DISLOCATION SPLITTING AND THE PLASTIC GLIDE PROCESS IN CRYSTALS

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Résumé. — L'auteur étudie l'interaction dislocation-réseau cristallin qui provient, en particulier, de la dissociation du cœur. Il faut ici distinguer deux cas, selon que le cœur est dissocié en dehors du plan de glissement, ou non.

Dans le premier cas, on trouve de nombreux exemples différents, mais intimement liés entre eux, tels que les métaux c. c., le glissement prismatique/hexagonal des métaux h. c., les barrières de Cottrell dans la structure c. f. c. et également d'autres cristaux comme le tellure ou le problème de la fragilité du soufre α . Pour calculer les mobilités de dislocation correspondantes, deux situations sont à distinguer selon que le glissement demande d'abord d'avoir une plus forte énergie de cœur ou au contraire, un cœur plus dissocié, c'est-à-dire de plus faible énergie.

Le cas d'un cœur dissocié dans le plan de glissement peut également être important dans les cas de *cisaillement synchronisé* (synchro-shear). En général, ce mécanisme introduit seulement un processus purement conservateur, du type de celui du glissement d'un ruban de faute extrinsèque (faute $2V$) dans la structure c. f. c. L'activation thermique ne devrait être nécessaire que pour nucléer la configuration du cœur des limites de fautes $2V$ de vecteur $2C\delta$ qui est nécessaire pour éviter un mauvais voisinage atomique dans certains composés. L'énergie d'activation est évaluée dans ce cas, semblable au *glissement visqueux*, et dépend de la contrainte. Ces considérations peuvent aussi s'appliquer à certains composés non stœchiométriques.

Abstract. — This paper is aimed at a review of the lattice-dislocation interaction, and more specially to the kind of interaction which stems from the splitting of the dislocation core. Two quite different situations are discussed whether the core is dissociated off the glide plane, or not.

In the first case, a number of various cases is reviewed, which all are intimately connected : crystallographic slip in b. c. c. metals, prismatic/pyramidal slip in h. c. p. metals, Lomer-Cottrell barriers in the f. c. c. structure and also some non metallic bonded crystals : tellurium and the brittleness of α -sulphur crystals. Finally, the general models proposed for modelling dislocation mobilities fall in two classes : whether a higher energy core configuration must be reached in order for the dislocation to start slipping, or, in contrary, the core splits wider in this plane thus decreasing its energy.

The case of a core dissociated in the glide plane is also considered in compounds where a « *synchro-shear mechanism* » has been assumed. In general, only a simple glide process is involved, quite similar to the slipping of an extrinsic ($2V$) stacking fault ribbon in the f. c. c. structure. Thermal help should be only needed for nucleating the suitable core of $2C\delta$ - $2V$ -fault boundaries which avoids making wrong nearest neighbour bonds in certain structures. The activation energy for such *viscous slip* is evaluated, and is found to be stress-dependent. A similar treatment could apply for some non-stoichiometric compounds also.

1. Introduction. — Only in the late five or six years it has become apparent that among the large variety of *pure* crystals investigated, their plastic slip depends primarily on the intrinsic lattice-dislocation interaction, as a general rule in Nature. The case of compact metals (face centered cubic or hexagonal compact) is in contrary rather a special case, with a weak lattice resistance and a yield strength controlled merely by propagation of slip through forest dislocations, the metallurgical importance of which has misguided a general appreciation of the slip process in Nature. In

contrast to these simple metals, numerous molecular, covalent (Si, Ge, ...) or ionic crystals (metallic oxides, although the role of impurities is not yet clear), even the b. c. c. transition metals exhibit a strong temperature dependence of elastic limit — increasing up to two orders of magnitude at helium temperature. Studying such strong thermal effects drew more and more attention to the dislocation core structure which is responsible for the intrinsic lattice resistance to plastic shear, at the origin of this behaviour.

The interaction between crystal lattice and dislocations is referred to as lattice friction, or also Peierls forces. This effect comes from core energy fluctuations

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when moving a dislocation. Core fluctuations are very much dependent on the type of atomic interactions existing in the solid, and fall mainly in two quite different classes. The older one is the well-known bond model [1] which applies typically for crystals with strongly directional atomic bonds, like covalent-bonded crystals; energy fluctuations arise there from the necessary breaking-reforming of directional bonds when core atoms glide past each other during the slip process. The words *Peierls forces* should be used specifically for terming this kind of lattice resistance.

In contrary, metallic bonds for example are not very directional and energy fluctuations there stem rather from a *splitting* of the dislocation core. It is often found to be so in other types of crystals, so that the slip behaviour of split core renews our understanding of the atomic slip process itself and is the key for explaining the relative strength of different slip planes in a given crystal (see for example section 2.1).

This paper is aimed at a review of this latter effect because of major advances in that field in recent years. In contrast, not much has been said about other splitting effects in spite of their importance, like the climb of extended dislocations for example, and it seems better to deal with these questions in a discussion session of this conference. In the following, two quite different situations are to be distinguished, whether the core is dissociated off the glide plane, or not.

Core dissociations off the glide plane are a frequent cause to make sessile those dislocations which lie along certain crystallographic directions in a number of cases: crystallographic slip in b. c. c. metals, prismatic or pyramidal slip in h. c. p. metals, Lomer-Cottrell barriers in the f. c. c. structure. Some of these configurations can be found also in some non-metallic bonded crystals, as in some weak Van der Waals-like solids (causing brittleness in orthorhombic sulphur) or in crystals with weakly overlapping electron orbitals like Tellurium.

A core dissociation confined in the glide plane may also sometimes control the glide mobility in more complex structures consisting of two or three different species of atoms. This is the so-called *synchro-shear mechanism*, first introduced by Kronberg for the plastic slip of alumina [2] then extended to spinels [3] and carbides [4, 5]. We would better call it *extrinsic glide* because of the close likeness with propagation of an extrinsic fault in the usual f. c. c. structure. On this basis we show that two types of synchro-shears should be distinguished depending on the net shift of the $2\sqrt{3}$ -fault which is involved in the process, either a simple Shockley vector δA , or a double vector $2A\delta$. Only simple dislocation glide occurs in the first case, without any need of thermal activation, contrary to a general assumption implied in some current terminology (e. g. the word *self-pinning*). The only case in which thermal activation is required is the second kind of synchro-shear which occurs in some closely related situations encountered in ordered alloys e. g. for

shearing γ' precipitates in superalloys and in the plastic deformation of long period ordered alloys. The *viscous slip* model proposed by Kear *et al.* [6] is reinterpreted and a reasonable stress dependent activation energy is computed; it is felt as being a much more general slip mode which should hold not only for long period ordered alloys, but also for some non-stoichiometric compounds (intermetallic compounds or carbides).

It is useful before entering those special aspects to review some typical examples recently investigated, which illustrate the general relation the splitting of dislocation core bears on the plastic slip properties of crystals. This is the purpose of the next section.

2. Core structures and slip planes of dislocations in crystals. — It is generally accepted that slip planes in a crystal lattice be the closest packed planes. However important exceptions are known to this rule (e. g. the *ionic slip* on $\{110\}$ planes in NaCl structure). It seems better to relate the habit of a dislocation line for lying and gliding in some lattice plane, to its possible dissociation in that plane, which lowers the total energy of the dislocation. This is illustrated below on some examples as different as: the case of h. c. p. metals, of ionic crystals, of tellurium, and finally of a molecular crystal: α -sulphur.

2.1 HEXAGONAL CLOSE PACKED METALS. — In h. c. p. metals the well-known splitting scheme:

(Thompson notations are used [7]) describes the most probable dissociation of dislocations in the basal plane, which is again the easiest slip plane for most of these metals: Cd, Zn, Mg, Co.

However secondary slip systems are known also to exist, namely the prismatic and the pyramidal glide, but with a much higher yield strength. Why so much higher is not a simple matter and has only been clarified a few years ago. It is not that *a*-dislocations ($a \equiv CB$) do not exist on $\{10\bar{1}0\}$ prismatic planes for it has been shown in Be by Regnier and Dupouy [8] that dislocation sources can readily be activated on these planes with proper stress orientation. Nor that dislocations experience a specially high resistance to proceed further on these planes, for these authors succeeded to make glide them under about the same stress as for basal glide providing the temperature was *low* enough. The real origin of a room temperature higher strength on prismatic slip planes can only be understood from the behaviour of dislocations with a *split* core, as indicated below.

