

The interaction of Lomer-Cottrell locks with screw dislocations

Journal:	<i>Philosophical Magazine & Philosophical Magazine Letters</i>
Manuscript ID:	TPHM-09-Jul-0300.R1
Journal Selection:	Philosophical Magazine
Date Submitted by the Author:	17-Jul-2009
Complete List of Authors:	Schoeck, Gunther; University of Vienna, Department of Physics
Keywords:	dislocation interactions, dislocation structures
Keywords (user supplied):	Lomer-Cottrell dislocation, Peierls model



The interaction of Lomer-Cottrell locks with screw dislocations

by

Gunther Schoeck

Faculty of Physics, University of Vienna, 1090 Vienna

E-mail: gunther.schoeck@univie.ac.at

Abstract

In fcc crystals dislocations are dissociated into partial dislocations and therefore restricted to move on $\{111\}$ glide planes. By junction reactions with dislocations on two intersecting $\{111\}$ planes Lomer-Cottrell dislocations along $\langle 110 \rangle$ directions can be formed which are barriers for approaching screw dislocations. Treating conventionally the interaction between a dissociated screw dislocation and a LC lock using classical continuum theory assuming the partials to be *Volterra dislocations* leads to erroneous conclusions. A realistic result can only be obtained in the framework of the Peierls model treating the partials as *Peierls dislocations* and taking explicitly account of the change in atomic misfit energy in the glide plane. At already moderate stresses (at less than $3 \cdot 10^{-3} \mu$ in Cu), the screw will combine with the LC lock to form a Hirth lock. As result the nature of the repulsive force will change drastically.

Keywords dislocation interaction, dislocation structure, Lomer-Cottrell dislocations, Peierls model.

1 Introduction

In the plastic deformation of fcc metals cross-slip plays an important role since it can lead to dynamic recovery. Because in these metals the dislocations are dissociated into partial dislocations connected by stacking-faults, they are restricted to move on $\{111\}$ glide planes. Cross-slip requires therefore some rearrangement of the dislocation core structure, in order that the screw dislocation in the primary plane can cross over into the cross slip plane. This can be accomplished with the aid of thermal activation. A review of the various theoretical models and attempts to derive expression for the cross-slip energy have been given by Püschl [1]. It has however been recently pointed out [2], that at present there are no theoretical methods available to calculate the cross slip energy reliably. When the two partials of the dissociated dislocation approach each other, the effective Burgers vector of the partials and the effective

1
2
3
4 stacking-fault energy change, effects which cannot be handled by conventional dislocation
5 theory in linear elastic continua. The different approaches in the literature may give the correct
6 order of magnitude of the activation energy, but they vary by a factor of two to three. For
7 thermally activated processes that means the difference between go and no-go.
8
9

10
11 A problem which can however be treated satisfactorily is the question whether an applied
12 stress is able to facilitate cross-slip by modifying the equilibrium configuration of the
13 dislocations. This will occur when under the action of an applied stress a screw dislocation is
14 pressed against an obstacle and the separation of the partials decreases. The possible reduction
15 of the activation energy for cross-slip resulting from such pile-ups has been invoked by
16 various authors [3-7].
17
18

19
20 Among the different obstacles for screw dislocations the Lomer-Cottrell dislocation [8]
21 (LC lock) has been considered to be of prime importance due its apparent great stability. LC
22 locks are formed when two attractive dislocations moving on intersecting {111} planes
23 combine. They lie along [110] directions are of pure edge character, with global Burgers
24 vector $a/2[1\bar{1}0]$ and possible glide plane {001}. Since they can dissociate somewhat into the
25 two intersecting {111} planes they are sessile and form barriers to hold up incoming screw
26 dislocations in {111} planes.
27
28

29
30 In the following we are therefore studying the stopping power of Lomer-Cottrell
31 dislocations for screw dislocations. We will not discuss the resistance of relatively short LC-
32 junctions against unzipping, generally found in dislocation dynamics simulations.[9-11] and
33 investigated with atomic models [12,13]. We rather consider the resistance which a long LC
34 lock exerts against an approaching screw dislocation. The possibility that the LC lock itself
35 can collapse under the action of a pile-up of screw dislocations has been proposed repeatedly
36 and investigated in detail by Stroh [14]. It has however been argued [4] that the escape of the
37 leading screw dislocation by cross-slip has a lower energy barrier. Since all these calculation
38 are based on classical dislocation theory dealing with dislocations at close distance, they are
39 not very trustworthy [2].
40
41

