, L from eq.(6).

Comparison of the calculations - The comparison of the pre-logarithmic factors K in eq. (8) ... (15) with the factors K' given by the orientation dependent line tension calculation (eq.(4a)) shows that they are identical in practice (Table 1).

Table 1 - Pre-logarithmic factors for the actual 60°-bend calculation K and for the
orientation dependent line tension calculation K' (eq(4a)).

Bend-type	K	K'
0°	1.517	1.554
30°	1.328	1.346
60°	0.949	0.931
90°	0.760	0.723

Both results for S only differ in the logarithmic term in a factor of the cut-off
parameter ϱ . Setting $\varrho = b$ and calculating the self stress for a bend of the
30°-type using eq.(2a) and L according to eq.(6) yields a larger increase of the
stress for small radii of curvature when using eq.(11) instead of eq.(4) (Fig.4,
lines 3 and 4). If L = R is used in eq.(4) the results are nearly equal to those of
eq. 11 (line 3 in Fig.4).
    If ϱ = b/8 as assumed by Hirth and Lothe is applied to eq.(11) the stresses
become remarkably higher (line 2 in Fig.4).
    Line 5 is the stress calculated for bends of 90°-type (eq.(15)). For the self
stresses of 90°-type bends calculated by eq.(4) (L = R, ϱ = b) slightly higher values
are obtained (5% for large radii of curvature (500nm) up to 10% for small radii
(25nm).
    Additionally the results using the rough estimate of eq.(3) (line 1) are shown
in Fig.4.

Results of the measurements and discussion
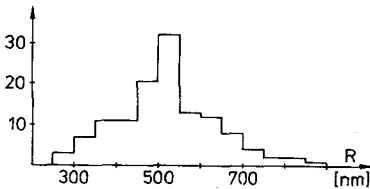1. Perfect dislocation under a stress of 30 MPa (Fig.3)

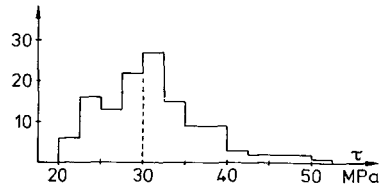Fig.5a Histogram of measured R of bends
of 30°-type in samples of type A.
    (From A. Tönnessen, H. Gottschalk,and H. Alexander, to be published)

Fig.5b Histogram of calculated stresses
from Fig.5a using eq.(2a;4;6) ϱ = b

Fig. 5b shows an accumulation at 30 MPa,the deforming stress. Because of the
interaction of dislocations in the deformed specimen it is reasonable that stresses
below and above 30 MPa are found. In this stress region the use of eq.(4) or eq.(11)
does not change the results (Fig.4, lines 3 and 4) if ϱ = b is chosen. If $\varrho \doteq$ b/8 is
used in eq.(11) (Fig.4, line 2) for all measured radii (R < 800nm) the calculated
stresses lie above the applied stress τ = 30 MPa which is not reasonable. When using
the simple line tension approximation according to eq.(3) the overestimation of the
stresses becomes even higher.
    Therefore the cut-off parameter ϱ = b which leads to a satisfying agreement
between the measurements and the calculations for low stresses shall be used for the
high stress experiments,too.
    For the bends A and B of different types in Fig. 3 the radii of curvature are: A
(30°-type bend), R = (540$\pm$ 30) nm; B (90°-type bend) R = (250 $\pm$ 20)nm. Both
curvatures lead to the same stress τ = (32$\pm$ 2) MPa which is in good agreement with
the applied stress.
2. High stress (τ = 350 MPa) acting on isolated partials (Fig.6)
In high stress deformed ⟨2,1,11⟩-oriented   specimens   dislocations   with   very   wide
separations (d > 1 μm) are found (Fig.6). In such a case the partials can be treated
as isolated and from the radii of curvature of their bends the local total force on
the dislocation can be calculated which is the sum of the driving force on the
dislocation and the stacking fault energy (γ(Si)= 58 mJ/m^2 /7/). The driving forces
in general are different for the leading and the trailing partial. In the given
crystallographic orientation of the stress axis one obtains for the driving force
on the leading partial F_{DL} and the driving force on the trailing partial F_{DT} :
$$F_{DL} = (7/12)b\tau \qquad\qquad F_{DT} = (5/12)b\tau$$

The total force on the leading partial F_L and on the trailing partial F_T is:

$$F_L = F_{DL} - \gamma = 2.0 \cdot 10^{-2} \text{ N/m} \qquad F_T = F_{DT} + \gamma = 11.4 \cdot 10^{-2} \text{ N/m} \qquad (\tau = 350 \text{ MPa})$$

These forces should be equal to the self forces of the bends what in fact is found from the experiment for the leading partials. For the average values of S/R of both types of bends (0°-type and 60°-type) using eq.(2), and (9) and (13) respectively ($\varrho = b_p$) one obtains: (n is the number of bends measured)

0°-type: n = 20 $S/R = (1.9 \pm 0.5) \cdot 10^{-2}$ N/m
60°-type: n = 15 $S/R = (2.2 \pm 0.5) \cdot 10^{-2}$ N/m

The bends of trailing partials in the isolated form are less frequent. Therefore only a few measurements could have been performed until now.

