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DISLOCATION RELAXATION IN A RANDOM ARRAY OF SOLUTES

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Abstract.- An amplitude-dependent internal friction peak occurs at \( T = 475 \) K in well-annealed, pure \( \alpha \)-Zr after slight deformation. Qualitatively, the results agree with a model for the motion of zig-zag dislocations in an array of obstacles. Comparison of theoretical and experimental results yields estimates of the effective activation enthalpy and activation volume of the process involved.

1. Introduction.- Recently, there have been advances in the understanding of high-temperature, solid-solution hardening (SSH) by dynamic simulation using computer techniques. For example, Schwarz and Labusch\(^1\) have employed such a technique to calculate the SSH component of the flow stress (\( \sigma_f \)), while Schwarz\(^2\) has used the same programs to calculate amplitude (\( \varepsilon \))-dependent internal friction (\( \Delta \)). The results reveal a simple quantitative correspondence between \( \Delta(\varepsilon) \) and \( \sigma_f \). These studies are providing new insight into the nature of strain-aging effects and the athermal plateau in \( \sigma_f \) vs. temperature (\( T \)) curves for solution-strengthened alloys.

In \( \alpha \)-Zr, anomalous mechanical behaviour (particularly creep) and the athermal plateau in \( \sigma_f \) vs. \( T \) curve is attributed to the strong interactions between dislocations and interstitial impurities (usually oxygen)\(^3\). In the same \( T \) range, peaks of \( \Delta \) vs. \( \varepsilon \) with some of the characteristic properties of a thermally assisted unpinning process have been reported\(^4,5\). It is shown in this paper that these peaks can be generated in well-annealed specimens of comparatively high purity \( \alpha \)-Zr after a very slight deformation at room temperature. Consequently, we can compare the results with calculations based on a very simple model proposed by Schlipf and Schindlmayr\(^6-8\), which is valid for the motion of zig-zag dislocations in a random array of solute obstacles in the low concentration limit.

2. Material.- Measurements of \( \Delta \) in flexure (frequency, \( f \approx 4 \) Hz) were carried out on specimens of a nominally 5N pure Zr. The interstitial impurity concentrations (\( \mu g/g \)) of the as-received (cold-rolled strip) material were found to be \( H < 5 \), \( N = 6 \), and 0 in the range 17 to 23. Specimens were used which had been annealed in a vacuum furnace at 1075 K (final grain size \( \approx 0.7 \) mm) and then slightly deformed in bending at room temperature. Even though precautions against the pick-up of 0 were taken, after annealing and testing analysis revealed some pick-up of both 0 and H. The final concentrations (\( \mu g/g \)) were \( H = 14 \pm 2 \) and \( 0 \approx 30 \). The equipment and measurement techniques employed have been described in detail elsewhere\(^9\).
3. Results.- Typical curves of $A$ vs. $T$ (E const.) and $A$ vs. $\varepsilon$ (T const.) are shown in figures 1 and 2, respectively. It must be pointed out, however, that identical results were not obtained on every specimen tested, presumably because the attempted "very slight deformation" did not always succeed. Nevertheless, once they had been obtained with a given specimen, the results were surprisingly stable and reproducible on heating and cooling, provided that the specimen was not heated above about 510 K. This is in agreement with the work of Atrens (4) who showed that a similar peak disappeared after heating for 20 minutes at 500 K.

Figure 1 can be described as a family of peaks of almost constant height, with a common high-$T$ tail, and increasing broadening on the low-$T$ side, as $\varepsilon$ increases. The results in figure 2 can be described by a $A$ vs. $\varepsilon$ peak which passes through the "window" of experimentally investigated $\varepsilon$, from high $\varepsilon$ to low $\varepsilon$, as $T$ increases. The shapes and behaviour of the peaks in figures 1 and 2 are similar to those predicted theoretically for thermally assisted unpinning of dislocations (10,11). Because of the preparation of the specimens, the fresh dislocations should be "zig-zagged" through a random array of interstitial solutes.