42
43 We first try to solve the problem of interaction in the classical way of conventional
44 continuum theory of dislocations by treating the partials as Volterra dislocations with constant
45 Burgers vector and assuming a constant stacking-fault energy as analyzed by Wolf [3]. It turns
46 out that the configuration would be stable up to a stress of the order of the theoretical shear
47 limit, and the separation between the partials could be reduced to a distance of less than a
48 Burgers vector. This result does however not agree with reality. A correct treatment requires
49
50
51
52
53
54
55
56
57
58
59
60

the use of the generalized Peierls model [15] treating the partial as Peierls dislocations including a detailed account of the changing atomic misfit energy in the glide plane. At the time of the previous treatment [3] these methods were not yet available. It turns out that at relatively moderate stresses the screw dislocation will combine with the LC lock to form a Hirth lock [8].

2. The interaction in classical continuum theory.

We consider here with conventional methods the interaction of a LC lock with an approaching dissociated screw dislocation in a linear elastic isotropic continuum. The screw dislocation may be pressed against the LC lock by a resolved shear stress τ_s acting in the direction of the screw components of the partials. For our consideration the origin of τ_s is inessential, it might result from the applied stress τ_a alone or be the stress $n\tau_a$ experienced by a dislocation at the head of a pile-up of n dislocations. We assume a LC lock at the origin along a $\langle 110 \rangle$ direction being of pure edge type. Since the approach distances of the screw dislocation is large compared to the possible dissociation width of the of the LC lock, its stress field corresponds to the one of its global Burgers vector $a/2 \langle 1\bar{1}0 \rangle$. The $\{111\}$ glide plane of the approaching screw dislocation is inclined by an angle $\alpha = 54.7^\circ$ to the possible glide plane $\{001\}$ of the LC dislocation. We treat the partial dislocations of the approaching screw dislocation conventionally as Volterra dislocations with screw components $b/2$ and edge components $h = \pm b\sqrt{3}/6$. The leading partial is assumed to be repulsive and positioned at the distance x from the origin. The partial separation is determined by the stacking fault energy γ and in equilibrium the separation is $d_0 = E_{int}/\gamma$, where E_{int} is the elastic interaction energy between the two partials. Under the action of the applied stress the trailing partial is situated at $x + d$ with separation $d \leq d_0$. With these assumptions it is possible to determine the forces experienced by the two partials. With shear modulus μ and Poisson ratio ν we have for the leading partial, with forces counted positive in the $+x$ direction

$$F_1 = \frac{\mu}{2\pi(1-\nu)} \frac{hb \cos \alpha}{x} + \gamma + \frac{\mu}{2\pi(1-\nu)} \frac{h^2}{d} - \frac{\mu}{2\pi} \frac{(b/2)^2}{d} - \tau_s b/2 \quad (1)$$

The meaning of the different terms is self-evident. They result from the interaction of the partials with the LC lock (term 1), their mutual interactions (terms 3 and 4) and the surface tension of the stacking-fault (term 2). The force on the trailing dislocation at $x + d$ is given by

$$F_2 = -\frac{\mu}{2\pi(1-\nu)} \frac{hb \cos \alpha}{x+d} - \gamma - \frac{\mu}{2\pi(1-\nu)} \frac{h^2}{d} + \frac{\mu}{2\pi} \frac{(b/2)^2}{d} - \tau_s b/2 \quad (2)$$

1
2
3
4 The total repulsive force $F = F_1 + F_2$ on the dislocation results from the gradient in the stress
5 field of the LC lock acting on the edge components balancing the pressure of the stress τ_s
6 acting on the screw components.
7

