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Dislocations in paratellurite TeO_2 : elastic energies and plastic deformation

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Résumé. — La paratellurite TeO_2 a des propriétés élastiques exceptionnellement anisotropes. Cela lui confère d'intéressantes possibilités d'applications acousto-optiques, qui dépendent de sa perfection cristalline, d'où l'importance des dislocations dont les propriétés dépendent également de l'élasticité. Nous avons calculé l'énergie des dislocations ayant des vecteurs de Burgers $[100]$, $[110]$ et $[001]$; dans certains cas, elle est maximale pour le caractère vis au lieu d'être minimale en élasticité isotrope. Par compression à vitesse constante, on a provoqué le glissement de dislocations, la contrainte a été appliquée le long de $[110]$, $[221]$, $[100]$ et $[001]$. Les cristaux de TeO_2 étaient fragiles au-dessous de 400°C (0,7 de la température de fusion). Les études macroscopiques (microscopie optique, topographie de rayons X) ont seulement permis d'observer des plans de glissement : $\{100\}$, $\{001\}$, $\{110\}$ et $\{101\}$ semblent être activés, les vecteurs de Burgers $\langle 010 \rangle$ et $\langle 110 \rangle$ ont été déduits.

Abstract. — Paratellurite TeO_2 is a crystal with exceptional anisotropic elasticity. This is the origin of interesting acousto-optical applications ; as they depend on crystalline perfection, dislocations are of particular importance and their properties are also directly linked to elasticity. We have calculated the energy of dislocations with $[100]$, $[110]$ and $[001]$ Burgers vectors : in some cases, it is maximum for screw character, instead of minimum for an isotropic medium. Constant strain rate compressions have been performed to induce dislocation glide ; the stress was applied along $[110]$, $[221]$, $[100]$ and $[001]$. TeO_2 crystals were brittle below 400°C (0.7 melting temperature). Macroscopic observations (optical microscopy, X ray topography) could only give information about slip planes : $\{100\}$, $\{001\}$, $\{110\}$ and $\{101\}$ seem to be activated. The existence of $\langle 010 \rangle$ and $\langle 110 \rangle$ Burger's vectors is suggested.

1. Introduction.

Single crystals of paratellurite (TeO_2) have excellent acousto-optical properties [1]. Their acousto-optical figure of merits for the slow shear mode is the highest known value for the visible region and it can be grown in high quality by the Czochralski method [2, 3]. Recently it has been concluded that the easiest method of characterization of TeO_2 single crystals involves the measurements of their internal stresses [4].

A crucial problem for the use of TeO_2 in different devices is the level of the acoustical losses in the crystal. It was shown that the dislocation density correlates with ultrasound attenuation in TeO_2 [5].

Moreover, the mechanical field of dislocations can disperse the slow shear mode of paratellurite due to its extremely high anisotropy in the $[110]$ direction. The same high anisotropy is likely to play a dominant role on dislocation properties ; e.g. their self-energy and stress field may determine the glide elements and the strength of obstacles to dislocation motion, instead of the anisotropy of the Peierls forces which is related to chemical bond strengths.

The crystal structure of paratellurite is tetragonal ($a = 0.48 \text{ nm}$, $c = 0.76 \text{ nm}$) ; it can be deduced from the rutile structure by stacking two unit cells along the $[001]$ axis. An additional distortion corresponds to a small displacement of Te atoms perpendicular to

[001] and a larger one for oxygen atoms (relative displacement 7 %) along [001] [6].

At room temperature, paratellurite has a ferro-elastic phase transition under about 900 MPa hydrostatic pressure. As it was pointed out in [7], the phase transition is reached at this pressure P due to the fact that the elastic shear modulus $C_s = (C_{11} - C_{12})/2$, which is already small at normal pressure, is vanishing because of $\frac{dC_s}{dP} < 0$ (though the value of $\left|\frac{dC_s}{dP}\right|$ is not especially large). Using the theory of anisotropic elasticity, we computed the dislocation stresses to see if some phase transition in the neighbourhood of the dislocation line can be predicted since such phase transition would have an impact on the dislocation mobility.

We have calculated the elastic energy factor Kb^2 for different dislocation orientation and Burgers vectors to determine the more probable slip systems. This approach has been partly successful in calcite [8] or rutile [9].