Regnier *et al.* [9] have accounted for the glide of *a*-dislocations in prismatic planes (*a* being the basal period) in suggesting the following dissociation scheme:

This suggestion is supported by the remark that an atomic displacement $\frac{1}{3}a$ turns the stacking of two

(1010) successive planes into two (112) b. c. c. ones, i. e. introduces a thin layer of b. c. c. phase, two atomic planes thick. Indeed some h. c. p. metals exhibit this phase transformation h. c. p. $\rightarrow$ b. c. c. at a critical temperature T_c . Amongst all the h. c. p. metals, a guess of their relative stacking fault energy can be obtained from comparison of ratios T_c/T_m , where T_m is the melting point. The smaller is this ratio, the smaller is the stacking fault energy in prismatic plane and so, the easier should be the prismatic glide versus the basal one since dissociation confines dislocations in the fault plane. This view fits very well with observations ; while Cd, Zn, Mg and Co do not present this phase transformation at all and correspondingly show basal glide as the easiest one, it can be noticed that Be, Re, Y, where $T_c \simeq T_m$, have the prismatic glide about as easy as the basal one, and most significant, Ti, Zr, and Hf which are known to slip much more easily on prismatic planes than on the basal one, are also those metals which exhibit the lower T_c/T_m ratios.

Now when testing the prismatic slip, experiments are designed for a zero applied stress in the basal plane and so, only prismatic slip is activated : the dislocations start moving in these planes but, when in screw direction, they may dissociate in the basal plane where a lower core energy is probable, due to a likely lower stacking fault energy in that plane. Once cross-slipped in the basal plane, dislocations experience there a zero applied stress and can be considered as frozen-in. However, when looking at the real cross-slip situation (Fig. 1) it is quite clear that changing the disso-

might only occur above certain finite temperature. In such a case, the corresponding macro-elastic limit should be expected to vary with temperature as shown in figure 1 [8] :

a) at very low temperatures, dislocations keep slipping and multiplying on prismatic planes, with only a weak thermal activation resulting in a slight decreasing flow stress ;

b) at medium temperatures, the cross-slip prismatic $\rightarrow$ basal is activated from some temperature T_b but the temperature is not high enough to activate the reverse cross-slip, back to prismatic planes. Then more and more dislocations become frozen up, leading to exhaustion of the available dislocation sources, and thereby *increasing* the flow stress needed to activate new sources : of course this process is help by internal stress concentrations (or by glide polygonisation) which are growing up from accumulation of frozen dislocations and are of increasing importance in this stage ;

c) finally, above some temperature T_p the frozen dislocations recover their mobility in cross-slipping back to their original prismatic plane and the flow stress decreases rather strongly with temperature as thermal activation is more and more available, while stress concentrations relax in the crystal. This has been observed for prismatic slip in Be [8] and Mg [10]. In Be, $T_b \simeq 170$ K and $T_p \simeq 290$ K : thus it is seen that the high room-temperature strength of prismatic slip in this crystal stem solely from the cross-slip induced freezing of prismatic dislocations in the basal plane at this temperature.

FIG. 1. — The transition glissile-sessile of a dissociated dislocation, or prismatic-basal for the case of h. c. p. metals. Note that the transition $g \rightarrow s$ (here prismatic-basal) is always easier than the reverse $s \rightarrow g$, because s is stable while g is only metastable. 1a shows the energy diagram ; 1b shows a bit of the dislocation dissociated in the basal plane, between two constrictions ; 1c shows the thermal dependence of flow stress : $T < T_b$, no sessile dislocations formed ; $T_b < T < T_p$ the transition $g \rightarrow s$ is activated ; $T > T_p$, the reverse, $s \rightarrow g$, is activated.

ciation plane requires in general some constrictions to be nucleated and brought apart along the core even though the frozen state has a lower energy. This means some energy barrier has indeed to be overcome, but of course much smaller than in the reverse direction basal $\rightarrow$ prismatic. So that, depending on the prismatic core width, it is expected that the freezing of dislocation lines along some crystallographic directions

Pyramidal slip $\{11\bar{2}2\} <11\bar{2}3>$ has been explained along similar lines by Stohr and Poirier [11] (where $<11\bar{2}3> = c + a$, c being the period normal to basal plane). Here, dissociation of $c + a$ -dislocations in pyramidal planes is a much more complex process of energy probably always higher than in the basal plane ; however splitting in the latter involves *climbing* of partial dislocations, so that pyramidal glide can be still preferred at low enough temperature. At room temperature, the cross-slip induced freezing of, here, pyramidal ($c + a$)-edge-dislocations in the basal plane has been evidenced by Blish and Vreeland in Zn [12], and by Stohr and Poirier using electron microscopy in Mg [11].

In principle such picture should apply in any of the cases where a sessile splitting of the core is to be expected. In fact, constrictions should be fairly easy to form on a split core of radius smaller than 2 to 3 b , where b is the *core radius* of the total perfect dislocation [13], so that no such behaviours should be observed in these cases. This is probably why it has never been reported in b. c. c. metals, but we should expect it for wider cores.

2.2 IONIC CRYSTALS WITH ROCK SALT STRUCTURE. — In these crystals, ionic slip $\{110\} <110>$ is the

easiest slip system, in contrast with the closest packed plane $\{100\}$ which is only a possible slip plane at high temperature. In other hand, although NaCl is a crystal rather hard, it was known for a long time by geophysicists that under hydrostatic pressure rock salt behaves as a much more ductile rock. These two features are accounted for by a certain extent of splitting of dislocation cores in these crystals.

This situation has been explained by Fontaine [14]. Interionic forces are reasonably known in ionic crystals, on the form of central pair interaction potentials which allow the most probable stacking fault energies to be computed and compared. In this way Fontaine showed theoretically that the more favourable splitting of $\frac{1}{2} < 110 >$ dislocations occur on $\{110\}$ planes following :

$$\frac{1}{2} < 110 > \rightarrow \frac{1}{4} < 110 > + \frac{1}{4} < 110 > .$$

It is easy to see that this fault shift brings nearer ions of opposite charge, so that it is *help* by coulombian interactions, contrary to what is generally said about fault in ionic crystals. The stacking fault energy comes then only from exchange interactions between those ions which now face each other, inducing some local dilatation normal to the (110) fault plane in order to relax the neighbouring lattice ions. Thus it is computed that neighbouring (110) planes are brought apart by a relative amount $\varepsilon_0 = \delta d/d \simeq 0.3$. The existence of such a relaxation makes the stacking fault energy higher and the core width narrower in presence of a hydrostatic pressure at least of the order of 4 kbar for NaCl [15]. Indeed, increased ease of cross-slip is clearly observed in this crystal at pressure ranging to 10 kbar at room temperature [16]. The stress for the onset of the third stage of deformation decreases linearly by 7 to 10 % per kbar, and a substantial reduction in flow stress of the polycrystal results (20 % at 10 kbar), causing a sensible increase in ductility.

On the other hand, the type of fault involved here has an important peculiarity as compared with usual (111) fault in f. c. c. structure. By no way the above fault shift $\frac{1}{4} < 110 >$ is physically meaningful, and the above reaction is not an adequate description of the stacking fault ribbon. As shown by Fontaine [14, 15], this shift does not produce a stable but an unstable fault ; this means that if the stacking fault energy γ is computed as a function of the shift x $[110]/\sqrt{2}$, the function $\gamma(x)$ does not show any minimum in the range $[0, b]$ but only a maximum for $x = 0.5 b$. This is probably a common situation for split cores ; Vitek has shown for example that this was also the case for b. c. c. metals [17]. From this result it follows that :

(i) such a stacking fault cannot develop all through the crystal. It is possible however for the dislocation core to dissociate because some elastic energy is gained from repulsion of the partials ;

(ii) no particular fault shift should play a role in the core structure, but instead this one must be described

in terms of a *continuous distribution* of partial dislocations of a density at point y , $\rho(y)$, and of Burgers vector $db = b\rho(y) dy$ so that :

$$b \int_{-\infty}^{+\infty} \rho(y) dy = b .$$

Mathematically, the treatment of this kind of splitting is not very different from the usual two-partial one, at least for simple distribution functions $\rho(y)$, and change only numerical factors in equations [14, 15]. In particular it leads to a core width somewhat more extended because γ values smaller than the maximum γ_0 are used for most of the y range (γ_0 is for the $\frac{1}{4} < 110 >$ shift).