8
9 The equilibrium configuration as function of τ_s can be obtained by solving the
10 system of simultaneous equations $\{F_1=0, F_2=0\}$ for d and x . The system has an analytical
11 solution comprising more than 20 rather clumsy terms including lengthy square roots. It can be
12 supplied upon request. Of interest is here especially the change in splitting widths d with
13 increasing stress τ_s . For a crystal with the elastic properties of Cu this is shown in Fig. 1 and
14 agrees essentially with the results of Wolf [3] who studied the behaviour of piled-up group of
15 screw dislocations in front of a LC lock. The partial separation d decreases rapidly with
16 increasing τ_s and for as stress of $\tau_s \approx 10^{-2} \mu$ it has been reduced from the original value $d_0 =$
17 $3.84 b$ to a value of $d \approx b$. The approach distance x as function of the applied stress is shown in
18 Fig. 2 This deduction seems to be straightforward and the conclusion reasonable but as we will
19 show the result does not agree with physical reality.
20
21
22
23
24
25
26
27
28
29

30 3. The interaction in the Peierls model.

31
32 The treatment of the partials as Volterra dislocations implies a rigid coupling between the
33 screw components $b/2$ and the edge components $\pm h$ of the partials and actually masks the
34 physical situation when the partials come close to each other. In isotropic media there exists
35 no elastic interaction between these components. Only in anisotropic media there may be a
36 small cross term which vanishes however for screw dislocations in fcc crystals. Therefore a
37 coupling between the screw and the edge component exists exclusively via the atomic misfit in
38 the glide plane which in order to minimize the misfit energy enforces a local coordination
39 between the two components. With decreasing partial separation the amplitude of the effective
40 edge components decreases however and vanishes for $d \rightarrow 0$. Hence one could expect a
41 situation where, when the partials are sufficiently compressed, the LC lock is unable to stop
42 the approaching screw dislocation.
43
44
45
46
47
48
49
50
51

52 Problems involving explicitly the atomic misfit energy in the dislocation core can be
53 treated within the framework of the Peierls model [15]. In the model the misfit energy density
54 in the glide plane is represented by the γ -surface which can be determined by ab-initio
55 calculations with density functional theory. For details of the analytical treatments we refer to
56 ref. [15]. Since the displacement discontinuity in the glide plane is represented by a density of
57 infinitesimal dislocations, the equilibrium configuration cannot be obtained on the stress level
58
59
60

but must be obtained by minimizing the total energy. We choose the coordinate system with z-axis along $\langle 110 \rangle$ (screw direction) and y-direction along $\langle 1\bar{1}2 \rangle$ (edge direction). The x-axis is perpendicular to the dislocation line and coincides in this case with the y-axis of the lattice. For the displacement caused by a screw dislocation at the position $x = x_0$ we use Peierls dislocations as trial functions for the components of the partials

$$Z(x) = \frac{b}{2\pi} \left(\arctan \frac{x - x_0 + d/2}{w} + \arctan \frac{x - x_0 - d/2}{w} \right) + b/2 \quad (3a)$$

$$Y(x) = \frac{h}{\pi} \left(\arctan \frac{x - x_0 + k/2}{v} - \arctan \frac{x - x_0 - k/2}{v} \right) \quad (3b)$$

The screw and edge components do not interact elastically and their separation d and k and the corresponding core widths w and v can be different. The elastic self energy is given by

$$E_{el} = H_{33} b^2 \ln \left(\frac{R}{2w} \right) - H_{33} (b/2)^2 \ln \left(1 + \frac{d^2}{(2w)^2} \right) + H_{11} h^2 \ln \left(1 + \frac{k^2}{(2v)^2} \right) \quad (4)$$

with outer cut-off radius R and anisotropic prelogarithmic energy factors for screw and edge H_{33} and H_{11} .