We have then deformed TeO_2 single crystals to determine the slip planes and slip directions and compare them to the theoretical predictions. Plastic deformation could be achieved only at high temperature ($T > 0.7 T_M$ where the melting temperature $T_M = 733^\circ\text{C}$) making optical observation of surface slip steps difficult and unreliable. We have therefore also used X-ray topography by the Berg-Barrett method.

2. Elastic energy calculations.

2.1 GENERAL PRESENTATION. — The computations of the elastic energy and the dislocation stresses were carried out using the well known linear elastic theory of dislocations in anisotropic materials.

The stresses around dislocations were computed by the formula (13-92) of Hirth and Lothe [10] :

$$\sigma_{ij} = \text{Re} \left[\left(-\frac{1}{2\pi i} \right) \sum_{k,n=1}^3 B_{ijk}(n) A_k(n) D(n) \eta_n^{-1} \right]. \quad (1)$$

The elastic energy E per unit length of a dislocation line in an anisotropic crystal is given by :

$$E = \frac{Kb^2}{4\pi} \ln \frac{R}{r_0} \quad (2)$$

where r_0 and R are the integration boundary limits [10].

The energy factors Kb^2 were computed from the formula (13-93) of Hirth and Lothe [10] :

$$Kb^2 = \sum_{i=1}^3 b_i \text{Im} \left[\sum_{k,n=1}^3 B_{i2k}(n) A_k(n) D(n) \right]. \quad (3)$$

These calculations are not taking into account the influence of the dislocation core which requires interatomic potentials to be used; this somewhat limits the validity of our results. However, we do not think

that an atomic approach would change considerably the implications of the calculations which stems from the very high anisotropy of TeO_2 elastic properties.

The computation was carried out with elastic tensors at room temperature and 450°C , the second one being obtained by an extrapolation of the temperature dependence data of the stiffness constants of Ohmachi and Uchida [11].

2.2 RESULTS. — We made an estimation of the elastic anisotropy of TeO_2 by calculating the ratio Y_M/Y_m of the maximum to minimum Young modulus. It was found equal to 11.3, a value much larger than those found for minerals regarded as very anisotropic e.g. orthopyroxene ($Y_M/Y_m = 1.4$), olivine ($Y_M/Y_m = 1.7$), quartz ($Y_M/Y_m = 1.9$) and calcite ($Y_M/Y_m = 2.9$) [12]. TeO_2 is an extreme case and we can expect some specific dislocation properties related to its elastic anisotropy.

The stress field around different types of dislocations was such that the phase transition at high hydrostatic pressure was achieved only in the very neighbourhood of the dislocation line, that is at distances of about $3b$ (b = length of Burgers vector) or smaller where linear elasticity is not valid. This phase transition would take place in the small volume in compression e.g. on the side of the « extra half-plane ». This is not enough evidence to conclude that, at normal pressure, the dislocations can cause a phase transition at their core. In our experimental conditions, we did not detect any effect which could be related to it.

In table I, we summarize the minimum energy factors Kb^2 for different Burgers vectors and the corresponding dislocation line orientations. As it can be seen, the results practically do not change between room temperature and 450°C as can be expected from the small differences between C_{ij} .

The paratellurite has a crystal structure very similar to rutile (TiO_2). Therefore, we have listed in table I the partial dislocations $1/2[001]$, $1/2[021]$ and $1/2[221]$ which would be perfect in the rutile lattice — [001], [011] and [111] respectively. The energy factors increase with the length of the Burgers vectors, with the exception of the [110] Burgers vector where a 40 % increase in length from [100] to [110] gives a 3 % decrease in energy. This is obviously due to the small shear modulus in (110) planes.

In figures 1 and 2, the energy factors belonging to different expectable slip systems are shown. The variation of Kb^2 for different slip planes is not too large for [100] and [001] Burgers vectors (Fig. 1). On the contrary, for $b = [110]$, the anisotropy is very large as expected from the peculiar elastic properties of TeO_2 for shear modes in {110} planes. The minimum to maximum ratio is about 3 (Fig. 1), much larger than in TiO_2 (where it is smaller than 1.1 [9]) and calcite [8]. The energy minimum for $u = [001]$ (Fig. 1) corresponds to a (110) slip plane and it seems reasonable that this effect dominates any core influence on the determination of the slip plane.