2.3 TELLURIUM. — In covalent bonded crystals, the structure of the dislocation core is generally controlled by the distortion of directional bonds and its mobility, by their breaking. The case of tellurium is interesting because both strong directional and weak directional bonds exist in the structure, so that both types of core-lattice interactions can occur in the same crystal, through a distortion of directional bonds and through a core splitting. This latter effect leads in particular to core dissociation off the slip plane, therefore sessile, in close resemblance with the well-known sessile dissociation of screws in the b. c. c. lattice. Because the case of the b. c. c. lattice has been often described elsewhere (see this conference) we think it is better to describe instead the plastic behaviour which follows from such a core structure on the less-known example of tellurium.

The lattice of Te can be viewed as hexagonal array of helicoidal chain of covalent bonded atoms with three atoms each turn ; the lattice periods of the hexagonal cell are c , the repeat period along the chains and a_1, a_2, a_3 the repeat periods of the hexagonal array in the basal plane perpendicular to the chain axis (Fig. 2).

FIG. 2. — Trigonal cell of the tellurium lattice.

In this structure there is a strong anisotropy of the atomic bonds. Within chains, each atom has a strong covalent bond with each of its two first nearest neighbours which is estimated to 0.68 eV ; between chains, there is only a weak overlap with electron orbitals of the four second nearest neighbours, each of which is estimated to 0.22 eV only.

Plastic slip occurs mainly on prismatic $\{10\bar{1}0\}$ planes with slip direction along $\mathbf{a}$ or $\mathbf{c}$ [18]; in that way, dislocation slipping avoid cutting the covalent chains, which explains why the basal plane (the closest packed plane in the structure) is never found as a slip plane.

Furthermore, both $\mathbf{a}$ and $\mathbf{c}$ dislocations are found to align themselves along the $\mathbf{c}$ direction after a few percent strain at liquid nitrogen temperature and both exhibit a strongly thermally activated elastic limit. These observations have been accounted for in terms of two kinds of lattice-dislocation core interaction [19]:

1) $\mathbf{a}$ -dislocations cannot dissociate off their prismatic glide plane, e. g. in the basal plane, unless cutting and distorting the covalent chains. On the other hand, these chains should be strongly distorted in the core region for any line orientation, except for the edge one which runs parallel to the chains [20]. Therefore a clear tendency to align $\mathbf{a}$ -dislocations into $\mathbf{c}$ directions is expected, and observed, in a close similitude with preferred dislocation orientations observed along closest packed rows of other covalent crystals like Si or Ge, and a strong lattice friction results;

2) $\mathbf{c}$ -dislocations have been proposed to dissociate when screw, in several prismatic planes at a time following the reaction [20]:

$$\mathbf{c} \rightarrow \frac{1}{3}\mathbf{c} + \frac{1}{3}\mathbf{c} + \frac{1}{3}\mathbf{c}.$$

The configuration is quite similar to sessile screws in b. c. c. metals (Fig. 3), and again the two faulted planes

FIG. 3. — Dislocation splitting of a $\mathbf{c}$ -screw dislocation in $\{10\bar{1}0\}$ planes of the tellurium lattice. *a*) sessile state of a $\mathbf{c}$ -screw dissociated into three $\mathbf{c}/3$ partials; *b*) partial recombination of a screw under the applied stress; *c*) glissile metastable state of a $\mathbf{c}$ screw.

should intersect along a $\frac{1}{3}\mathbf{c}$ -partial. Here the introduced stacking faults involve only a fault in the chain arrangement but keep unchanged the atomic chain itself. Such a stacking fault should not have a prohibitive energy, the defect in chain stacking being somewhat similar (but not exactly equivalent) to prismatic twins which have been observed [19]. Unfortunately it has not been possible so far to visualize by electron microscopy the screw alignment of $\mathbf{c}$ -dislocations after straining as it is beautifully observed in b. c. c. metals, because screws escape the foil under the large image forces due to the external surfaces. Such forces indeed can easily exceed the room temperature elastic limit, for the foil cannot be much thicker than 300 to 400 $\mathbf{c}$ owing to the large absorption in tellurium. Nevertheless their wake

is evidenced by numerous edge dipoles and debris left behind.

Other support for this splitting model comes indirectly from the plastic behaviour of the $\mathbf{c}$ -glide [21]. Clearly, this sessile core configuration gives rise to a progressive freezing of the slip dislocations as they reach the screw character, at the origin of the same kind of slip resistance as the one acting on prismatic slip planes in h. c. p. metals, explained above. Again, the same sort of thermally activated cross-slip allows the screw to be glissile again, resulting in a severe decrease of macroelastic limit with temperature, in complete agreement with observations. By the same token, the extended microplasticity stage observed below the macro-elastic limit (Fig. 4) is also explained, with a very smooth transition in stress-strain curves between the micro and macroplastic range.

FIG. 4. — The stress-orientation effect on $\mathbf{c}$ -glide in tellurium at 77 K. Both dissociation planes of $\mathbf{c}$ -screws are equally stressed in C-II orientation, while in C-III orientation one of these planes (the slip plane) is two times more stressed than the other one. The strain dependence of the activation area is also shown, given in unit $\mathbf{ac}$, $\mathbf{a}$ and $\mathbf{c}$ being respectively the basal and the $\mathbf{c}$ -repeat periods; such strain dependence is used to choose a proper elastic limit. σ is the stress resolved on the slip plane, and γ the strain resolved on the same plane.

Another feature characterizes specially those core dissociations off the slip plane: it is found as well in b. c. c. metals, but *not* in prismatic glide of h. c. p. metals. The stress orientation dependence of the elastic limit for $\mathbf{c}$ -slip *does not* obey the Smid law (while $\mathbf{a}$ -slip does obey this law). The argument follows simply from figure 3*b* which pictures how a screw starts moving under the applied stress. It is quite clear that the stress component resolved on the gross slip plane is

no longer the only component which matters, for the other stress components on the dissociation planes have to do with the necessary constrictions of the faulted ribbon in these planes, in order for the total dislocation to move in its primary slip plane. Figure 4 shows this effect in the case of tellurium. There the stress-strain curves for compressive prismatic glide along the c axis are presented at 77 K for two orientations of the single crystal [21]. The so-called C-II orientation has the same resolved shear stress on both the dissociation planes in figure 3, while for C-III orientation, one is two times larger than the other, the gross-slip plane being the more stressed one. When plotted in terms of the resolved stress on this gross slip plane, as is shown in figure 4, the elastic limit is seen to be just two times higher in C-III than in C-II. Alternatively, the elastic limit would be about the same in the two orientations if it was resolved on this dissociation plane which is not the slip plane. Therefore, the need for screw recombination appears to be the rate controlling step for the macro-elastic limit. Also, it can be seen that the less favourable is the stress orientation for recombination, the more developed is the microplastic stage and the smoother is the micro-macroplastic transition.

Finally how effective is this kind of lattice friction in the overall plasticity, and specially in the low temperature work-hardening beyond the elastic limit is an important problem for this class of crystals. For the sake of simplicity the case of tellurium is below described but similar trends begin to be worked out also for b. c. c. metals, α -iron in particular [22, 23].

In short, at lower temperatures we expect the lattice friction to be too large to allow any dislocation rearrangement such as those interactions between primary and conjugated slip systems which give rise usually to a hard stage II in stress-strain curves. Accordingly these curves should only show a *slight* dipole hardening due to trails and other debris left behind in the wake of screws; as a result the whole plasticity should be controlled in this temperature range by the one lattice friction. Indeed this is the outline the stress-strain curves of numerous b. c. c. metals look like at very low temperature.

In the upper part of the thermal activation range however, some dislocation screening, and tangling, should always occur as the lattice friction decreases until becoming too weak to oppose these rearrangements. These latter are made as much easier in these lattices, on the other hand, than cross-slipping is obviously facilitated by the kind of core structure so that a true glide tangling can be developed even at such temperatures still relatively low. Thus, some kind of transition behaviour where a strain dependent hardening superimposes upon a Peierls friction (still rate controlling at yielding) is generally expected at temperatures in between the athermal and the lower range, and therefore *below* the athermal threshold. This should hold very generally in nature, for any crystal showing this kind of core structure.

A glide polygonisation of this sort has indeed been observed in tellurium single crystals [21]. Below 150 K, the activation parameters behave quite normally, the activation volume is strain independent, and the activation energy is linear in temperature. Also stress-strain curves are typical of a high lattice friction, with no workhardening visible beyond yielding, as shown in figure 5. At 77 K and above, the only polygonisation is the one of c -edges which cluster and form some slight kink bands when the flow stress is not too high. In contrary, figure 6 shows that above 150 K stress-strain

FIG. 5. — Stress-strain curves of prismatic c -glide in tellurium, at low temperatures.