0°-type: n=5 $S/R = (8/8/5.3/4.4/4.4) \cdot 10^{-2}$ N/m
60°-type: n=4 $S/R = (6.3/6.1/5.2/4.6) \cdot 10^{-2}$ N/m

For both types the measured radii are found too large and the self forces too small. Though the number of measurements must be increased it may be concluded that there is no equilibrium between driving force and back force in case of the trailing partials. As the driving force is higher than the back force one may assume obstacles beeing present at the trailing partial /8/.
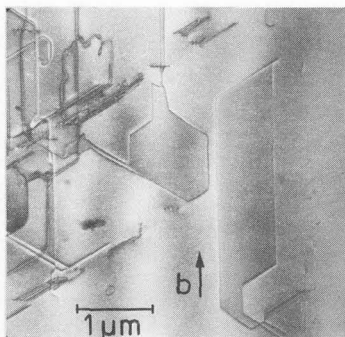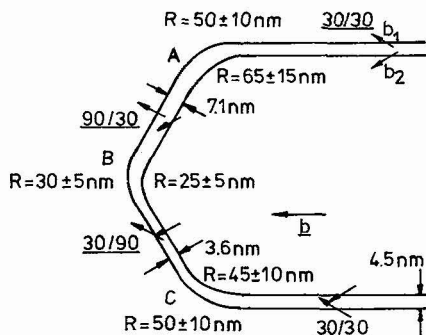

Fig.6 - Isolated partials (350 MPa), stress axis ⟨2,1,11⟩

Fig.7 - "Average" dislocation loop (250 MPa), stress axis ⟨213⟩

3. High stress ($\tau = 250$ MPa) acting on complex bend configurations (Fig.1)

For the partial dislocations in specimens of type B beeing deformed by compression along ⟨213⟩ the driving forces are

$$F_{DL} = (5/12)b\tau = 4 \cdot 10^{-2} \text{ N/m} \qquad F_{DT} = (7/12)b\tau = 5.6 \cdot 10^{-2} \text{ N/m}$$

By taking the averages of the bend curvatures and of the separations measured for a large number of dislocation loops an average dislocation loop is constructed which is shown in Fig.7. According to the different positions of the partials three different bend-types occur, called A, B, C.
Taking the mean values of the outer and inner bend for the three types though they are found to be different and considering the loop dislocation as a perfect one the following stresses are calculated:

A	166 MPa (eq.(2a),(4))	190 MPa (eq.(1a),(11))
B	145 MPa (eq.(2a),(4))	163 MPa (eq.(2a),(15))
C	189 MPa (eq.(2a),(4))	220 MPa (eq.(1a),(11))

With this simple method a fairly good agreement with the deformation stress is only achieved for the bend type C using the improved line tension calculation (eq.(11),(15)). It fails for bend types A and B.

For a detailed calculation of the line tension the complicated actual situation of the partials in the bend has to be taken into account. The geometrical approximation according to Fig.2 is shown in Fig.8. A further approximation is made by taking the self force (eq.(2),(9) or(13)) of the isolated partial contributing to the force on the segment L and L' respectively. Then the forces of the three partial segments lying opposite to the segment L or L' in consideration must be added. For the calculation of the interaction forces of these segmented partial dislocations a
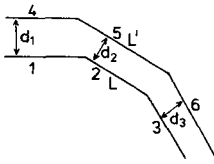
Fig.8 - Dissociated dislocation bend

method given by Hirth and Lothe /9/ is applied. The resulting forces on the segments L and L' are slightly locally variing but only the value at the apex of each bend is considered here. Table 2 contains the results of the computations for the three leading and the three trailing bends. The interaction force F_{ij} means the force exerted by dislocation i on dislocation j. The dislocations are numbered according to Fig.8. The forces pointing in the direction of the driving forces are counted positive.

Table 2 - Forces on the dislocations in a dissociated dislocation bend (10^{-2} N/m)

Bend type	A(lead.)	A(trail.)	B(lead.)	B(trail.)	C(lead.)	C(trail.)
S/R	-2.10	-2.92	-3.07	-3.51	-3.58	-2.28
F_{25} or F_{52}	+2.61	-2.31	+4.63	-5.60	+6.65	-6.55
F_{15} or F_{42}	+0.01	-0.45	+0.53	-0.66	+0.18	-0.30
F_{35} or F_{62}	-0.17	-0.09	+0.71	+0.10	-0.62	-0.28
τ	-5.80	+5.80	-5.80	+5.80	-5.80	+5.80
F_D	+4.00	+5.60	+4.00	+5.60	+4.00	+5.60
Sum	-1.45	+5.98	+1.00	+4.53	+0.74	+1.99

The sum in the last line of Table 2 should yield zero. While the results for the leading partials in bend B and C are fairly satisfying, if the error is considered which arises when adding up so many contributions, the results for the trailing partials in particular do not fit to the assumption of an equilibrium between the driving force and the back force in the bend.

Conclusion - It is shown that the calculation of the line tension and the stresses in a bend is very sensitive to the choice of the cut-off parameter ρ . Setting it equal to the Burgers vector excellent agreement of the stress derived from the bend curvatures with the applied stress is achieved. Using an improved calculation of the line tension taking the actual dislocation arrangement into account the applied stress can be derived from the bend curvatures for isolated leading partials, too. That fails, however, completely for the trailing partials.

These results mean that for the dislocation under low stress conditions and for the isolated leading partials under high stress conditions a steady state motion of the bends can be assumed for which a perturbation of the equilibrium state can relax in a short relaxation time. This seems not to be valid for the trailing partials for which interaction with unidentified obstacles may occur. These assumptions are confirmed by the results for dissociated dislocation bends. As in these cases the measured radii of curvature for the leading and the trailing partial are fairly similar a breakdown of the computations because of quite different radii of curvature is impossible.

The special role the trailing partials apparently play should be further investigated by additional measurements of isolated dislocation bends and by an improvement of the calculation of the complicated configuration of dissociated bends. The application of the linear anisotropic elasticity theory to curved dislocations, however, as outlined e.g. by Scattergood /10/, should only result in slight modifications since the anisotropy factor of Si is only A = 1.56.

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