Table I. — Minimum energy factors and corresponding type of dislocations for various short Burgers vectors in paratellurite TeO_2 .

b	b nm	RT	$T = 450^\circ\text{C}$	R.T. and 450°C	
		$[Kb^2]_{\min}$ $10^{-10} \text{ J.m}^{-1}$	$[Kb^2]_{\min}$ $10^{-10} \text{ J.m}^{-1}$	dislocation characteristics type u	
[100]	0.48	36.8	35.7	edge	[001]
[110]	0.68	35.9	37.1	screw	
[001]	0.76	155.9	150.6	screw	
[011]	0.90	190.7		mixed ~	[001]
[111]	1.02	216.6		mixed	[112]
$1/2[001]$	0.38	39		partial, screw	
$1/2[021]$	0.61	75.3	72.9	partial mixed	[001]
$1/2[221]$	0.78	89.6		partial, ~ screw

Fig. 1. — Energy factor Kb^2 variations of pure edge dislocations for three Burgers vectors in TeO_2 . U refers to the line directions. In an isotropic elastic medium, there is no variation. The minima suggest possible slip planes.

The energies of $[110]$ dislocations in $\{1\bar{1}0\}$ planes (Fig. 2b) are related to $C_s = (C_{11} - C_{12})/2$ which is small. They vanish for $C_s \rightarrow 0$ at the phase transition, i.e. the lower curve in figure 2b goes to zero, giving vanishing energy for dislocations in the $(1\bar{1}0) [110]$

slip system. For the same reason, it was found that the energies of $[100]$ edge dislocations gliding in (010) can go to zero (Fig. 2c). One can see another interesting consequence of the high anisotropy i.e. the screw dislocation energy is larger than that of edge or mixed ones in the $(001) [100]$ (Fig. 2a) and $(010) [100]$ (Fig. 2c) slip systems. There is also an extraordinary large ratio of energy between edge and screw dislocations in the $(001) [110]$ slip system (Fig. 2a). This ratio is about 6, when for isotropic elasticity it is $1/(1 - \nu) \sim 1.4$. It is therefore likely that this $(001) [110]$ slip system cannot be activated.

From elastic energy point of view (Fig. 2), the more likely slip systems are $\{1\bar{1}0\} [110]$, $\{010\}$ and (001) with the same slip direction $\langle 100 \rangle$. This assumes perfect dislocations and does not take into account possible dissociations, in particular of dislocations with Burgers vectors having a component along $[001]$; they may give rise to two partials, which are perfect dislocations in the corresponding rutile structure, the associated stacking fault being possibly small.

3. Plastic deformation.

3.1 SPECIMEN PREPARATION. — Single crystals have been grown by the Czochralski technique from 5 N purity raw material [2, 3]. The growth axis was $[110]$. Specimens were then cut from the boules using X-ray diffraction for orientation (precision 0.5°).

They had various sizes to allow easy identification of orientations; the smallest ones were $2.5 \times 3.4 \times 7.8$ mm and the largest were $4.4 \times 4.5 \times 9$ mm. The stress σ was applied along the greatest dimension. The lateral faces were mechanically polished using Linde alumina paste down to $0.3 \mu\text{m}$.

In view of the various possible slip systems, specimens with four different stress orientations were cut (Fig. 3). The stress axis $[110]$ should allow to activate glide along $[100]$ and $[010]$, the shortest repeat distance of the structure (Table I); for $\sigma \parallel [100]$, the next close-packed directions $[110]$ and $[1\bar{1}0]$ should be activated.