FIG. 6. — Same as figure 5, but above 143 K : note the quite different effect of temperature.

curves do not show any more a very clear temperature dependence, and exhibit an apparent strong work-hardening. Most important, detailed recordings of these curves show continuous serrations along the test (Fig. 7).

FIG. 7. — Example of serrations along the stress-strain curve. The direct load-elongation chart is shown for prismatic c-glide in tellurium single crystal at 263 K.

A parallel study of the dislocation substructure by Berg-Barrett topography shows a strong polygonisation above 150 K. The long c-screws accumulated on their slip planes can relax the long range stresses they build up in attracting a-screws. Twist walls result in the prismatic plane which have been clearly evidenced by Berg-Barrett topography (Fig. 8) and confirmed by

FIG. 8. — Berg-Barrett topography of a deformed specimen (c-glide) at 210 K. Horizontal strips show prismatic slip planes polygonized into twist-walls. Vertical contrast lines which exhibit offset at the crossing of prismatic twist sub-boundaries are rough kink bands formed by polygonisation of c-edges in the basal plane. These offsets typify a twist about a vertical (basal) axis. (4040) reflection.

electron microscopy. This polygonisation is only possible at a temperature higher than 150 K, because 150 K is just that temperature at which glide of a-dislocations is observed becoming very easy, being no more hindered by the strong lattice friction which opposes this slip system also at lower temperatures. Thus a situation arises in which all slip dislocations become entangled within walls: c-edges form kink walls and c-screws form twist walls. Therefore straining can only proceed by collective displacement of dislocation walls, which result in the observed sudden stress drops. The drop frequency determines solely the apparent work-hardening rate on the gross stress-strain curve, and the apparent elastic limit, while the limit stress for having the isolated screw mobile is probably much lower than this, although being still thermally activated.

A somewhat similar glide tangling is also observed above about 200 K (depending on the stress orientation) in α -iron; it has been followed by Berg-Barret topography, the details of which is reported in reference [22].

Finally, we would end this section with a remark about f. c. c. crystals, the preceding discussion brings forth.

2.4 A REMARK ABOUT LOMER-COTTRELL BARRIERS, AND THE BRITTLINESS OF α -SULPHUR. — It is worth noticing that formation and recombination of Lomer-Cottrell barriers formed at the intersection of two slip bands in the f. c. c. structure is again the same problem as the above paragraph.

Let the total Burgers vector of the recombined barrier be $\vec{AB}$, and $\vec{CD}$ its line direction, in Thompson notations (Fig. 9). Its slip plane would thus be the

FIG. 9. — Geometry of the usual Lomer-Cottrell barrier in the f. c. c. lattice. The slip plane of the total recombined barrier is a cube plane $\{001\}$. Thompson tetrahedron is shown for convenience.

plane $(\vec{AB}, \vec{CD})$, i. e. $\{100\}$. Of course this plane is never observed as a slip plane; this can seem unexpected because $\{100\}$ planes are the second closest packed planes in that structure, while $\{110\}$ planes for example (less dense than $\{100\}$) are sometimes observed [24]. Figure 9 gives the explanation: a dislocation $\vec{AB}$ which would slip on $\{100\}$ would dissociate when edge, on two $\{111\}$ planes at a time and so could only slip against a very high lattice friction as compared with other possible slip planes.

However the above considerations may be usefully extended to explain the plastic behaviour of some *pseudo f. c. c.* crystals. Such an example is the brittleness of α -sulphur [25].

α -sulphur is a molecular crystal with ring shaped molecules; each ring contains eight covalent bonded atoms, and Van der Waals forces tighten the rings together into an orthorhombic lattice with sixteen rings per unit cell. This complex structure can be viewed as derived from the f. c. c. one, with (111) stacking in the usual sequence ... ABC ABC ...; here A, B, or C is a block of four successive (111) planes within which rings are rather tightly entangled together while a gap is left open in between the blocks. There are six $\frac{1}{2} \langle 110 \rangle$ repeat periods of which three are repeat periods within the (111) plane of the blocks, and the three others turn a block A into B or C. Because of these similarities, Thompson notations can still hold for describing the possible dislocations.

However in the sulphur lattice that tetrahedron is very much elongated in the *c*-axis (Fig. 10), for the *c*-unit

FIG. 10. — Thompson tetrahedron for the orthorhombic (sulphur)-lattice.

is at least two times longer than the *a* and *b* ones ($a = 10.46 \text{ \AA}$, $b = 12.87 \text{ \AA}$, $c = 24.49 \text{ \AA}$). This causes Burgers vectors with a non-zero *c*-component to be less stable than others, which introduces strong differences with the f. c. c. case in dislocation mobilities. As a result sessile barrier similar to Lomer barriers are more easily produced along slip lines and α -sulphur shows a brittle behaviour while f. c. c. crystals are ductile.

An example is given if one considers the possible splitting of a dislocation with Burgers vector $\mathbf{CB} = \frac{1}{2} [01\bar{1}]$:

$\mathbf{C}\delta$ is of the Shockley partial type, of index $[11\bar{2}]$; because of its large *c*-component, it decomposes to give a $[121]$ or $[211]$ one and a *stair-rod* according to:

So, when a $\mathbf{CB}$ dislocation reach a screw orientation, it should dissociate on two $\{111\}$ planes at a time, as:

Similarly, when it is parallel to AC, i. e. to $[101]$:

Such barriers are obviously sessile and should be readily formed during simplex or duplex slip; they cause a strong hardness for these slip systems, which are very difficult to activate in compression tests for example.

On the other hand the large values obtained for total dislocation energies due to the length of available $\frac{1}{2} \langle 110 \rangle$ Burgers vectors, and the weakness of Van der Waals forces suggest strongly the existence of these dissociations, and barriers. No direct evidences has yet been obtained but the sessile nature of the above $\frac{1}{2} [01\bar{1}]$ screw has been clearly proved by transmission X-ray Lang topography (25). Accidental introduction of a crack in course of experiment allowed to observe individual motions of $[01\bar{1}]$ dislocations under the crack induced stresses, thereby providing direct evidences on mobilities of dislocations of different character. It has thus been shown that a $\mathbf{CB}$ dislocation can easily move locally under stresses as weak a $10^{-6} \mu$ (μ , shear modulus) when out of AC or AD directions, while being completely sessile even under high stresses when screw, thereby prohibiting any long range slip.

3. Activation energy for slip of dislocations with a core dissociated off their slip plane. — We wish to show now the general background of theoretical models proposed for evaluating dislocation mobilities when the core splitting occurs off the slip plane.

As shown above, this situation is fairly often encountered. In many physical cases, it happens that the most favoured slip plane is not the dissociation plane: whether the dislocation core is spread out in several planes at a time (b. c. c. metals, tellurium, Lomer-Cottrell barriers), or the core splits in only one plane but which is not the one favoured by the applied or even the local stresses (prismatic and pyramidal glide in h. c. p. metals). In a sense the usual cross-slip which becomes so profuse in f. c. c. metals at the end of stage II of deformation falls in this class of situations, because the primary slip plane is no more the easiest one, with more and more numerous obstacles and tangles left by the deformation itself. Then primary dislocations, although dissociated in that plane have to slip in another (111) plane. Consistently the same experimental trends should apply as well for elastic limits as for the flow stress at the onset of

stage III of deformation (wavy screw slip lines, gradual transition on stress-strain curves as straining increases, strong thermal dependence of any stress value characteristic of this transition).

In all these situations, two different cases are to be considered separately for modelling the core mobility. Whether a higher energy core configuration must be reached in order for the dislocation to start slipping on the new plane, and the driving force is then these stresses which favour a bowing out of the *total* dislocation in that plane, or, in contrary, the core splits wider in the new plane, thus decreasing there its energy, and the driving force is the widening of ribbon under eventually these stresses which push the *partials* apart in acting on their opposite components.

3.1 SLIP OF DISLOCATIONS IN PLANE OF HIGHER CORE ENERGY. — In numerous examples, slip can only proceed further if a higher energy core configuration is reached all along the dislocation line. Among these we can list :

— Recombination of a sessile core split on several planes at a time.

— Recombination for cross-slipping on a new plane in which dissociation is much narrower (part (c) of figure 1c ; see ref. [26]).

— Core modification for synchronizing atomic shears adjacent to the slip plane in some ordered alloys to avoid making wrong bonds within the slip interface (see further, section 4).