The atomic misfit energy in the glide plane can be described by the γ -surface $\gamma(y,z)$ which can be expressed analytically by a 2D Fourier series reflecting the threefold rotational symmetry of the $\{111\}$ plane. The Fourier series and the corresponding γ -values for Cu have been derived recently in ref. [2]. The characteristic features can be described by a five-term series fitting three specific γ -values and the shear modulus. The resulting atomic misfit energy in the glide plane of the dissociated dislocation is

$$E_A = \int_0^R \gamma(Y(x), Z(x)) dx \quad (5)$$

In order to calculate the stress field we can neglect the splitting of the LC lock and assume a single edge dislocations of Peierls type with core width v_0 situated at the origin. Its possible glide plane $\{001\}$ is inclined by $\alpha = 54.7^\circ$ to the $\{111\}$ glide plane of the approaching screw. The resolved shear stress acting on the edge components of the approaching partials is

$$\tau_{LC} = 2H_{11} b \cos \alpha \frac{x}{v_0^2 + x^2} \quad (6)$$

with $v_0 \approx 0.6b$. At the closest approach of the screw dislocation $x_0 \approx 4b$ the stress τ_{LC} agrees practically with the one of a Volterra dislocation at the origin with a $1/r$ dependence but avoids the physically unrealistic divergence at $x = 0$.

The interaction energy of the approaching screw with the LC lock is given by

$$E_{LC} = \int_0^R \sigma_{LC}(x) Y(x) dx \quad (7)$$

With the stress τ_S acting on the screw dislocation the enthalpy H of the configuration (considering that the stress acts in the $-x$ direction) is given by

$$H(d,k,w,v,x_0,\tau_S) = E_{el} + E_A + E_{LC} + \tau_S b x_0 \quad (8)$$

The equilibrium configuration can be obtained when for each value of τ_S the enthalpy is minimized with respect to the five geometrical parameters. The geometrical parameters without applied stress in equilibrium are: $d = 3.89 b$, $k = 3.98 b$, $w = 0.48 b$, $v = 0.57 b$

Of special interest is the change in splitting distances d and k as shown in Fig. 1 and the approach distance x_0 shown in Fig. 2. With increasing stress the separation k of the edge components begins to become smaller than the separation d of the screw components. At a stress $\tau_S \approx 2.9 \cdot 10^{-3} \mu$ a critical situation is reached and the configuration becomes mechanically unstable. The equilibrium separations of the edge components has been reduced to a value $k \approx 1.04 b$ and as result the maximum height of the edge component is reduced to $h_m = 0.14 b$. As consequence the repulsive gradient force of the LC lock is no longer sufficient to hold up the approaching screw. It will recombine with the LC lock and as result a Hirth lock [8] is formed. This will drastically change the nature of the interaction with screw dislocations which follow in the same glide plane.

4. Discussion

We have studied the interaction of a screw dislocation with a LC lock which is considered to be the prime obstacle for pile-ups of such dislocations. The LC lock has a unique property among all locks formed by junction reactions as being of pure edge type. It is oriented along a [110] direction and hence can block either 60° dislocations or screw dislocations. A 60° dislocation which is pressed against the LC lock has an edge component of $b\sqrt{3}/2$ and hence there exists a strong elastic interaction with the LC lock thus preventing a close approach. For a screw dislocation however there exists no elastic interaction with the LC lock. A repulsion results only when the dislocation is dissociated and then only by the interaction with the relatively small edge components $\pm h$ of the partials. Since they form a dipole the repulsive force results only from a *gradient* in the lock stress and hence the screw dislocation can approach to a close distance. The partial separation d however is controlled by the *magnitude*

1
2
3
4 of the lock stress and hence can be reduced considerably. This in turn leads to a decrease in the
5
6 amplitude of the edge components and hence to a weakening of the interaction. As result there
7
8 exists a critical stress where a mechanical breakdown occurs and the screw dislocations will
9
10 combine with the LC lock to form a Hirth lock. For Cu this occurs at a stress $\tau_s = 2.9 \cdot 10^{-3} \mu$. As
11
12 shown above this process can only be studied within the framework of the Peierls model since
13
14 the coupling between the components of the partials occurs by the atomic misfit energy. A
15
16 treatment in conventional continuum theory would lead to erroneous conclusions.

