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CONTINUOUS-DISTRIBUTION DISLOCATION MODEL OF INTERNAL FRICTION ASSOCIATED WITH THE INHOMOGENEOUS SLIDING ALONG HIGH-ANGLE GRAIN BOUNDARIES

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Abstract.— Basing on a continuous-distribution dislocation model of high-angle grain boundaries, an integral-differential equation governing the inhomogeneous sliding along the boundaries was set up. This equation consists of three terms. The first term is the shear stress produced by the dislocations with a given continuous distribution linear density, the second term is the applied shear stress and the third term is the Newtonian viscous resistant stress. This equation was solved approximately and the approximate formulae for the internal friction and modulus defect were obtained. For high-purity isotropic metals, the viscosity for grain-boundary sliding is correlated with the diffusion coefficient along grain-boundary, Dₚ, by an expression similar to Einstein-Stokes formula. The optimum temperature of grain-boundary internal friction peak for a number of pure metals calculated according to this model and sliding mechanism are fairly close to the corresponding experimentally observed values. It is shown that for impure metals, the viscosity of some grain boundaries is considerably changed by the selective segregation of impurities along them, so that another internal-friction peak (the solute peak) appears at a different temperature. Also, in anisotropic pure metals and in the presence of internal stress, the migration of grain boundaries may cause another high temperature internal-friction peak or a higher internal-friction background in addition to the grain-boundary peak associated with grain-boundary sliding.

I. Introduction.— Using a torsion pendulum, Kê observed in polycrystalline 99.991 % Al an internal-friction (IF) peak around 285°C (f = 0.8 Hz) which was absent in fully annealed bamboo structure "single crystals" /1/. He therefore attributed this peak ("grain-boundary peak") to a relaxation process in the grain boundaries. Recently, Woirgard et al /2/ reported that a notable relaxation effect is present in slightly strained Cu single crystals in the same temperature range as the grain-boundary (GB) peak in polycrystals and also a very weak relaxation effect in unstrained Al single crystals. They concluded that the GB peaks must be explained by mechanisms which are not specific of the GB itself, but involve more generally the climb and glide of lattice dislocations. Similar proposition has been made by Gondi et al /3/. They reported that single crystals or macrocrystalline sheets of 99.6 % Al

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show IF instabilities in the temperature range of the K\& peak, and slight deformations of these specimens cause the K\& peak to appear. The possibility is considered that the K\& peak depends on free or polygonized dislocations inside the grains. The present report will suggest a concrete dislocation model illustrating that the GB peak (or the so-called "K\& peak") can be associated with a relaxation process in the GB itself.

It is evident that any realistic mechanism of the GB peak must conform to the structure of the high-angle grain boundaries. The coincidence superlattice model of high-angle GB recently proposed was very successful in explaining many properties of high-angle grain boundaries /4/. A close approach to the coherency condition can be achieved for high-angle boundaries with a periodic segmented structure and there is a region where the "fit" is relatively good and one where it is poor. This is basically similar to the early models put forward by Kröner /5/ and by Mott /6/ for explaining the assumed viscous behavior of high-angle grain boundary in atomistic terms. It has been pointed out that the coherency condition is achieved by the constraint applied to each lattice by the regions of "good fit" between the two lattices. Disturbance of the regularity of this highly constrained structure, by the introduction of "misfit" segments, can be effectively described in terms of dislocations with Burgers vector not of a lattice translation vector but of the appropriate high index interplaner spacings /7/. This leads naturally to a continuous-distribution dislocation model of high-angle grain boundaries.

II.- Continuous-Distribution Dislocation Model of High-Angle Grain Boundaries and the Mechanism of Inhomogeneous Sliding along the Grain Boundaries.- Let us consider an arbitrary high-angle GB as shown in Fig. 1 in which AB is the GB plane separating grain 1 and grain 2. Assume the thickness of GB layer be d and ro the atomic radius. We can imagine that when grain 1 and grain 2 approach each other, the frontier atoms of one grain will be acted by a misfit force from the frontier atoms of the other grain, so that these atoms will be displaced through \( u_{1i} \) and \( u_{2i} \) (i represents the i-th atom) and give rise to a certain internal stress. Eventually a stable high-angle GB is formed as an equilibrium state is reached. The GB layer is therefore equivalent to a continuous distribution of alternatively +ve and -ve (in the sense of statistical average) edge-type and screw-type dislocations.