Fig. 2. — Energy factor Kb^2 variations with the character of dislocations for various possible slip systems in TeO_2

- a) slip plane (001) Burgers vectors [100] or [110]
- b) slip plane (110) Burgers vectors [110] or [001]
- c) slip plane (010) Burgers vectors [100] or [001]

$\sigma \parallel [221]$ allows to check for a possible [001] slip direction. Finally, the direction [001] was chosen to check if paratellurite had some similarity with rutile where the slip system $\{101\} \langle \bar{1}01 \rangle$ is the most easily activated [13]. In this case, samples with $\{010\}$ or $\{110\}$ lateral faces have been prepared (Fig. 3). Specimens have been tested, either as-grown, or after an anneal of 10 h at 620 °C in air; no major influence on plastic properties was detected. The crystalline perfection has been assessed by X-ray reflection topography. The image of the as-polished specimens was almost uniformly grey. This means that there is no sub-boundaries nor misorientations larger than $24'$ which is the divergence of the X-ray beam used for Berg-Barrett examination. As the crystal perfection was very good, double crystal topography could also be used.

Fig. 3. — Various specimens with compressive stress orientations and lines corresponding to various slip systems.

3.2 DEFORMATION EXPERIMENTS. — All mechanical tests have been run in air, the samples being compressed between two alumina rams. Above 630 °C, it was necessary to insert platinum foils to avoid melting at the contact between TeO_2 and Al_2O_3 . The tests were performed in an Instron-machine at a constant cross-head velocity of 20 $\mu\text{m}/\text{min}$ ($\dot{\epsilon} \sim 3$ to $4 \times 10^{-5} \text{ s}^{-1}$) with the set-up already used in previous studies [14]. Stress relaxations were also recorded after stopping the cross-head motion. A few typical stress-strain curves are shown in figure 4. It can be seen that the softest direction is [221] while the hardest is [001]. Small yield drops are observed for $\sigma // [221]$, even when reloading after initial deformation. For $\sigma // [110]$ there was no yield drop except for annealed specimens. For compression along [100], the $\sigma - \epsilon$ curves display large maxima similar to those observed in covalent crystals at low temperature [15]. Finally, for the hardest direction [001], the stress changes gradually from the elastic to plastic regime. The $\sigma - \epsilon$ curves exhibit a linear work-hardening stage at $\epsilon \sim 2\%$, with $\theta = d\sigma/d\epsilon$ values at $T > 450$ °C of 360 MPa for $\sigma // [110]$ and 700 MPa for $\sigma // [221]$.

We take the stress at the onset of plastic deformation as the ratio of the applied load to initial surface for a deformation of $\epsilon = 0.2\%$, $\sigma_{0.2}$; when there is a yield drop, the upper and lower stresses, σ_U and σ_L have been taken. They are plotted in figure 5. It was not possible to deform TeO_2 single crystals below 400 °C ($0.67 T_M$) even after predeformation. Some cleavage along $\{100\}$ was easily induced in specimens stressed along [001]; along this direction a very large yield stress has been found at 685° ($0.95 T_F$) (Fig. 5). For

Fig. 4. — Engineering stress (σ) versus engineering strain (ϵ) for compression of TeO_2 crystals at various temperatures along different directions $\dot{\epsilon} \sim 4 \times 10^{-5} \text{ s}^{-1}$.

specimens loaded along [110] and [221], the $\sigma - T$ variations look similar, suggesting that the same slip system has been activated. Analysing stress relaxations gives information on the thermal activation of the deformation process and therefore, on the obstacles to dislocation motion. We use the equation :

$$\dot{\gamma} = \dot{\gamma}_0 \exp\left(-\frac{\Delta H - V\tau}{kT}\right) \quad (4)$$

where $\dot{\gamma}$: shear strain rate

τ : shear stress

$\tau = \sigma f$ where f is the Schmid factor

V : « activation volume ».

If $\dot{\gamma}_0$, ΔH and V are constants, it can be shown that during relaxation, the stress is related to time t by the relation :

$$\tau = -\frac{kT}{V} \ln(t + C) + D \quad (C \text{ and } D \text{ constant}). \quad (5)$$

Fig. 5. — Yield stress ($\sigma_{0.2}$, σ_u , σ_l) versus temperature (T) for various orientations of σ . The straight lines connecting points at various T mean that the same specimen has been deformed. The curves drawn through the data were calculated to be : $\ln \sigma = -0.0107 T + 12.04$ for $\sigma \parallel [221]$; and $\ln \sigma = -0.0074 T + 10.01$ for $\sigma \parallel [110]$; σ in MPa and T in K. T_M is the melting temperature. F is to indicate that the specimen was fractured during the test.

