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# 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](mailto: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

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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.  
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10 A problem which can however be treated satisfactorily is the question whether an applied  
11 stress is able to facilitate cross-slip by modifying the equilibrium configuration of the  
12 dislocations. This will occur when under the action of an applied stress a screw dislocation is  
13 pressed against an obstacle and the separation of the partials decreases. The possible reduction  
14 of the activation energy for cross-slip resulting from such pile-ups has been invoked by  
15 various authors [3-7].  
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18 Among the different obstacles for screw dislocations the Lomer-Cottrell dislocation [8]  
19 (LC lock) has been considered to be of prime importance due its apparent great stability. LC  
20 locks are formed when two attractive dislocations moving on intersecting  $\{111\}$  planes  
21 combine. They lie along  $[110]$  directions are of pure edge character, with global Burgers  
22 vector  $a/2[1\bar{1}0]$  and possible glide plane  $\{001\}$ . Since they can dissociate somewhat into the  
23 two intersecting  $\{111\}$  planes they are sessile and form barriers to hold up incoming screw  
24 dislocations in  $\{111\}$  planes.  
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27 In the following we are therefore studying the stopping power of Lomer-Cottrell  
28 dislocations for screw dislocations. We will not discuss the resistance of relatively short LC-  
29 junctions against unzipping, generally found in dislocation dynamics simulations.[9-11] and  
30 investigated with atomic models [12,13]. We rather consider the resistance which a long LC  
31 lock exerts against an approaching screw dislocation. The possibility that the LC lock itself  
32 can collapse under the action of a pile-up of screw dislocations has been proposed repeatedly  
33 and investigated in detail by Stroh [14]. It has however been argued [4] that the escape of the  
34 leading screw dislocation by cross-slip has a lower energy barrier. Since all these calculation  
35 are based on classical dislocation theory dealing with dislocations at close distance, they are  
36 not very trustworthy [2].  
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39 We first try to solve the problem of interaction in the classical way of conventional  
40 continuum theory of dislocations by treating the partials as Volterra dislocations with constant  
41 Burgers vector and assuming a constant stacking-fault energy as analyzed by Wolf [3]. It turns  
42 out that the configuration would be stable up to a stress of the order of the theoretical shear  
43 limit, and the separation between the partials could be reduced to a distance of less than a  
44 Burgers vector. This result does however not agree with reality. A correct treatment requires  
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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  $\tau_s$  acting in the direction of the screw components of the partials. For our consideration the origin of  $\tau_s$  is inessential, it might result from the applied stress  $\tau_a$  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  $\gamma$  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  $\mu$  and Poisson ratio  $\nu$  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

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

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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  $\tau_s$   
6 acting on the screw components.  
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9 The equilibrium configuration as function of  $\tau_s$  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  $\tau_s$ . 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  $\tau_s$  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.  
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### 30 3. The interaction in the Peierls model.

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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.  
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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  $\gamma$ -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  
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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  $\gamma$ -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  $\gamma$ -values for Cu have been derived recently in ref. [2]. The characteristic features can be described by a five-term series fitting three specific  $\gamma$ -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  $\tau_{LC}$  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  $\tau_S$  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  $\tau_S$  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  $60^\circ$  dislocations or screw dislocations. A  $60^\circ$  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*



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4 of the lock stress and hence can be reduced considerably. This in turn leads to a decrease in the  
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6 amplitude of the edge components and hence to a weakening of the interaction. As result there  
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8 exists a critical stress where a mechanical breakdown occurs and the screw dislocations will  
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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  
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14 the coupling between the components of the partials occurs by the atomic misfit energy. A  
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16 treatment in conventional continuum theory would lead to erroneous conclusions.

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

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4 obtained by an equal resolved shear stress  $\tau_s$  as found above. However the influence on the  
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6 cross-slip process requires careful consideration. The compression of the partials in the  
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8 primary plane leads to a reduction of the enthalpy. Cross-slip can however only spread in the  
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10 cross-slip plane when the enthalpy of the system is lowered by the transition into the cross-slip  
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12 plane [2]. This requires that in the cross-slip plane an even larger Escaig stress  $\tau_E^C$  must be  
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14 present. Contrary to a widely held belief it can therefore only take place, when the dislocation  
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16 in the cross-slip plane is either more compressed or correspondingly 'more extended', with the  
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18 condition  $|\tau_E^C| \geq |\tau_E|$ . This must be considered when trying to correlate the occurrence of cross-  
19  
20 slip with the axis-orientation of the applied stress.  
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8 Figure captions:  
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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  $\tau_s$  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 )  
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22 Fig. 2 The approach distance  $x$  of a screw dislocation forced by a stress  $\tau_s$  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.  
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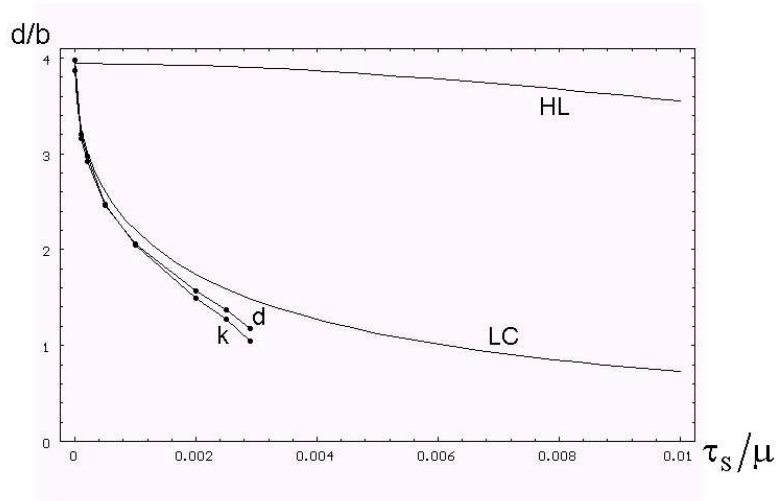


Fig. 1

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  $\tau_S$  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 (  $k$  )

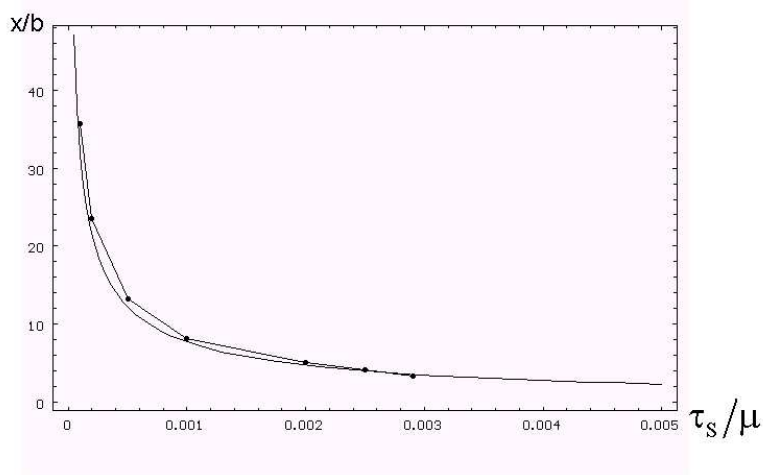


Fig.2

Fig. 2 The approach distance  $x$  of a screw dislocation forced by a stress  $\tau_s$  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)