According to Kröner /8/, the continuous distribution dislocation density tensor in the GB layer may be expressed as

\[
\mathbf{\kappa} = - \mathbf{n} \times \nabla (u_2 - u_1),
\]
where \( n \) is the normal unit vector. Although the specific form of \( \phi \) is unknown, but the mean value of \( \phi \) along GB should be zero according to simple physical arguments, so that \( \phi = 0 \). Moreover, \( \phi \) depends on the direction and magnitude of the Burgers vector and the direction of dislocation line which all have a random distribution. We may classify the GB dislocations into four typical types as shown in Fig. 2. (a) +ve and -ve edge dislocations with Burgers vector \( \mathbf{B} \) along \( \mathbf{i} \) and dislocation line \( \mathbf{D} \) along \( \mathbf{j} \); (b) +ve and -ve screw dislocations with \( \mathbf{B} \) and \( \mathbf{D} \) both along \( \mathbf{j} \); (c) +ve and -ve edge dislocations with \( \mathbf{B} \) and \( \mathbf{D} \) along \( \mathbf{k} \) and \( \mathbf{j} \); (d) GB vacancies which can be considered as dipoles composed of a pair of dislocations of +ve and -ve c-type.

It can be seen from Fig. 2 that the elementary process for GB sliding is the slip of the dislocations of a- or b-type and that for GB migration is the climb of the dislocations of a-type or the slip of c-type. The elementary process of GB diffusion is the climb of dislocation dipoles of d-type.

III. Internal Friction given rise by the Inhomogeneous Sliding along Grain Boundaries.- When a shear stress \( \tau \) is applied along the GB in the direction \( x \), some of the elementary dislocations of a-type or b-type can overcome the potential barrier to move into a neighbouring valley by thermal activation. This will facilitate the neighbouring elementary dislocations to overcome the potential barrier, so that the slip takes place in the form of an "avalanche" involving the group motion of a chain of elementary dislocations. Such a cooperative process was recently proposed by Ishita et al /9/ basing on their studies of GB diffusion in colloid polystyrene latex and gold sol crystals.

Consider the inhomogeneous sliding of a flat and smooth GB layer extending indefinitely along the y-direction and having a width (Fig. 2). Consider only the case of isotropic metals so that the slidings on both sides of the boundary are equal and opposite. The inhomogeneous slide \( u(x,t) \) at the point \( x \) along GB satisfies the equation:

\[
\frac{\mu}{\pi(1-\nu)} \int_{-\ell/2}^{\ell/2} \frac{\partial u(x',t)}{\partial x'} \, dx' - \tau_0 e^{i\omega t} + \eta \frac{\partial u(x,t)}{\partial t} = 0, \tag{2}
\]

where \( \mu \) is the shear modulus, \( \nu \) is the Poisson ratio, \( \tau_0 \) is the applied stress amplitude, \( \omega \) is the angular frequency and \( \eta \) is the assumed viscosity coefficient associated with the GB sliding. The first term on the left-hand side of Eqn. (2) is the shear stress produced at \( x \) by the dislocations with a continuous distribution linear density of \( \partial(2u)/\partial x \), the second term is the applied stress, and the third term is the Newtonian viscous resistant stress. The boundary condition for \( u(x) \) is \( u(\pm \ell/2) = 0 \).