We have plotted τ versus $\log t$ which is linear for $t \gg C$. Using the parameters σ (initial stress of relaxation test) and Vf , further analysis can be done : fits for the data from $\sigma \parallel [110]$ and $[221]$ can respectively be described by the equations :

$$\sigma = 10 + 8 \times 10^{-26} (Vf)^{-1} \quad (6)$$

$$\sigma = 5 + 8 \times 10^{-26} (Vf)^{-1} \quad (7)$$

For the four orientations tested, the values of Vf at 600 °C are all of the order of $2 \times 10^{-27} \text{ m}^3$ which for $f = 0.5$ corresponds to about $20 V_{uc}$ ($V_{uc} = 1.75 \times 10^{-28} \text{ m}^3$, unit cell volume). This represents the magnitude of the volume involved when a dislocation overcomes an obstacle.

3.3 SPECIMEN OBSERVATIONS.

3.3.1 Optical observations. — Optical observations provide normally the easiest way to determine the elements of slip. The shape of the crystal after large deformations ($\epsilon \sim 10\%$) gives indications on the slip direction. We never observed symmetrical deformation, either because only one slip direction was active, or because of mechanical instability leading to buckling. Slip steps are not easy to observe after high temperature deformation. Moreover, some thermal grooving may occur and be misleading. We could draw the following conclusions :

For $\sigma \parallel [110]$, the $(1\bar{1}0)$ lateral face of the specimen remained flat. This suggests a slip direction contained in this plane i.e. a $\langle hhl \rangle$ direction.

For $\sigma \parallel [221]$ samples were twisted. On the $(1\bar{1}0)$ faces, only the lines at 30° from $[221]$ were visible (Fig. 3). They correspond to (001) slip plane.

For $\sigma \parallel [100]$, the (001) face remained flat suggesting

a $[hko]$ slip direction : as slip steps are parallel to $[001]$, this makes $\{hko\}$ slip planes likely.

For $\sigma \parallel [001]$, samples were strained to very small values (Fig. 4) which prohibited shape analysis. Horizontal steps were observed in (010) and (100) faces which led to assume (okl) and (hol) slip planes.

Optical observations helped but nevertheless did not give enough information to determine the glide elements of TeO_2 .

3.3.2 X-ray topography. — Berg-Barrett topography can give further information on the plastic deformation. X-ray copper radiation has been used, with an experimental method already described in previous papers [16, 17]. The intensity of the beam reflected by a single crystal can be modified in two cases :

(i) When there is a misorientation due to different grains or subgrains. The image can disappear or else the images can exist but overlap or separate; this is called orientation contrast, the image displacement giving rise to a grey or white contrast.

(ii) When a distorted reflecting plane is used the intensity can be increased [17]. This is called extinction contrast. It is the case for internal stresses due to dislocations which give a black contrast. Therefore, when imaging e.g. with a plane containing the dislocation Burgers vector, no contrast is expected. This rule has been observed in the case of single slip, but some trouble arose for multiple slip [16]. Furthermore, this kind of visibility criterion is valid only for isotropic elastic crystals. In the case of paratellurite, it has to be used with some caution since as, shown above, the elastic anisotropy is fairly large.

$\sigma \parallel [110]$:

Figure 6 shows features which are related to plastic deformation. Black lines are generally surrounded by white regions : this is due to extinction contrast associated with dislocations while resulting misorientation gives orientation contrast. It was not possible to obtain diffraction conditions giving a vanishing of the black contrast to determine the Burgers vector. The observations (Fig. 6a and 6b) suggest, that the slip planes are (100) and (010) . Our previous optical observations lead us to assume a $\langle hhl \rangle$ slip direction which would then be the $[001]$ direction. This slip direction cannot be activated since it is perpendicular to σ . Buckling was probably due to mechanical instability with activation of secondary slip systems. We then assume that the slip directions are $[100]$ and $[010]$. The dislocation emergences in the $(1\bar{1}0)$ face are therefore pure screw and explain the intense cross-slip observed in figure 6b. It is very likely that the slip systems activated are $(100) [010]$ and $(010) [100]$, previous elastic considerations (§ 2.2) justifying the Burgers vectors.