— Core debris (dipoles) left at the crossing of intersecting stacking faults widely extended [27].

Let us consider a straight dislocation line in the low core energy configuration, with line tension t (Fig. 11). In order to start slipping, a certain critical length of core AB has first to reach the high energy state ; AB must be long enough to bow out in the new plane, thus reaching an unstable position under the work of applied stresses σ , and finally making the whole length mobile, in the high energy state. Taking account of the energy increase, lengthening, and the work of stresses acting on the total dislocation, the energy of critical bow-out AB is simply [26] :

$$U_0 = \frac{2}{3} \rho t' \theta^3, \quad t' = \sigma b \rho, \quad \cos \theta = t/t' \quad (1)$$

with t' the high energy line tension, ρ the curvature radius, and θ the critical angle for line tension equilibrium at point A, being small enough to approximate the sine and cosine functions by their development :

$$\theta \simeq (2(t' - t)/t')^{1/2}.$$

This result may be expressed in terms of the critical length $l_c = AB$:

$$U_0 = \frac{2}{3} l_c (t' - t) \quad (2)$$

$$l_c = 2 \rho \theta = 2(2(t'(t' - t))^{1/2}/\sigma b \quad (3)$$

$$y_c = (t' - t)/\sigma b \quad (4)$$

with y_c , the critical sag. Hence an activation energy varying as σ^{-1} and an activation volume as σ^{-2} .

FIG. 11. — Critical bow-out for making glissile again a straight sessile dislocation ; t and t' are respectively line tensions of the lower and higher energy state ; they equilibrate at A or B, taking into account the radius ρ of the bow-out under the applied stresses.

To this term, one has to add eventually a constriction term if there is a change in splitting mode. From linear elasticity, the energy needed to constrict a two-partial ribbon into a point can be computed as [13, 28, 29] :

$$U_c = A \mu b^2 (d - b)^2 / d \quad (5)$$

with d , the stress dependent dissociation width, μ the shear modulus and A a constant depending on the dissociation geometry. Accordingly the activation energy becomes $U = U_0 + 2 U_c$. It has been shown theoretically [29] and verified experimentally [30] that the constriction term prevails ($U_0 \ll 2 U_c$) at very low temperatures, when the process is almost solely due to mechanical stresses, so that the core mobility becomes controlled by constriction formation ; the thermal dependence of flow stress can in this case be used as an experimental check of eq. (5). In this way Kubin *et al.* [30] have shown that tensile deformation of very pure niobium between 2 K and 80 K exhibits an activation energy which fits eq. (5), except for the constant A which is found to be ten times larger than calculated. A better fit might be expected in using a continuously distributed dislocation density for describing the core, instead of the partial scheme, which should result in a wider spread of core and a higher constriction energy.

Finally, when the dislocation core can fluctuate

between two splitting modes, one has to take into account the possible transition of the freed loop AB back to its low energy state. As first discussed by Duesbery and Hirsch [31, 28] the preceding critical bow-out may thus be never reached. At stress low enough (high temperature) the freed loop should extend so far in the slip plane (eq. (4)) that several atomic planes should be crossed over, which are neighbouring and parallel to the initial dissociation plane. In fact at the first plane reached the loop dissociates again in it, back to its initial sessile core configuration. The preceding critical bow-out is then replaced by a critical *kink* separation and the process is turned into an usual double kink mechanism with a lower energy than predicted by eq. (2). Such a transition between the two processes has been observed recently by Kubin *et al.* [30] in niobium.

3.2 CROSS-SLIP OF DISLOCATIONS IN PLANE OF LOWER CORE ENERGY. — As it has been seen in section 2, it is expected to encounter during plastic slip, situations where the slip dislocations split in those intersecting planes in which their core can dissociate much wider. Examples are the basal cross-slip of prismatic or pyramidal dislocations h. c. p. metals (part (b) of figure 1c), or the $\{110\}$ slip in f. c. c. metals recently observed by Le Hazif *et al.* [24].

In general, the stacking faults involved in the initial slip plane and in the cross-slip plane are not of the same nature. Such cases have not been worked out theoretically. Up to now only the well-known cross-slip in f. c. c. lattice has been considered, which is indeed the same problem, the *effective* stacking fault energies being made different there only because differences in resolved stresses in the two planes. This similitude is emphasized by a recent treatment of Friedel suggestions [32, 33, 13].

Let us start from a constriction which has nucleated on a fault ribbon spread on the primary slip plane of a f. c. c. crystal. Cross-slipping on another plane occurs when the two halves of the constriction are separated along the line, allowing some dislocation length in between to be bowed out and to dissociate in the cross-slip plane *as soon as* the halves are brought apart (Fig. 12). For some critical separation, AB, the configuration energy goes through a maximum, beyond which A and B are pushed apart under the work of stresses, making the whole dislocation cross-slipped.

It is clear that this process is quite different from the one of section 3.1. The maximum energy falls between U_c and $2 U_c$, U_c being the constriction energy (eq. (5)). Most important, it can be shown that the stress component which bows out the total dislocation in the cross-slip plane is always *negligible* in the energy as compared with those components which push the partials apart. So that the active stresses for cross-slipping, whatever be their origin, are the local stresses which widen or narrow the fault ribbon; thus they can be introduced only through an *effective* stacking fault

FIG. 12. — Successive steps of a cross-slip process into a plane of wider dissociation; a) starting constriction in the original slip plane; b) and c) widening of the cross-slipped loop AB in the new cross-slip plane.

energy $\gamma \pm k\sigma b$, where γ is the stacking fault energy, σ the resolved shear stress on the primary plane and k a geometrical factor depending on stress orientation; alternatively only the ratio $\sigma b/\gamma$ is of interest. Finally the nucleation length is short, a few d , the ribbon width, so that the activation volume should be small, of the order bd^2 .

At small stresses ($\sigma b/\gamma \ll 1$) the asymptotic expression :

$$U = 2 A \mu b^2 d_0 \left[\left(1 - \frac{b}{d_0} \right)^2 - \alpha \sigma b \gamma^{-1} \right] \quad (6)$$

holds for the activation energy (for the *two* constrictions in the primary and in the cross-slip plane), α being an orientation dependent parameter given in [13, 33]; d_0 is the zero stress dissociation width and A is the same as in eq. (5) :

$$A = \frac{1}{8\pi} (0.92 \sqrt{\ln(\mu b/15\gamma)} - 0.60). \quad (7)$$

Other stress values require numerical solutions.

The model, eq. (6), (7), explains reasonably well the thermal dependence of σ_{III} , the resolved stress at onset of the stage III of deformation, and gives correct evaluations of γ , in the range $\sigma b \ll \gamma$ where it can be assumed that profuse cross-slip occurs at this stage under the applied stress *alone* without any need of hypothetical piled-ups, and contrary to previous treatment of Schoek, Seeger and Wolf [34]. The other assumption is that cross-slip nucleates heterogeneously, there where the applied stresses make narrower the primary ribbon.

Assuming an Arrhenius law for the strain rate :

$$\dot{\epsilon} = \dot{\epsilon}_0 \exp - \frac{U(\sigma_{III})}{kT}$$

one deduces : $U(\sigma_{III}) = kT \ln (\dot{\epsilon}_0/\dot{\epsilon})$, hence from eq. (6) :

$$\alpha\sigma_{III} = T \cdot \frac{\gamma^2 (\ln \dot{\epsilon} - \ln \dot{\epsilon}_0)}{A\mu b^2} \left(\frac{8\pi k}{\mu b^3} \right) + \frac{\gamma}{b}$$

Assuming $\mu b^3 \simeq 5$ eV, and eq. (7) for A (with $d_0 \gg b$) it is :

$$\alpha\sigma_{III} = T \frac{\gamma^2 (\ln \dot{\epsilon} - \ln \dot{\epsilon}_0)}{\mu b^2 \left(87 \left[\ln \frac{\mu b}{15\gamma} \right]^{1/2} - 57 \right)} + \frac{\gamma}{b} \quad (8)$$

Eq. (8) should hold for $\sigma_{III} b \ll \gamma$, i. e. for metals not too much dissociated (e. g. *pure* metals) and not too high σ_{III} that is to say not too low temperature. Effectively Beneteau and Coulomb [35] have recently observed a *linear* $\sigma_{III}(T)$ law at high temperature (200 K-400 K) and have deduced quite reasonable γ -values from (8) for polycrystalline Cu, Ni, Ag and alloys Cu-Si, Ni-Cr.

