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POINT DEFECT - DISLOCATION INTERACTION IN MgO

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Abstract.- Amplitude Dependent Internal Friction has been measured from 77 K to 593 K in MgO single crystals plastically deformed at room temperature. Experimental results have been tested with several theoretical models of dislocation breakaway. A reliable value of interaction energy (0.5 eV) is deduced from the model of Teutonico, Granato and Lücke, but only a partial agreement between experimental results and the model is obtained. For that reason, a numerical analysis of thermomechanical breakaway has been undertaken.

1. Introduction.- Different behaviours of mobile dislocations in MgO single crystals plastically deformed at Room Temperature (R.T.) have been presented in previous papers [1], [2]. Among these aspects, one of the most important is the high sensitivity of Internal Friction (IF.) to annealing; for treatments above RT., the level of the IF. spectrum decreases very quickly as annealing temperature increases. Such a reduction of IF. has been already explained by pinning of dislocations with migrating point defects. In our last paper [3], we tried to apply - in order to determine binding energy between pinning point defects and dislocations - the classical theoretical models (reviewed by Pérez et al. [4]) (such as the models of Granato and Lücke [5], Saul and Bauer [6], Friedel [7]; Teutonico, Granato and Lücke (TGL.) [8]). For the most part, these models did not fit correctly our results along the whole temperature range; besides, the different values of dislocation-point defect interaction energy U_0 , deduced from the few measurements consistent with these models, seemed to be unreliable except for the model of TGL ($U_0 = 0.5$ eV).

New experiments have been performed for the present paper and now the theoretical models have been tried on computed local internal friction data. However none of those models fit exactly experimental results. About the TGL model, partial agreement is obtained in the low temperature range. This fact could be due to the thermal breakaway of other species of pinning points activated in the higher part of temperature range. Moreover these two temperature parts seem to overlap one another making more complex the dissociation of these various processes and their understanding.

For this reason, numerical analysis of thermomechanical breakaway has been undertaken involving various parameters such as interaction energy U_0 , average loop length, number of pinning points. Amplitude dependent Internal Friction Δ_H is calculated as a function of stress σ for a given temperature. Such a calculation is

obtained from the statistical depinning and repinning of a dislocation along which several pinning points are non regularly located. Depinning and repinning energies, for each pinning point are determined from the energy diagram considering dislocation-point defect binding energy, tension line and stress work. Then, the results of that numerical analysis are compared to experimental measurements.

2.- Experimental results.- Detailed experimental conditions have been described

elsewhere [3]. Experimental results are presented using the real Local Amplitude Dependent Internal Friction Δ_{HL} corresponding to the strain amplitude ϵ . Δ_{HL} is deduced from amplitude dependent Internal Friction Δ_H (experimentally measured) by the Lazan's method [9] leading to the following relation :

$$\Delta_{HL} = \Delta_H + 0,77 \Delta_H \frac{\partial \Delta_H}{\partial \epsilon} + 0,11 \Delta_H^2 \frac{\partial^2 \Delta_H}{\partial \epsilon^2}$$

For example, Figure 1 shows the large difference between Δ_H and Δ_{HL} plotted versus ϵ . For each annealing temperature (293 K, 366 K, 429 K, 521 K, 593 K), a set of $\Delta_{HL}(\epsilon)$ curves are plotted for measurements performed between 77K and the annealing temperature. Two of these sets of curves are presented in Figures 2 and 3 respectively for the annealing temperatures 293 K and 593 K. Thermal activation of depinning, already observable on Figures 2 and 3, is particularly pointed out by the plot of Δ_{HL} versus temperature at constant strain amplitude ϵ presented on Figure 4. Such $\Delta_{HL}(T)$ curves are obtained from data of Figure 2.

Fig. 2 : After plastic deformation at 293K, variations of Δ_{HL} versus ϵ at various temperatures a : 77K, b : 102K, c : 151K, d : 183K, e : 240K, f : 293K.

Fig. 1 : Difference between measured Δ_H and computed Δ_{HL} by Lazan's method.

Fig. 3 : After annealing at 593 K, variations of Δ_{HL} versus ϵ at various temperatures. a : 77K, b : 105K, c : 133K, d : 193K, e : 246K, f : 425K, g : 523K.

Fig. 4 : After plastic deformation, variations of Δ_{HL} versus T at various strain amplitudes. a : 5.10^{-6} , b : 10^{-5} , c : $1.5.10^{-5}$, d : 2.10^{-5} , e : $2.5.10^{-5}$, f : 3.10^{-5} .

Discussion : All the experimental results show obviously that thermal activation is already operative at 77K. So, only thermally activated models have been tested. For instance the model developed by Saul and Bauer leads to the following expression for Δ_{HL} .

$$\Delta_{HL} = \Delta_0 (1 + \sigma v / kT) \exp \left\{ - U_0 / kT \right\}$$

where σ is the resolved shear stress acting on a dislocation

v is the activation volume

Δ_0 is the relaxation strength factor.