$\sigma \parallel [221]$:

Extinction contrast associated with dislocations was seen on both faces. On the $(1\bar{1}0)$ face we observed

Fig. 6. — Berg-Barrett topograph of TeO_2 deformed along $[110]$. $T = 546^\circ\text{C}$, $\varepsilon = 1\%$. a) (001) face, g $[004]$. Black lines are due to extinction contrast, white regions to orientation contrast. b) $(1\bar{1}0)$ face, g $[2\bar{2}0]$. The wavy aspect of the lines is due to cross slip of dislocations. The different horizontal and vertical scales take into account the fact that the film is parallel to the incident beam but not to the sample. Black lines correspond to enhanced reflections.

traces at 60° from $[221]$, i.e. approximately parallel to $[001]$ and also at 30° from $[221]$, that is approximately parallel to $[110]$ and perpendicular to the previous ones (Figs. 3 and 7). Slip traces at about 40° from $[221]$ were seen on the (114) face. Many slip planes may correspond to these traces. To clear completely the problem, a specimen was cut in order to make observations in (001) and (100). Figure 8a shows traces parallel to the $[100]$ and $[010]$ directions in the (001) plane while figure 8b shows traces parallel to $[010]$ in the (100) plane. Slip planes can therefore be (010), (100) and (001). However the different aspect of the topographies as well as further considerations led us to assume (001) as slip planes and (010) and (100) as dislocation walls.

$\sigma // [100]$:

The lines on the face (010) (Fig. 9a) correspond to the steps observed by optical way. In the orthogonal (001) face (Fig. 9b), features at about 45° to σ could be seen,

Fig. 7. — Berg-Barrett topograph of TeO_2 deformed along $[221]$ first at 537°C , then 461°C , with $\varepsilon = 1.5\%$. $(1\bar{1}0)$ face. a) g $[2\bar{2}0]$, b) g $[310]$.

Fig. 8. — Berg-Barrett topograph of the sample shown figure 7 : a) (001) cut, g $[004]$; b) (100), cut, g $[302]$.

Fig. 9. — Berg-Barrett topograph of TeO_2 deformed along $[100]$. $T = 599^\circ\text{C}$, $\varepsilon = 4\%$. a) (010) face, g $[032]$; b) (001) face, g $[106]$.

although in some cases a single operative slip system lead to an asymmetry of the sample shape. These features correspond to $(\bar{1}\bar{1}0)$ and (110) slip planes. The extinction contrast observed in the (001) face using (106) diffracting planes disappears using (004) diffracting planes. This supports the conclusion that $[110]$ and $[\bar{1}\bar{1}0]$ slip directions were operative in the slip planes (110) and $(\bar{1}\bar{1}0)$. Dislocations emerging in the (010) face have a screw character; this is in good agreement with the cross-slip activity which has been observed (Fig. 9a).

$\sigma // [001]$:

X-ray topography shows steps parallel to $[010]$ and $[100]$ on (100) and (010) faces. The other samples with (110) faces could not provide conclusive informations. Some doubt arose for attributing the steps to slip traces taking into account the very high temperature (630°C) for plastic deformation. Cut parallel to (001) in the middle of the sample confirm the intersection with slip planes (011) and (101) . New cuts of these samples parallel to (110) exhibit traces nearly parallel to $[\bar{1}\bar{1}0]$; the glide planes are therefore almost perpendicular to the $[001]$ axis.

4. Discussion.

4.1 SLIP SYSTEMS. — At this stage our conclusions about the slip planes as deduced from optical and X-ray topography observation, are summarized in table II; slip directions and C.R.S.S. values were further considered.

Let us now examine the results of table II in view of the dislocation energy calculations (Sect. 2) and the mechanical data (Sect. 3.2).

4.2 GLIDE SYSTEMS AND DISLOCATION ENERGY CALCULATIONS. — The predictions of glide elements from dislocation elastic energy calculations have not been very successful in covalent compounds like sapphire [18], rutile [9], or calcite [8]. It seems that the choice of slip planes may be determined by the details of chemical bonding i.e. by the core energy, rather than by the minimum elastic energy. However, TeO_2 is so anisotropic that the elastic approach should give

realistic insight on *perfect* dislocation activity. It can hardly be safely extended to the case where dissociation is involved since the energy of dislocations can substantially be reduced, as observed for instance in sapphire [18, 19].