17
18 This opens the question whether under realistic conditions a pile-up of screw dislocations
19
20 under the action of a resolved shear stress τ_s is able to facilitate cross-slip by creating a
21
22 favourable starting position as often invoked in the literature [3-7]. Let us consider for an
23
24 order-of-magnitude estimate the stress τ_{III} at which the transition from stage II to stage III of
25
26 work hardening occurs, which is believed to result from massive onset of cross-slip. For Cu a
27
28 value of $\tau_{III} \approx 3 \cdot 10^{-3} \mu$ at 78 K has been reported [16]. With a critical stress $\tau_s \approx 2.9 \cdot 10^{-3} \mu$ a
29
30 'pile-up' of more than two dislocations would already convert the LC lock to a Hirth lock.
31
32 This changes the nature of the repulsion for the following dislocations drastically. Since in
33
34 contrast to the LC lock the barrier now contains screw components, the repulsive force on
35
36 approaching screw dislocation depends now on the *magnitude* of the lock stress which will
37
38 stop the approaching dislocation at a much larger distance. The decrease in partial separation
39
40 depends however now on the *gradient* of the lock stress, which will be small. As we see for
41
42 barriers containing screw components the influence of the *magnitude* and the *gradient* of the
43
44 lock stress is now just reversed when compared with the LC lock. This difference shows up
45
46 clearly in Fig. 1 where we have plotted the change in splitting width when the screw
47
48 dislocation approaches a LC lock and a Hirth lock. For a Hirth lock shear stress $\tau_s = 10^{-2} \mu$
49
50 (which is close to the theoretical strength) would now only lead to a decrease in the separation
51
52 width from $d_0 = 3.97 b$ to $d = 3.53 b$. Though pile-ups of screw dislocations still may exist
53
54 their ability to facilitate cross-slip is therefore only marginal. The TEM observations of
55
56 Mughrabi [17] in stage II (with the dislocations pinned under load by neutron irradiation)
57
58 show that the barriers for the dislocation groups are more likely grids or walls of dislocation
59
60 and hence we expect always screw components to be present in the barriers.

The separation of the partials is much more affected by an 'Escaig stress' τ_E acting on the
edge component of the partials [5]. For instance an Escaig stress of $\tau_E = 10^{-2} \mu$ would lead to
a reduction of the splitting width to a value of $d = 2.53 b$ [2] considerably less than the value

obtained by an equal resolved shear stress τ_s as found above. However the influence on the cross-slip process requires careful consideration. The compression of the partials in the primary plane leads to a reduction of the enthalpy. Cross-slip can however only spread in the cross-slip plane when the enthalpy of the system is lowered by the transition into the cross-slip plane [2]. This requires that in the cross-slip plane an even larger Escaig stress τ_E^C must be present. Contrary to a widely held belief it can therefore only take place, when the dislocation in the cross-slip plane is either more compressed or correspondingly 'more extended', with the condition $|\tau_E^C| \geq |\tau_E|$. This must be considered when trying to correlate the occurrence of cross-slip with the axis-orientation of the applied stress.

References

- [1]. W. Püschl, Prog. Mater. Sci. **47**, 415. (2002)
- [2] G. Schoeck, Phil. Mag. Lett. In print (2009)
- [3] H. Wolf, Z. Naturforsch. **15a** , 180 (1960)
- [4] A. Seeger, in : Dislocations and Mechanical Properties of Crystals (J. C. Fisher, W. G. Johnston, R Thomson, T Vreeland Jr, ed) Wiley 1957 p. 243
- [5] B. Escaig, in: Dislocation Dynamics, (Rosenfield, A. et al. ed. Mc Graw Hill, New York) 1968, p.655.
- [6] J. Bonneville and B. Escaig Acta Metall. **27**, 1477 (1979)
- [7] G. Saada, Mater. Sci. Engng. **137**, 177 (1991)
- [8] J. P. Hirth and J. Lothe, Theory of Dislocations, Wiley, New York (1982)
- [9]] B. Devincere, L.P. Kubin, C. and T. Hoc., Scripta Mater. **54**, 741 (2006)
- [10] Martinez, E., Marian, J., Arsenlis, J. A., Victoria, M., Perlado, J. M., Journ. Mech. Phys. Solids, **56**, 969 (2008)
- [11] B. Devincere, L.P. Kubin, C. and T. Hoc., Science **320**, 1745 (2008)
- [12] D. Rodney and R. Phillips. Phys. Rev. Lett. **82**, 1704 (1999)
- [13] V. B. Shenoy, R. V. Kutka and R. Phillips Phys. Rev. Lett. **84**, 1491 (2000)
- [14] A. N. Stroh, Phil. Mag, **1**, 489 (1956)
- [15] G. Schoeck, Mater. Sci. Eng. A **400-401**, 7 (2005)
- [16] R. Berner, Z. Naturforsch. **15a**, 689 (1960)
- [17] H. Mughrabi, Phil. Mag. **23**, 897 (1971)