Let \( \tilde{x} = 2x/\ell \),

\[
\tilde{x} = 2x/\ell, \tag{3}
\]
and \[ V = \left[ 2M/(1-\gamma) \right] \frac{e^{-i\omega t}}{\omega} \quad \text{and} \quad C = \pi (1-\gamma) \frac{\omega n \mu d}{\omega} \quad \text{(4, 5)} \]
then Eqn. (2) can be written as
\[
\int_{-\infty}^{\infty} \frac{dV}{d\xi} \left( \frac{1}{\xi - \xi'} - 1 + CV \right) i = 0 \quad \text{and} \quad V (\xi') = 0. \quad \text{(6, 7)}
\]
Now let us try to find an approximate solution of the form
\[ V = q \frac{\sqrt{1-\xi^2}}{(1+\xi (1-\xi))} \quad \text{(8)} \]
Obviously this solution satisfies the boundary conditions given by Eqn. (7). Substituting Eqn. (8) into Eqn. (6) and let \( \xi = 0 \), we get on putting the real part and the imaginary part equal to zero respectively:
\[ 2p + (1/\sqrt{1+p^2}) \log \left[ \frac{(1+p^2+p \sqrt{1+p^2})/(1+p^2-p \sqrt{1+p^2})}{(1+p^2)^{3/2}} \right] = C, \quad \text{(9)} \]
\[ (1+p^2)^{3/2} / (1+pC(1+p^2)) = q. \quad \text{(10)} \]
The anelastic strain \( \dot{\varepsilon}_a \) associated with the GB sliding is
\[ \dot{\varepsilon}_a = \frac{2d}{(1-C/2)^2} \int_{-\infty}^{\infty} \frac{e^{-i\omega t}}{\omega} \quad \text{(11)} \]
The total strain is \( \varepsilon = \varepsilon'_a + \varepsilon''_a \), where \( \varepsilon'_a = \varepsilon_0/M \) (the elastic strain).
The internal friction and modulus defect can be obtained from the imaginary and the real part respectively from \( \dot{\varepsilon}'_a/\varepsilon'_a = \varepsilon'_a/\varepsilon_0/M \) and we have
\[ Q^{-1} = -\text{Im}(\dot{\varepsilon}'_a/\varepsilon'_a) = \left[ \frac{\pi (1-\gamma)}{2} \right] \left[ (4p-C)q/p^2 \right], \quad \text{(12)} \]
\[ \Delta M/M = \text{Re}(\dot{\varepsilon}'_a/\varepsilon'_a) = \left[ \frac{\pi^2 (1-\gamma)}{2} \right] \left[ (1-1/\sqrt{1+p^2})q/p^2 \right]. \quad \text{(13)} \]
In Fig. 3, \( Q^{-1} \) and \( \Delta M/M \) (or \( \Delta M/\varepsilon_0 \)) are plotted as function of \( C \), the unit of the ordinate has been chosen as \( \pi (1-\gamma) /2 \). The dotted curves represent the corresponding curves for single relaxation time. It can be seen that a peak appears at
\[ C = \pi (1-\gamma) \frac{\omega n \mu d}{\omega} = 4.269, \quad \text{(14)} \]
and the height of the peak is
\[ Q^{-1 \max} \approx 0.29 \pi (1-\gamma) /2. \quad \text{(15)} \]
The relaxation strength \( \Delta M \) can be determined from the extreme values taken from the \( \Delta M/M - C \) curve in Fig. 3 as
\[ \Delta M = \Delta M/M \quad \text{for } C=0 \quad - \Delta M/M \quad \text{for } C=\infty = 0.5 (1-\gamma) /2. \quad \text{(16)} \]
From this we get \( Q^{-1 \max} = \frac{1}{2} \Delta M = 0.25 (1-\gamma) /2 \), which is close to the value determined directly from the \( Q^{-1} - C \) curve.

IV.- Comparison with Experiments. Assuming that only the GB dislocations near the GB vacancies are feasible to sliding, then the force acting on a dislocation segment of average length \( \bar{\ell} \) is \( F \) where \( b \) is the total Burgers vector of these mobile dislocations. If we apply Einstein's relationship approximately to the present case, then we have the average sliding rate \( v_H = D_b \bar{\ell} b \kappa / \kappa \), where \( D_b \) is the coefficient of GB diffusion. Since by definition, \( \eta = \bar{\ell} / (v_H / d) \), we get finally
\[ \eta = \frac{\gamma d}{\nu} = kTd/\alpha D_b = kT/2r_0 D_b, \]  
\[ (17) \]
on assuming that \( a = b = d = 2r_0 \). Thus the viscosity \( \eta \) for GB sliding is correlated with the diffusion coefficient along grain boundaries. If \( D_{bo} \) is the diffusion constant and \( H \) the activation enthalpy associated with GB diffusion, then we have