For TeO_2 , the three slip systems predicted by calculations (see Sect. 2, Figs. 1 and 2), have been observed :

— For $\{\bar{1}\bar{1}0\} \langle 110 \rangle$ and $\{010\} \langle 100 \rangle$, cross-slip was observed (Figs. 9a and 6b respectively) indicative of the screw character of probably undissociated dislocations. The energy factor is, however, minimum in the first case (Fig. 2b) and maximum in the second case (Fig. 2c); this does not seem to influence the cross-slip behaviour of screw dislocations.

— The third predicted system $(001) [100]$ (Fig. 2a) can be activated only for $\sigma // [221]$ which is the only orientation with non-zero Schmid factor (Table III). It may have been observed for $\sigma // [221]$. However, the slip direction could not be determined by observation of slip steps.

Finally, in the case of $\sigma // [001]$ large energy perfect dislocations have to be activated. Possible simple Burgers vectors are $\langle 011 \rangle$ or $\langle 021 \rangle$. They correspond to dislocations with large elastic energies (Table I), which would therefore dissociate according to reactions such as :

$$[011] \rightarrow 1/2[021] + 1/2[001] \quad (8)$$

$$[021] \rightarrow 1/2[021] + 1/2[021] \quad (9)$$

The two partial dislocations introduced in reactions (8) and (9) are perfect dislocations of the rutile structure; a small stacking fault energy can be expected. However, we could not deduce these Burgers' vectors, as our Berg Barrett observations led us to assume $\{01l\}$ planes with $l \geq 4$ for $\sigma // [001]$.

4.3 GLIDE SYSTEMS AND PLASTIC DEFORMATION. — When deforming a crystal along different directions, we may activate the same slip system; then, the yield stresses (σ_1 or σ_2) must be in the inverse ratio of the Schmid factor f :

$$\frac{\sigma_2}{\sigma_1} = \frac{f_1}{f_2} \quad (10)$$

Table II. — *Slip systems and their corresponding critical resolved shear stress (CRSS) for TeO_2 compressed along various directions.*

$\sigma //$	slip planes	slip directions	600 °C CRSS (MPa)
$[110]$	$(100), (010)$	$[010], [100]$	17
$[221]$	(001)	$[010], [100]$	4.2
$[100]$	$(110), (\bar{1}\bar{1}0)$	$[\bar{1}\bar{1}0], [110]$	22
$[001]$	$(101), (0\bar{1}1)$	$[101], [011]$	
	$(101), (01\bar{1})$	$[101], [0\bar{1}1]$	

If there are different slip systems, with different critical resolved shear stresses (CRSS) and if a hard slip plane is activated, the shear stress on softer slip planes must always remain below their CRSS. We examine our results on these basis, with the Schmid factor values displayed in table III.

Specimens with $\sigma // [110]$ and $[221]$ have only a few cases with $f = 0$ (Table III). Moreover, their yield stress-temperature behaviours are similar (Fig. 5). Let us investigate the tentative conclusion that the same slip system has been activated, although the

Table III. — Schmid factors for different slip systems in the various types of specimens.

slip plane	slip direction	$\sigma //$			
		[110]	[221]	[100]	[001]
010	100	0.5	0.38	0	0
	101	0.27	0.46	0	0
	10 $\bar{1}$	0.27	0.05	0	0
	201	0.39	0.49	0	0
	20 $\bar{1}$	0.39	0.11	0	0
	001	0	0.30	0	0
001	100	0	0.30	0	0
	110	0	0.43	0	0
110	1 $\bar{1}$ 0	0	0	0.5	0
	001	0	0.43	0	0
	2 $\bar{2}$ 1	0	0.21	0.44	0
	22 $\bar{1}$				
10 $\bar{1}$	010	0.42	0.16	0	0
	101	0.23	0.19	0.45	0.45
101	010	0.42	0.48	0	0
	10 $\bar{1}$	0.23	0.07	0.45	0.45
10 $\bar{2}$	010	0.31	0	0	0
	201	0.24	0	0.49	0.49
102	010	0.31	0.47	0	0
	20 $\bar{1}$	0.24	0.14	0.49	0.49

$\sigma - \varepsilon$ curves show some differences (Fig. 4). The ratio of yield stress σ_1 , for $\sigma//[110]$ to σ_2 for $\sigma//[221]$ is between $1/(0.42)$ and $1/(0.58)$; we must search in table III the slip systems having $0.42 < f_1/f_2 < 0.58$ for the two σ directions. The only case which suits this requirement is $\{010\} \langle 101 \rangle$.