At lower temperatures, in contrary, the experimental fitting with numerical computations is far less convincing, indicating probably an increasing role of internal stress concentrations at favourable nucleation places. Apart from these difficulties, however, it has to be emphasized that the whole activation problem has never been completely investigated experimentally, in any temperature range, as far as activation energy and activation volume are concerned. Such measurements should be needed for a meaningful comparison with theory.

4. Plastic slip of dislocations with *extrinsic* cores dissociated in the slip plane. — It is worth considering now also those dislocations in more complex structures which, although being extended in the slip interface, give rise to the *synchro-shear mechanism* of Kronberg. We wish to analyse somewhat in details such processes, because its close resemblance with the simpler propagation of an extrinsic fault (or 2V-fault) in f. c. c. lattice. The reason for such similarities is apparent from the next section. As a result, two types of synchro-shears should be considered separately, depending on the shift of the involved 2V-fault, whether it is a simple Shockley vector δA , or a double vector $2A\delta$.

4.1 SYNCHRO-SHEARS OF THE δA 2V-FAULT TYPE. —

4.1.1 *Extrinsic nature of (111) stacking faults in carbides.* — Kronberg [2], fifteen years ago drew attention on the particular motion the ions near the slip plane should undergo, when a Shockley-type partial dislocation is moving through the basal plane of an alumina crystal. Anions and cations should not follow the same path, in order to avoid very bad stacking of identical ions of the type A-A, just above one another across the slip interface. As a result, some synchronism has to work between these different ionic motions to keep them in time, which has been proposed to cause another kind of lattice friction.

The essentials of this mechanism can be described most clearly in the carbide lattice, which is the simplest lattice of the type and where some evidence for it has been recently claimed [4, 5]. The lattice of transition metal carbide can be described as a stacking of $\{111\}$ planes of octahedral sites :

where metallic ions form the A, B, C planes and carbon planes are represented by α, β, γ .

It is quite clear that no *intrinsic* fault can exist in the structure, as noted by Kelly and Rowcliffe [4]. This type is the 1V-type in Frank notations, such as obtained when removing only one plane, like :

or

$$\dots A \beta C \alpha \downarrow C \alpha B \gamma \dots, \\ \dots \Delta \Delta \Delta \blacktriangledown \Delta \Delta \Delta \dots$$

or

$$\dots A \beta C \downarrow \beta C \alpha B \dots \\ \dots \Delta \Delta \blacktriangledown \Delta \Delta \Delta \dots$$

In all the examples, faults like either $\dots C \alpha \gamma A \dots$ or $\dots C \alpha C \alpha \dots$ are quite improbable because a very bad stacking is introduced owing to large differences in size and electronic structure of the two atom species. Only these faults which belong to the *extrinsic* scheme (2 V-faults) are expected :

which avoid piling-up of metallic ions just above one another through only a thin carbon layer.

It is known then, that such a fault is two atomic planes thick, so that its boundary cannot be a simple Shockley partial but has a core consisting of *two* Shockley partials one above the other, the Burgers vector sum of which is equal to a Shockley vector. This is exactly the same situation for an usual extrinsic fault ribbon in f. c. c. structure. Thus the shear process in carbides is typified by the propagation of such extrinsic ribbons, so that we should better call these atomic motions *extrinsic glide*. We show below, looking at this process, that moving an extrinsic ribbon through a f. c. c. lattice, displaces atoms of the two fault layers past each other along two 60°-directions, obviously in a synchronized way, and reproduces exactly the same atomic motion as the so called synchro-shear mechanism. But as such, only a simple dislocation glide is involved without any need of thermal activation.

4.1.2 *Propagation of extrinsic fault in f. c. c. structure.* — We show first that a boundary of extrinsic fault in f. c. c. lattice consists of a partial dislocation of total Burgers vector δB for example, the core of which can be described as superposition of two Shockley cores with 120°-Burgers vectors $A\delta$ and $C\delta$ on the two fault layers.

Figure 13 pictures such a boundary. On the left side is the perfect ... ABCABC ... stacking, and on the right side is the extrinsic stacking fault :

Only atoms onto the fault layer are shown, and the boundary character is chosen screw, of total vector $\delta\mathbf{B}$, for the sake of simplicity.

FIG. 13. — Sketch of an extrinsic-screw partial in the f. c. c. lattice. Extrinsic stacking fault is on the right, perfect lattice on the left. Atomic shears for boundary motion to the left are shown for different boundary core structures : full lines are for a ($A\delta$, $C\delta$) core ; dotted lines are for other core structures : ($B\delta$, $2\delta B$) or ($2\delta B$, $B\delta$). For the first core structure, note that Δ -atoms and $+$ -atoms move along 60° -routes in a correlated way.

To describe the core of a two layers $\delta\mathbf{B}$ -fault boundary with Shockley vectors, only two solutions exist : either ($2\delta\mathbf{B}$, $B\delta$) or ($C\delta$, $A\delta$). From the minimum energy argument, the couple ($C\delta$, $A\delta$) is to be preferred ; for, it can be viewed as a dipole $\pm b/2$ plus two $\delta\mathbf{B}/2$ components on each layer, as compared with $\delta\mathbf{B}$ on one plane plus a $\pm\delta\mathbf{B} = \pm b/\sqrt{3}$ dipole. But the couple ($C\delta$, $A\delta$) is definitely more plausible when looking at corresponding atomic displacements if fault boundary is moved. Such displacements are sketched figure 13 for different core structures assuming the bottom atom layer (symbol 0) to be fixed while the two upper layers are moved as the boundary is slipped to the left.

(i) Core ($B\delta$, $2\delta B$). That means a $B\delta$ relative shear between 0 and Δ -layers, and a $2\delta B$ relative shear between Δ and $+$ layers, or a $B\delta + 2\delta B = \delta\mathbf{B}$ shear relative to 0 and $+$ -layers. Here it is seen that Δ and $+$ atoms exchange their projections onto the (111) plane in slipping one above the other, thereby disrupting the close packed character of the structure.

(ii) Core ($2\delta B$, $B\delta$). In this configuration, Δ -atoms move a $2\delta B$ distance, thereby being obliged to climb directly over 0-atoms below and thus disrupting again the closepacked character of the structure.

(iii) Core ($C\delta$, $A\delta$). Δ -atoms and $+$ -atoms move along 60° routes in a way much more favourable since it avoids any climb of two adjacent layers one above the other. It can be noticed that these routes feature exactly the same process as claimed for *synchro-shear partials* [2] and that their correlation is automatically ensured by the obligation to maintain the extrinsic nature of the stacking fault. In other

words, no thermal activation is needed and the process is of a pure glide nature ⁽¹⁾.

We show briefly now that similar considerations holds also in oxides where a synchro-shear mechanism has been claimed.

4.1.3 The case of oxides : corundum and spinels : synchro-shear as a pure, non activated glide. —

4.1.3.1 Corundum lattice (Al_2O_3). — The corundum lattice can be described as a close-packed stacking of planes of octahedral sites :

where oxide ions form a hexagonal close-packed frame ACAC ... with aluminium planes in β interstices. The index i of a plane β_i refers to the unoccupied aluminium sites (one third) ; it is related to partition of the octahedral sites in a (0001) plane into three sub-lattices [36] and shown figure 14 ; we note β_i a (0001) plane with all sites numbered i , unoccupied.

For the same reasons as for carbides, only 2 ∇ -faults have reasonable energies, i. e. faults in which two apexes are turned :

The sequence of indices depends on the boundary core structure. Two kinds of sequences, i. e. two kinds of unoccupied sites arrangements, can be generated (see Fig. 14) :

(i) Core of the type ($A\delta$, $B\delta$) generates any of the equivalent sequences :

(ii) Core of the type ($2\delta B$, $B\delta$) generates sequences with double-repeated indices :

It is not simple to say something about relative energies of these two types of faults, in absence of detailed computations (type (i) of 2 ∇ -fault is the one introduced by Kronberg, with equivalent notation, in [2]). However, the same discussion as above, section 4.2, holds also in this case and favours a core structure ($A\delta$, $B\delta$) ; it gives rise to the same ion

⁽¹⁾ It has been claimed in the case of a boundary edge character [5] that a core ($C\delta$, $A\delta$) must have depleted atom sites to be able to accommodate easily the incoming atoms at the moving boundary ; if a site happens to be occupied by some atom in the core, it should be first diffused away before the partial goes on slipping, hence the need of an activation energy. However, we disagree on this point. Some depleted region must *always* exist near an edge core, for geometrical reasons. If an atom happens to be trapped there, it means only that a jog pair has been nucleated, which makes the slip interface to take a kind of rumple but does not impede the glide : a new depleted room appears immediately above the jog pair.