\[ T_p \exp(H/T_p) = 4.269(2r_0)^2 D_{bo}/\ell(1-\nu)^2 k(2\pi f), \]
\[ (18) \]
where \( T_p \) is the peak temperature of the GB IF peak and \( f \) is frequency of vibration. The \( T_p \) values calculated according to Eqn. (18) for a number of pure metals are summerized in Table 1 with experimental values. The values of \( D_{bo} \) and \( H \) were in general taken from Ref./10/. Data for Al, Cu, Au were estimated according to the empirical formula given in Ref./11/. In cases when \( \ell \) and \( f \) are not known, we assumed that \( f = 1Hz \) and \( \ell = 0.05 \) mm taking account of the fact that \( \ell \) may be smaller than the actual grain size if the boundary is not flat and smooth enough so that ledges and protrusions may act as obstructing sites for GB sliding. As the origins of the experimental data are quite diversified and the experimental values are varied according to experimental conditions and specimen purity, the agreement between estimated values and experimental values shown in Tab. 1 seems to be quite satisfactory. For Al, Sn and some other metals, the estimated values are much lower than the experimental values and these may be connected with an impurity effect.

<table>
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<tr>
<th>Metals</th>
<th>Ag</th>
<th>Fe</th>
<th>Sn</th>
<th>W</th>
<th>Zn</th>
<th>Mo</th>
<th>Ta</th>
<th>Al</th>
<th>Cu</th>
<th>Au</th>
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</thead>
<tbody>
<tr>
<td>( T_p ) estimated</td>
<td>426</td>
<td>638</td>
<td>139</td>
<td>1587</td>
<td>236</td>
<td>1365</td>
<td>1590</td>
<td>385</td>
<td>528</td>
<td>478</td>
</tr>
<tr>
<td>( T_p ) experimental</td>
<td>440</td>
<td>704</td>
<td>340</td>
<td>1500</td>
<td>323</td>
<td>1325</td>
<td>1400</td>
<td>560</td>
<td>500</td>
<td>455</td>
</tr>
</tbody>
</table>

V. Discussion. In metals containing soluble impurities, it is well known that there is a selective segregation along certain boundaries /12/. If the viscosity associated with the inhomogeneous sliding in the pure solvent region of the boundary is \( \eta_1 \), and that in the solute region is \( \eta_2 \), then Eqn. (6) still holds but \( C \) will depend upon \( \xi \). This will give rise to a solute IF peak at a temperature above the original solvent peak if \( \eta_2 \) is larger than \( \eta_1 \). The solute peak will appear at a temperature below that of the solvent peak only when precipitation has occurred at the grain boundaries in which case \( \eta_2 \) may be smaller than \( \eta_1 \). This may be the case observed in Cu containing Bi /13/. Although dislocations of a-type and c-type shown in Fig. 2 can climb or slip to give rise to GB migration, but actually the net migration is zero since there are equal numbers of positive and negative dislocations in the boundaries. However, in highly anisotropic pure metals as Mg, Zn, etc., or in the presence of internal stress (e.g. the occurrence of excessive dislocations near GB layer), the elastic modulus and the
stress are different at the two sides of the boundaries and it can be shown that the migration rate of the boundary toward the side having a smaller shear modulus (e.g., \( \mu_1 \)) under the action of a shear stress is

\[
v_\perp = \left( \frac{D_b}{kT} \right) \left( \frac{1}{\mu_1} - \frac{1}{\mu_2} \right) \tau_{ab}^2 \approx v_\parallel \left( \frac{1}{\mu_1} - \frac{1}{\mu_2} \right) \tau_{<<} v. \quad (19)
\]

This stress-assisted GB migration rate \( v_\perp \) may cause a high temperature IF background or another GB peak which is amplitude dependent. But it can be seen from Eqn. (19) that the contribution of GB migration to GB internal friction should be much smaller than that of GB sliding.

References


Fig. 1. An arbitrary high-angle grain boundary.

Fig. 2. Grain-boundary sliding (upper) and four types of grain boundary dislocations (lower).

Fig. 3. \( Q^{-1} \) vs C and \( \Delta M/M \) vs C curves.