The $\{010\} \langle 101 \rangle$ slip system can explain only part of the lines observed for specimens with $\sigma//[221]$ (Figs. 7, 8) and $\sigma//[110]$. In the latter case, the $\langle 101 \rangle$ Burgers vector does not allow to explain the wavy lines (Fig. 6b) by cross-slip which is the most common explanation for such a feature. Finally, such a Burgers vector corresponds to large energy dislocations (Table I) requiring dissociation possible according to reaction (8), but which would render difficult slip out of the primary glide plane. We therefore conclude that different slip systems have been activated for $\sigma//[221]$ and $\sigma//[110]$. As we had experimental evidence for the $\{100\} \langle 010 \rangle$ system in the case of $\sigma//[110]$, we can hence eliminate this system for $\sigma//[221]$ which comforts our previous suppositions for $\{100\}$ as dislocation walls.

We have computed the CRSS values using f from table III and slip systems from table II. The results at 600 °C where we have a large number of data, are reported in table II. The CRSS values for $\sigma//[221]$ are the smallest; the (001) $\{010\}$ slip system gives a Schmid factor equal to zero for all other σ directions (Table III). It cannot be activated for any other σ orientation. The next CRSS values are for $\sigma//[110]$ and $[100]$: for $\sigma//[110]$ the slip system is $\{100\} \langle 010 \rangle$;

it has $f = 0$ for the other stress orientations except for $\sigma//[221]$ where the resolved shear stress on $\{100\} \langle 010 \rangle$ is 5.3 MPa at yielding, below its CRSS (Table II). For $\sigma//[100]$, the slip system is (110) $[1\bar{1}0]$; it can have $f \neq 0$ only for this stress orientation (Table III). Our results displayed in table II are therefore coherent in terms of mechanical data and slip systems.

4.4 DEFORMATION MECHANISM. — We now discuss the possible obstacles to dislocation glide for $\sigma//[110]$, $[221]$ and $[100]$ specimens. As we have only a limited amount of mechanical data (Fig. 5), we shall not detail too much the question. The brittleness of TeO_2 at $T < 0.7 T_M$ is a quite general observation for covalent compounds [20]. It is then expected that dislocation mobility is dominated by overcoming Peierls stress. There is no satisfactory description of the periodic variation of Peierls stress in the slip plane, especially in a compound. However, there are many models for the thermally activated glide of dislocations. A form with general validity for the activation energy ΔG in the equation of deformation is [21]:

$$\Delta G = U_0(1 - \sigma/\sigma_0)^\beta \quad (U_0 \text{ and } \beta \text{ are constant}). \quad (11)$$

One consequence of equation (11) is that the activation volume $V = (\delta \Delta G / \delta \sigma)$ decreases with increasing σ and reaches zero when $\sigma = \sigma_0$ (σ_0 is

the Peierls stress). This trend has been observed for $\sigma // [221]$, $[110]$ and $[100]$. A representation of ΔG can be obtained from equations (6) and (7) by integration, following the procedure used in reference [14]; it gives a linear relation between $\ln \sigma$ and T , as suggested in figure 5. Mechanical data are, therefore, consistent with a Peierls mechanism for the plastic deformation of TeO_2 .

5. Conclusions.

Paratellurite TeO_2 shows a large plastic anisotropy which is not dominated by the anisotropy of Peierls stresses as it is usually the case for such brittle covalent compound. The large elastic anisotropy permits to explain the slip systems on the basis of minimum elastic energy for dislocations. The analogy with the

rutile structure is not so obvious as $\{102\} \langle 201 \rangle$ glide planes were not directly determined. The determination of slip directions or Burgers' vectors of gliding dislocations will be completed by transmission electron microscopy studies.

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