FIG. 14. — Al_2O_3 structure (structure 6³ in Schläfli notations). Each (111) planar net (0-atoms : $z = 1$; Δ -atoms $z = 2$; + -atoms : $z = 3$) is divided into three subnets in such a way as an axis of symmetry order 3 be obtained : indexes of a planar net are obtained from the ones of the sheet just below by $\text{C}\delta$, $\text{A}\delta$, $\text{B}\delta$ translations (in the projection plane) : $\text{C}\delta$: $0 \rightarrow \Delta$; $\text{A}\delta$: $\Delta \rightarrow +$; $\text{B}\delta$: $+$ $\rightarrow 0$. Smallest repeat periods in a 6³-planar net are shown. Perfect corundum lattice is then represented by sequence of 12 planes : ... $\text{A } \beta_1 \text{ C } \beta_2 \text{ A } \beta_3 \text{ C } \beta_1 \text{ A } \beta_2 \text{ C } \beta_3 \text{ A } \dots$ where β_i planes are incomplete Al^{3+} planes, A or C planes are O^{2-} planes.

motions as illustrated by Kronberg, and should not involve any thermal help.

Of course, we do not take into account here the possible additional Peierls forces effect, from the breaking-reforming of atomic bonds involved in the propagation of a partial core through the lattice. Whatever be this effect dislocation splitting can only attenuate it, and nothing notable is to be expected from corundum structure.

4.1.3.2 *Spinel lattice* ($\text{Al}_2\text{O}_4\text{Mg}$). — We introduce first a simple convenient notation for the close packed stacking of (111) planes of this lattice :

Oxide ions form a f. c. c. frame ... ACBACBA ... with cations planes in its octahedral (Al) and tetrahedral (Mg) interstices. The notation α'_i means an aluminium *kagome* plane with one fourth of sites unoccupied ; the index i refers to a partition of the octahedral sites in a (111) plane into four sublattices [36] shown figure 15 ; we note α'_i a (111) aluminium plane with all sites numbered i unoccupied.

FIG. 15. — L_{12} structure (structure 3⁶ in Schläfli notations). Each (111)-planar net (0-atoms : $z = 1$; Δ -atoms : $z = 2$; $\dagger$ -atoms : $z = 3$) is divided into four subnets ; indexes of a planar net are obtained from the ones of the sheet just below in such a way as i-sites form a f. c. c. packing (of repeat periods 2 AB, 2 BC, 2 CA). Perfect spinel lattice is represented by sequence (see text) : ... A β'_1 C α_1 B γ'_1 A β_1 C α'_1 B γ_1 A ... Also shown are atomic shears $2\delta B = C\delta + AB$, which turns γ'_1 into α'_1 and $2C\delta = (C\delta + AB) + (C\delta + BA)$, which turns β_1 into α_1 .

Finally the notation α_i means in contrary a *mixed* layer with Al and Mg cations ; α_i is a contracted notation equivalent to three layers, $b_i \alpha_i c_i$:

... C α_j B ... is : ... C b_j α_j c_j B ...

Here b_i stands for a Mg-(111) plane of tetrahedral sites in which only sub-lattice i out of the four ones is occupied, and α_i stands for a Al-(111) plane of octahedral sites in which only sub-lattice i out of the four ones is occupied. There where detailed notation of such mixed layers is not useful, only contracted notation is used for the sake of simplicity.

Again 1 ∇ -faults introduce a very bad piling of two oxide layers one on the top of the other, and only 2 ∇ -faults are to be considered. Because same arguments as above apply also here, we consider only the 2 ∇ -fault with core boundary $(B\delta, C\delta) = \delta A$ (see Fig. 15):

If faulting occurs on a mixed layer one has a slightly different stacking :

These faults are identical to faults of type I-I of Hornstra [3], and again, ion motions corresponding to a boundary slip are in fact only *extrinsic glides* of the above type which should *not* cause any special lattice friction.

Note that here, faulted index sequences change from the perfect scheme, which makes use of only one number. From this, it is easy to see that it makes a change in the first nearest neighbors of an oxide ion sitting onto the fault, so that this type of fault does not keep invariant first nearest neighbors. However, it is possible to find another type of fault with all first nearest neighbors around any ion kept unchanged : the perfect index sequence has only to be reset. This is done if a BC oxide-oxide spacing is added to δA ; then a 2 V-fault shift of the type 2 C δ is formed :

or on a mixed cation layer (see Fig. 15) :

These faults are identical to faults of type III of Hornsta, who has shown that a *twin* is obtained if such a fault sweeps each successive cation layer [3]. Because

core structure of its boundary has to be more complex when it lies on a mixed layer, sweeping on successive cation layers requires core modifications since mixed and kagome layers alternate. Such core modifications could be at the origin of a *thermal activation* of the sort discussed in section 3.1 or below, in 4.5. Finally, we see that extrinsic glide on mixed layers involves 60° routes for four ion pairs : O-Mg, Mg-Al, Al-Mg, Mg-O, on four successive ion planes.

In contrary to δA -2 V-faults, 2 C δ -2 V-faults introduce boundaries with a dipolar core structure, as it is seen when looking at the corresponding plausible atomic shears. We discuss this point below, in relation with the L_{12} structure which is found in numerous ordered alloys, like AuCu₃.

4.2 SYNCHRO-SHEARS OF THE 2C δ -2 V-FAULT TYPE.

— 4.2.1 *Core structure of 2 C δ -extrinsic boundaries in the L_{12} structure (AuCu₃).* — The AuCu₃ structure is given figure 15, with Au atoms on all the sites numbered 1 for example, i. e. forming kagome (111)-planes with Cu atoms on all the other sites. In this way, and noting as above A_i a A-(111) plane in which Au occupies all sites of sub-lattice i, the L_{12} structure can be represented by the stacking :

$$\dots A_1 B_1 C_1 A_1 B_1 C_1 \dots$$

Recent understanding of plastic deformation processes in this structure [6] has brought forth an important idea. Plastic slip proceeds there in developing preferentially pure geometrical faults, i. e. stacking faults without any wrong nearest neighbor bond. So that it is particularly important to look for the partial dislocations which can lead such faults.

From the perfect sequence $\dots A_1 B_1 C_1 A_1 \dots$ it is readily seen that any different indices on two successive letters means a wrong nearest neighbor pair Au-Au. It follows that a pure geometrical stacking fault must not change the letter index, i. e. has for shift any vector which connects two sites of the same sublattice. Figure 15 shows that the shortest vectors of this kind are of the type 2 A δ or 2 δA . Of course such faults can be as well 1 V-fault as 2 V-one. In the last case, it can be remarked the complete similitude with the 2 C δ -2 V-fault type introduced in the preceding section as preserving first nearest neighbors in the spinel lattice.

Let us consider now, the core structure of the boundary of an extrinsic 2 C δ -2 V-fault. As shown in section 4.1.2, it can be thought as a superposition of two Shockley cores with 120° Burgers vectors (2 δB , 2 δA) on the two fault layers. However when looking at the atomic shears it means, it is realized that here a 2 δB shift makes slip the Δ -atoms for example, figure 15, directly through the top of O-atoms just below, thus disrupting the close packed character of the structure. It is much more plausible for these atoms to follow the equivalent path C δ + AB which avoids such climbing one atom above the other ; in the same way the formal displacement 2 δA should be really compos-

ed of C δ + BA, so that the core structure can be written :

$$\begin{pmatrix} 2 \delta B \\ 2 \delta A \end{pmatrix} \equiv \begin{pmatrix} C\delta + AB \\ C\delta + BA \end{pmatrix} \equiv 2 C\delta.$$

Summarizing, extrinsic boundaries of the type 2 C δ should have a dipolar core structure, but once formed, should propagate through the lattice in a pure glide process, without any need of thermal help (as far as the true Peierls friction is assumed negligible). Here again, the net shifts of the two successive layers within the fault differ by a 60° angle, like it is for the first kind of synchro-shear discussed previously.

However the *formation* of such dipolar cores can lead to a thermally activated glide process, also termed *viscous slip* we discuss now for some ordered alloys.

4.2.2 « *Extrinsic activated glide* » in super-alloys and in long range ordered alloys (L. R. O. A.). — Shearing of coherent Ni₃Al precipitates (γ' phase) is the origin of precipitation hardening in nickel-base alloys. Ni₃Al is an ordered phase with L_{12} structure. Like discussed above, pure geometrical faults can only be led by partials of the type 2 C δ or 2 δC .