This relation is available for early states of depinning. i.e. for the case where the fraction of unpinned loops. $f(t)$ is very small ($f(t) \ll 1$) and for high temperature ($\sigma v \ll kT$). Then, Δ_H is expected to vary exponentially with $\frac{1}{T}$. Experimental results fit only partially this model; the value of interaction energy U_0 deduced from this partial agreement is too small (0.1 eV) comparatively to the temperature range along which thermal activation is operative.

In fact the model of TGL is the most important one that we have used. According to this model, a triangle force-distance law gives a rather good approximation for all stress levels and leads to the activation energy for breakaway :

$$U = U_0 (1 - \sigma/\sigma_H)^2$$

with U_0 interaction energy
 σ_H mechanical depinning stress.

Along the temperature range where the TGL model 10 is valid, such a relation allows us to expect a linear variation of strain amplitude ϵ ($\epsilon = \frac{\sigma}{E}$) as a function of $T^{1/2}$ for a given level of Δ_{HL} . Besides, a critical temperature T_C can be determined by the intercept of this straight variation with temperature axis i.e. for zero stress. The mathematical development of this model [9] links such a critical temperature T_C to interaction energy U_0 with the following relation :

$$U_0 \approx 23 \text{ k } T_C$$

Fig. 5 : Variation of ϵ versus $T^{1/2}$ for the same level of Δ_{HL} (10^{-3}) and for various annealing states. a : 293K, b : 366K, c : 429K, d : 521K, e : 593K.

In order to get a more extensive analysis of these experimental results, a numerical analysis of internal friction Δ_H due to dislocation breakaway has been undertaken extending a study developed by Vincent et al. [11].

Basically, the same triangle force-distance profile (determined in the TGL model) have been applied to interaction between a dislocation and each of its pinning points assumed to be of the same species. The configuration of a pinned dislocation chosen for this calculation is presented on Fig. 6. The central part is

Figure 5 shows variation of experimental strain amplitude ϵ versus $T^{1/2}$ for a given level of internal friction Δ_{HL} (10^{-3}) and for different annealing states. Only along the low temperature part, experimental data seem to be consistent with the predicted results of the model. All these extrapolated straight lines determine an approximated critical Temperature T_C of 250K which leads, using the preceeding relation, to an interaction energy $U_0 \approx 0.5 \text{ eV}$. About the high temperature part, the TGL model is no more verified. This deviation could be due either to the interaction of dislocations with another type of pinning point, or to the fact that the TGL model is no more valid in this temperature range.

pinned like a symmetrical double loop and the other pinning points are regularly spaced.

Fig. 6 : Configuration of a pinned dislocation

A reliable value for interaction energy U_0 (0.5 eV) is chosen and then, activation energies for depinning U_D and repinning U_R for each pinning point are computed assuming that the dislocation depinning starts from the largest loop and continues one point at a time. U_D , U_R are computed by the relations (1),(2):

$$(1) U_D \propto A U_0 (1 - \sigma/\sigma_D)^2 ; \quad (2) U_R \propto B U_0 (\sigma/\sigma_R - 1)^2$$

where : A and B are coefficients depending upon several parameters which determine the dislocation configuration σ_D : mechanical stress for depinning
 σ_R : repinning stress.

Both of these stresses depend upon the number of each pinning point. The relations (1) and (2) are valid for $\sigma < \sigma_D$ and $\sigma > \sigma_R$. The rate theory allows to compute the area swept by dislocations and consequently the strain-stress cycle from which Δ_H is deduced.

Fig. 7 : σ/μ versus $T^{-1/2}$ at constant Δ_H

Figure 7 shows the first results of this calculation; the applied stress amplitude σ is plotted versus $T^{-1/2}$ at constant level of Δ_H . The main parameters are given hereafter :

- number of pinning points $N = 9$
- central loop length $L = 100b$ (b : Burger's vector)
- ratio $L/l = 2$.

Along the main part of the temperature range a linear plot is obtained. Such a result is consistent with the relations (1) and (2). Indeed, for an internal friction level, the depinned fraction (i.e. the depinning probability) is almost constant; thus we have :

$$U_D(\sigma)/T \approx C(\text{constant}) \rightarrow \sigma = \sigma_D(1 - C T^{1/2})$$

Unfortunately the critical temperature derived by extrapolation is about 480K which leads to about 1eV for interaction energy; such a value is not consistent with the value chosen for the computation.

Fig. 8 : Diagrams of energy for various stresses.

Furthermore the diagrams of energy presented on Figure 8a, b confirm that in the low temperature range, the thermally activated depinning of the first pinning point is sufficient to initiate the mechanical breakaway of the whole dislocation. Along the high temperature part Figure 8c shows that successive thermally activated depinnings are

necessary to trigger the whole breakaway. Then, the linearity of the TGL law $\sigma(T^{1/2})$ is naturally no more expected in these conditions. This result is consistent with the conclusion of Teutonico et al. [12]. Therefore, this work shows that the analysis of the experimental results according to the TGL model has to be confirmed. In order to fit better the experimental conditions, we must complete our calculation in particular including a distribution of different parameters (loop lengths for example).

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