4. Theoretical Model (6-8).- It is assumed that the freshly created network lengths can be treated by the vibrating-string model but, because of their interactions with the random array of obstacles, each network length ($L$) will take on a zig-zag configuration characterized by an amplitude ($z$) and a length ($l$) as shown in figure 3. Attractive and repulsive obstacles are supposed to be present in equal numbers, and the "idealized" basic step in the dislocation motion is taken to be the jump from one zig-zag configuration, $A_n B_n A_{n+1}$, into an equivalent one, $A_n C_n A_{n+1}$ (see figure 3). In the process, the dislocation is unpinned at the attractive obstacle $B_n$, pushed
past the repulsive obstacle \( R_n \), and recaptured by the attractive obstacle \( C_n \). The corresponding potential energy diagram (figure 4) has four minima that must be taken into account. At the lowest \( \varepsilon \), the dislocations interact with the attractive obstacles only. This gives rise to a Debye peak which is \( \varepsilon \)-independent \((7)\). At higher \( \varepsilon \), the dislocations are forced to interact with the repulsive obstacles also. According to Schlipf and Schindlmayr \((8)\), the dislocation velocity \( \dot{y} \) is given by

\[
\dot{y} = \frac{Z \omega_o \sinh (gb^3 \sigma_{\text{eff}}/ckT)}{E}
\]

where \( \omega_o \) = jump frequency at \( \sigma = 0 \), \( g = 1 \) (geometrical factor), \( b \) = Burgers vector, \( c \) = concentration of obstacles, \( k = \) Boltzmann's constant and \( \sigma_{\text{eff}} \) = effective stress. If internal stresses are neglected, \( \sigma_{\text{eff}} \) is composed of the external stress \( (\sigma) \) and the back stress, \( (T/b)d^2y/dx^2 \), due to the line tension \( (T_b) \). \( T_b \) is taken to be 0.5 \( Gb^2 \) where \( G \) is the shear modulus. For \( \varepsilon > ckT/RE^3 \), eqn. [1] defines an \( \varepsilon \)-dependent dislocation mobility and a solution in closed-form is not possible. Assuming interstitial 0 obstacles, \( c = 2 \times 10^{-4} \), and since Young's modulus \( (E) = 99 \) GPa, and the average orientation factor \( R = 2/(3\pi) \) (for a random assemblage of grain orientations), the above inequality predicts \( \varepsilon \)-dependence for \( \varepsilon > 4 \times 10^{-7} \) at 475 K. This is in keeping with the results in figures 1 and 2, indicating that a solution of eqn. [1] is necessary.

\[ \Delta = \frac{(2/\pi)^3(ML^2)(E/G_0)}{2 \ln((p^2+1)/p)} \]

\[ + (2\omega/\pi B)[\text{Li}_2(q_1 \exp(-\pi B/2\omega)) - \text{Li}_2(q_1 \exp(\pi B/2\omega))] \]

\[ + \text{Li}_2(-q_2 \exp(\pi B/2\omega)) - \text{Li}_2(-q_2 \exp(-\pi B/2\omega)) \]

Fig. 3: Upper diagram shows the basic jump of the dislocation from one attractive obstacle \( B_n \), over a repulsive obstacle \( R_n \), to an attractive obstacle \( C_n \). The lower diagram also defines zig-zag bow-out of a network length \( L \).

If it is assumed that the average bow-out of the network length (under stress) is given by a cosine function (an excellent approximation when non-linear effects are negligible\((7)\)), an approximate solution can be obtained for a linearized cyclic stress, which in turn leads to a closed-form expression for \( \Delta \). The equations given by Schlipf and Schindlmayr \((8)\) are incorrect. We have repeated the calculations and find

\[ \Delta = \left(\frac{2}{\pi}\right)^3 M L^2 \frac{E}{G_0} \left[ 2 \ln\left(\frac{p^2+1}{p}\right) \right] \]

\[ + \left(\frac{2\omega}{\pi B}\right) \left[ \text{Li}_2\left(q_1 \exp\left(-\frac{\pi B}{2\omega}\right)\right) - \text{Li}_2\left(q_1 \exp\left(\frac{\pi B}{2\omega}\right)\right) \right] \]