Now dislocations in the nickel matrix can only produce C δ Shockley dislocations, which in contrary would lead a complex fault (stacking plus order fault) when entering a γ' precipitate. One of the most probable mechanism is then to make two paired C δ partials, lying on two successive (111) layers, enter the precipitate at a time provided that some higher core energy be reached following the transformation :

$$2 C\delta \equiv \begin{pmatrix} C\delta \\ C\delta \end{pmatrix} \rightarrow \begin{pmatrix} C\delta + AB \\ C\delta + BA \end{pmatrix} \equiv \begin{pmatrix} 2 \delta B \\ 2 \delta A \end{pmatrix} \equiv 2 C\delta.$$

That the new core has a higher energy, can be immediately seen from the added dipole AB/BA, with AB $\perp$ C δ . In this way the two paired partials can enter the precipitate, trailing behind a 2 C δ -2 V-fault of a pure geometrical nature, providing that thermal activation helps making the core energy higher.

The same pairing process plus a core activation has been shown to be needed to propagate geometrical faults, i. e. plastic deformation, in L. R. O. A. also [37]. There the slip partials are of the type 4 C δ (when $M = 2$, M , the spacing between periodic antiphase boundaries, expressed in terms of the parameter) ; they have to be paired as (4 C δ + AB, 4 C δ - AB) in order to shear the one of the three possible domains (a domain is defined by the { 100 } direction of the superperiod). The spatial distribution of this particular domain resembles very much the configuration of a dispersed second phase with a volume ratio of about 33 % ; therefore the analogy is complete with the superalloy case.

4.2.3 *Possible extension of the model to non stoichiometric compounds.* — Let us consider a non stoichiometric compound AB_x, $x \lesssim 1$, where A is a

metallic atom and B, for example, is a carbon atom or an oxide ion. In a certain number of cases a stoichiometry x is obtained as homogeneous mixing of the stoichiometric phase AB, with a second phase in which vacant B sites, in definite ratio, are distributed in an ordered arrangement on (111) planes. This second phase forms in this case coherent domains, or clusters, dispersed in the stoichiometric phase, in a way much similar to γ' precipitates in superalloys. If that second phase happens to be of composition $A_4 B_3$, with B atoms forming kagome-(111)-planes (i. e. with vacant B sites on sub-lattice 1, Fig. 15), then the situation is quite the same as the one described previously; dislocations from the stoichiometric phase AB should be paired on the form of two superimposed Shockley partials ($C\delta$, $C\delta$), then turned into ($C\delta + AB$, $C\delta + BA$) partials, in order for the domains $A_3 B_4$ to be sheared without bringing two B-vacancies into first nearest neighbors. Of course, other phase compositions, or vacancy orders, might give rise to other kinds of core rearrangements, or other pairing processes as well, which have to be explicated for each given situation. In this way, the thermally activated glide in such non-stoichiometric compounds could in principle be taken into account. No such treatments have been worked out for the time being, in any compound.

Finally we show below how the activation energy can be computed in these classes of situations.

4.2.4 Evaluation of activation energy for the « extrinsic activated glide ». — Let us consider the shearing of a γ' precipitate by two superimposed $C\delta$ partials. They have to form a higher energy core, on the form of an added dipole AB/BA, thus leading to similar problem as in section 3.1. Only the geometry differs, because the dislocation is bent against the round shape of precipitates. So that one has to consider rather the situation of figure 16 instead of figure 11.

Fig. 16. — Geometry of the configuration for extrinsic activated shear of L_{12} -ordered precipitates.

Let be R , the precipitate radius, ρ the loop radius which enters the precipitate under the stresses, t the line tension of the two $C\delta$ partials in the matrix and t' with the modified core, in the precipitate.

The energy of an advancing loop AB, writes :

$$U = 2 \rho t' \theta_2 - 2 R t \theta_1 - \frac{\sigma^* B}{2} [\rho^2 (2 \theta_2 - \sin 2 \theta_2) + R^2 (2 \theta_1 - \sin 2 \theta_1)]$$

with $\sigma^* = \sigma - (\gamma/B)$, γ the stacking fault energy (pure geometrical fault), $B = 2 C\delta$. With the two equations :

$$\theta_1 + \theta_2 = \theta_c, \quad R \sin \theta_1 = \rho \sin \theta_2$$

θ_1 and θ_2 can be eliminated. The critical configuration is again defined by :

$$\cos \theta_c = t/t', \quad \sigma^* B \rho = t'.$$

Developing $\sin \theta$ and $\cos \theta$ up to θ^3 terms yields the analogs of eq. (2), (3), (4) for the critical quantities :

$$U = \frac{2}{3} (t' - t) l_c, \quad (9)$$

$$l_c = 2 \rho \theta_2 = 2 R \theta_1 = \frac{2 \rho R}{(R + \rho)} \theta_c = \frac{2 R}{(R + \rho)} [(2 t'(t' - t))^{1/2} / \sigma^* B] \quad (10)$$

$$y_c = \frac{R \rho \theta_c^2}{2 (R + \rho)} = \frac{R}{R + \rho} \left[\frac{(t' - t)}{\sigma^* B} \right]. \quad (11)$$

Finally, the result can be written in the convenient form :

$$U = \frac{4}{3} \mu B^3 n^{-3/2} \varphi(x), \quad (12)$$

with $n : t' - t = \mu B^2 / n$, $\varphi(x) = 2 x / (1 + kx)$, $x = R/B$, and $k = 2 \sigma^* / \mu = B/\rho$. Here a line tension $t' = \mu B^2 / 2$ is assumed.

And the activation volume :

$$V = - \frac{dU}{d\sigma} = \frac{4}{3} n^{-3/2} \left(\frac{kx}{1 + kx} \right)^2 \left(\frac{\mu}{\sigma} \right)^2 B^3. \quad (13)$$

The parameter n is difficult to estimate like any core problem within the framework of linear elasticity. It refers to an added perfect dipole to the core of the Shockley pair ($C\delta$, $C\delta$); only an order of magnitude, say a few tens, can be guessed. It is better to take it as a parameter to fit experimental data.

To illustrate, the case of Waspaloy (Ni 58 %, Cr 19 %, Co 13 %, Mo 4 %, Ti 3 %, Al 1.5 %) is taken, because such processes have been experimentally evidenced and studied between 600 °C and 800 °C [38]. Here $\mu = 5.7 \times 10^{11}$ c. g. s. at 700 °C, $\delta A = 1.45 \text{ \AA}$, $\gamma \approx 20 \text{ erg/cm}^2$, and $R = 325 \text{ \AA}$. We compute from

eq. (12) the following values for the activation energy in kcal/mole (the stress is in kg/mm²) :

$\sigma \backslash n$	29.05	34.34
—	—	—
21	245	190
35	180	140
64	118	92

Note that in this table, σ is a resolved shear stress. For comparison, creep experiments between 600 °C and 800 °C give in this alloy (published values have an estimated error of about 25 %) in the same unities [38]:

σ	U
—	—
27	185
40	185
56	140
74	135

In this table σ is the load stress (F/S). It is thus seen that a reasonable n -value can fit the experimental range of data. Same kind of agreement is obtained for

activation volumes, of the order 2 000 Å³. For illustration, the values $n = 29$ or $n = 34$ correspond to $t' - t = \mu b^2/22$ or $\mu b^2/26$ respectively, where b is the smallest repeat period.

Finally we would emphasize the expected size effect in this model. From eq. (12) it is seen that decreasing the precipitate radius (i. e. $x = R/B$) is like increasing the stress, that is to say *decreases* the energy. This effect can be important for small x values ($x < 100$) and should be the best verification of the model. For example, in the case of Ag₃Mg, a long period ordered alloy in which B is very long ($B = 2 \times 4 C\delta \simeq 12$ Å), an energy as low as a few electron-volts can be obtained for $R = 1\,000$ Å ($x = 83$), and for a stress relatively low, $\sigma^* \simeq 10^{-3}$ μ ($\sigma \simeq 7$ kg/mm²). In other examples, the large value of U can completely inhibit this mode of slipping when the size x is too large ; other competitive processes such as climb, ... may then be prevailing ; in the contrary, small sizes x favour this type of shearing mode and may better correspond to activation energies such as eq. (12). Such transitions in deforming processes can perhaps take place as the non-stoichiometry x in compounds like AB_x is varied by sufficient amount.

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