1
2
3
4
5
6
7
8 Figure captions:
9

10
11 Fig. 1 The separation of the partials of a screw dislocation in front of a LC lock (LC) or of
12 a Hirth lock (HL) based on conventional continuum theory of dislocations as function of the
13 stress τ_s acting on the screw components the partial dislocations. The results of the Peierls
14 model (points with linear interpolation) represent the separation of the screw components (d)
15 and the edge components (k)
16
17
18
19
20
21

22 Fig. 2 The approach distance x of a screw dislocation forced by a stress τ_s acting at the screw
23 components of the partial dislocations in front of a LC lock. Continuous curves based on
24 conventional continuum theory of dislocations The results of the Peierls model are points with
25 linear interpolation.
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

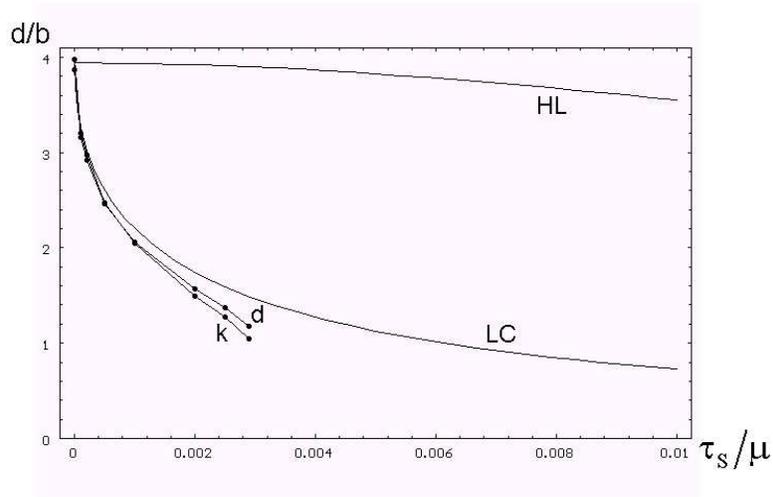


Fig. 1

Fig. 1 The separation of the partials of a screw dislocation in front of a LC lock (LC) or of a Hirth lock (HL) based on conventional continuum theory of dislocations as function of the stress τ_S acting on the screw components the partial dislocations. The results of the Peierls model (points with linear interpolation) represent the separation of the screw components (d) and the edge components (k)

254x190mm (96 x 96 DPI)

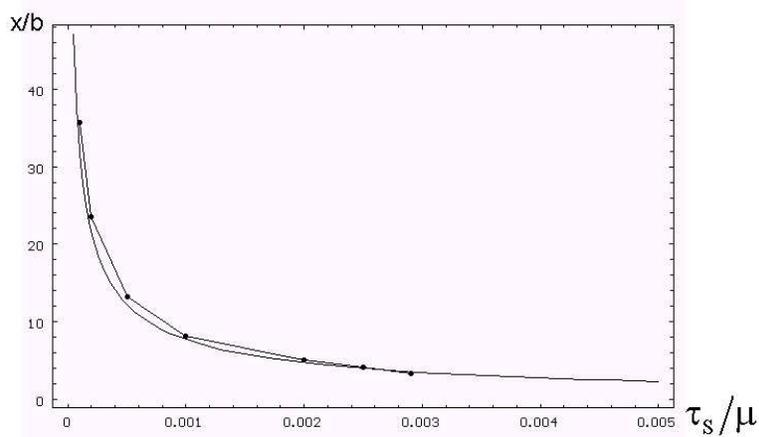


Fig.2

Fig. 2 The approach distance x of a screw dislocation forced by a stress τ_s acting at the screw components of the partial dislocations in front of a LC lock. Continuous curves based on conventional continuum theory of dislocations. The results of the Peierls model are points with linear interpolation.
254x190mm (96 x 96 DPI)