\[ + \text{Li}_2\left(-q_2 \exp\left(\frac{\pi B}{2\omega}\right)\right) - \text{Li}_2\left(-q_2 \exp\left(-\frac{\pi B}{2\omega}\right)\right) \]
where \( \text{Li}_2 = -\int_0^x \frac{\ln(1-\xi)}{\xi} \, d\xi \) (the dilogarithm function), \( \omega = 2\pi f \), \( a_o = \sigma_o b^3/c kT \) (\( \sigma_o \) is the stress amplitude), \( p = (\pi/2)/a_o \omega T \), \( \tau = L^2 c kT/\pi^2 \omega_0 T b^2 \), \( \omega_0 = \omega_0 \exp(-U_{\text{eff}}/kT) \) where \( \omega_0 \) is an attack frequency and \( U_{\text{eff}} \) is the effective activation enthalpy, and \( B = (p^2 + 1)^{1/2}/\pi \). The equations for \( q_1 \) and \( q_2 \) are

\[
q_1 = \frac{[(p^2+1)^{1/2}-1]}/[(p^2+1)^{1/2}+1]S; \quad q_2 = S
\]

with

\[
S = \left[ p/((p^2+1)^{1/2}-1) \right] \left[ (p^2 \cosh^2 (\pi b/2 \omega)+1)^{1/2}-p \cosh (\pi b/2 \omega) \right].
\]

A plot of \( \Delta_N \) (normalized \( \Delta \)) vs. \( \omega T \) for various values of \( a_o \) is shown in figure 5. This family of curves can be described as a peak of almost constant height, which broadens on the high \( \omega T \) (low \( T \)) side as \( a_o \) (or \( \epsilon \)) increases, while the low \( \omega T \) (high \( T \)) asymptote is unchanged. These curves are qualitatively very similar to the experimental results shown in figure 1.

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**Fig. 5**: Normalized internal friction as a function of \( \omega T \) for various values of \( a_o \).

To make a more detailed comparison between theory and experiment, we have calculated \( \Delta_N \) vs. \( T \) (\( \epsilon \) const.) and \( \Delta_N \) vs. \( \epsilon \) (\( T \) const.) curves for the same ranges of \( \epsilon \) and \( T \) explored experimentally. These calculations have been carried out using eqn. [2] adapted to the strain distribution in our flexure specimens (9). The parameters used in the calculations were: \( \omega_0 = 1 \times 10^{12} \) s\(^{-1} \), \( U_{\text{eff}} = 1 \) eV (simply estimated from the peak position), \( \omega = 8\pi \), \( Gb^3 = 7.47 \) eV, \( c = 2 \times 10^{-4} \) and \( L = 1000 \) b. The activation volume \( V \) of the process (b times the diamond area swept-out by the dislocation, figure 3) is \( 2b^2 \), or more simply, \( V = b^3/c = 5000 \) b\(^3\). The calculated results corresponding to figures 1 and 2 are given in figures 6 and 7, respectively. In figure 7, the arrows indicate the approximate range of \( \epsilon \) explored experimentally in figure 2. Comparison of the experimental and theoretical curves shows that qualitatively the agreement is very good.

5. **Discussion.** - The magnitudes of \( U_{\text{eff}} = 1 \) eV and \( V = 5000 \) b\(^3\) are consistent with those determined for thermally activated deformation mechanisms attributed to oxygen
Fig. 6: Normalized internal friction as a function of temperature calculated for the various indicated strain amplitudes.

Fig. 7: Normalized internal friction as a function of strain amplitude calculated for the various temperatures indicated. Arrows indicate the experimental strain amplitude range.

SSH in α-Zr\(^{12}\). Fernandez and Povolo\(^{5}\) have attributed an ε-dependent Λ peak at about 475 K in large-grained Zr to the interactions between oxygen and extended dislocations. However, their results obtained at 50 kHz yield a much broader peak (extending to 800 K on the high-T side) than the results in figure 1. Comparison of their results with theoretical predictions for the unpinning of extended dislocations\(^{13}\) yields a reasonable value for the binding energy of 1.3 eV, but an unreasonably large dislocation loop length (= 5 x 10⁴ b). In the model presented here, \(U_{\text{eff}}\) is not simply related to the binding energy (see figure 4) but is not inconsistent with the high values reported for the binding energy\(^{3,5,14}\). It should be noted that the parameters used in the calculations for figures 6 and 7 are not the only set which give qualitative agreement between theory and experiment. Nevertheless, the very good agreement obtained using plausible parameters is very promising. It suggests that a quantitative comparison between theory and experiment can be attempted using single crystals (i.e. with R known), if an independent determination of the network length, L, can be obtained and the concentration of interstitials is known.

REFERENCES