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PARAMETRIZATION OF LOW TEMPERATURE DEFORMATION  
CHARACTERISTICS IN SINGLE CRYSTALS OF MOLYBDENUM

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ABSTRACT

A rate-temperature parameter is defined through Dorn-Rajnak model for Peierls mechanism, and has been shown to be useful in characterizing the low temperature deformation of single crystals of molybdenum. This parameter was utilized in testing the mechanical equation of state and also in proving the failure of such an equation in molybdenum. Whereas the rate of work hardening was found to be uniquely defined by strain and parameter, the flow stress depended in addition on thermo-mechanical history of the material.

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## I. INTRODUCTION

It is an established fact that a variation in the strain-rate during plastic deformation of metals may be compensated by an appropriate temperature change thereby leaving the stress for a given strain unaltered.[1] In addition, several attempts [2-4] were made to define the deformation characteristics of metals through an equation of state such as

$$\sigma \equiv \sigma \{ \dot{\epsilon}, \epsilon, T \} \quad (1)$$

where  $\sigma$  is the flow stress,  $\dot{\epsilon}$  the strain rate,  $\epsilon$  the strain and  $T$  the temperature. Such an equivalence fails to apply whenever some recovery process takes place during deformation. The purpose of the present investigation is to characterize the flow stress through a rate-temperature parameter [5] derived from the Peierls mechanism [6,7] and study the failure of the mechanical equation of state accompanying a change in this parameter.

## II. ANALYSIS

Dorn and Rajnak [6], and Guyot and Dorn [7] established that the low temperature deformation behavior of bcc metals is controlled by the Peierls mechanism through the formation and motion of pairs of kinks. Their mathematical formulations lead to the following expression for the strain-rate:

$$\dot{\epsilon} = \frac{\rho L a b^2}{2 w^2} v \exp - \frac{2 U_k}{kT} \left( 1 - \frac{\sigma^*}{\sigma_p} \right)^2, \quad (2)$$

where  $\rho$  is the length of all thermally activatable dislocation segments per unit volume;  $L$  is the average length of a dislocation that might be swept out by a pair of kinks following their nucleation;  $\frac{vb}{w}$  is the frequency of vibration of a dislocation with  $v$  being the Debye frequency,

b the Burgers vector of the dislocations and w the width of the critical pair of kinks; a is the interatomic spacing;  $U_k$  is the energy of formation of a single kink under zero effective stress  $\sigma^*$ , and  $\sigma_p$  is the Peierls stress.

The effective stress is given by

$$\sigma^* = \sigma - \sigma_G \quad (3)$$

where  $\sigma$  is the applied stress, and  $\sigma_G$  is the back or athermal stress.

The effective stress is the thermally activated component resulting from short-range obstacles (such as Peierls stress) to dislocation motion, and depends on both the temperature and the strain-rate. It has been shown in single crystals of iron by Spitzig and Keh [8], that the effective stress is independent of strain. On the other hand, the athermal stress component which results from long-range obstacles to dislocation motion (such as dislocation tangles and Cell walls) is a function of strain (or the dislocation distribution) [8], and depends on the work-hardened state of the material. It is essentially independent of the strain-rate and the temperature except for the slight variation with the shear modulus.

Thus

$$\sigma = \sigma^* \{T, \dot{\epsilon}\} + \sigma_G \{\epsilon\} \equiv \sigma \{T, \dot{\epsilon}, \epsilon\} \quad (4)$$

Equation 2 may be rewritten as

$$T \ln (A/\dot{\epsilon}) = \frac{2 U_k}{k} [1 - \sigma^*/\sigma_p]^2 = P \quad (5)$$

where  $A = \frac{\rho L a b^2 v}{2w^2}$  is the material constant and P is the rate-temperature parameter. Equation (5) implies that for constant values of the parameter P, the effective stress should be the same. For specimens with identical

initial treatment the athermal stress ( $\sigma_G$ ) must be the same, changing only with the strain (provided that the work-hardening characteristics are the same, independent of T and  $\dot{\epsilon}$ ) so that:

1. Tests conducted at suitable combinations of temperature and strain-rate should result in identical ( $\sigma$ - $\epsilon$ ) curves for the same value of P.
2. As a result of (1), the flow stress can be represented by  $\sigma(\epsilon, P)$  so that an equation of state may be written to be

$$\sigma = \sigma \{ \epsilon, P \} \quad (6)$$

3. Consequently the dislocation substructure, which determines the flow stress, should be the same for the same value of P (equivalent stress-strain curves) and different for different values.
4. Finally, from equation (5) above, a change in P caused by appropriate variations in temperature and/or strain-rate should result in a change in  $\sigma^*$  corresponding to the new value of the parameter. Thus if at a certain value of strain ( $\epsilon_0$ ) the parameter is abruptly changed then the new effective stress value achieved thereupon should correspond to that for the new parameter at that strain  $\epsilon_0$ . If the athermal stress depends only on strain, and an equation of state described by (6) is valid, then the above argument should hold also for the flow stress ( $\sigma = \sigma^* + \sigma_G$ ) for specimens with identical initial treatments.

### III. EXPERIMENTAL PROCEDURE

Molybdenum single crystals were prepared by electron beam zone melting techniques and specimens with tensile axes orientation at the center of the standard triangle were machined from these. After checking

the orientations of the prepared samples they were electropolished, annealed at 2050°C for 24 hours in an ultra-pure helium atmosphere, and electropolished again to mirror finish. Tension tests at strain-rates between  $10^{-1}$  and  $10^{-6}$   $\text{sec}^{-1}$  in a temperature range of 77 to 400°K were performed with these crystals using an Instron machine. One specimen was tested in addition at 45°K in obtaining the temperature dependence of the yield stress.

#### IV. RESULTS AND DISCUSSION

Fig. 1 depicts the stress-strain curves for equivalent combinations of temperature and strain-rate at various values of the parameter P. All curves are parabolic in shape, characterized by high initial work hardening rates. Suitable combinations of strain-rate and temperature which gave identical stress-strain curves were sought essentially by trial and error. Temperatures, strain-rates, values of A and the parameter P obtained from equation (5) are tabulated in Table 1. The values of A range from  $1.34 \times 10^5$  to  $4.79 \times 10^6$   $\text{sec}^{-1}$  with a mean of  $1.45 \times 10^6$ . Using reasonable values [5,6] for  $\rho$ , L and w of  $10^8$   $\text{cm}^{-2}$ ,  $\text{cm}^{-4}$  and 30b, A is estimated to be  $8 \times 10^6$  which is of the same order as obtained above. P values obtained using the average value of  $1.45 \times 10^6$   $\text{sec}^{-1}$  for A are shown in Table 1 as  $\bar{P}$ , and the maximum deviation between P and  $\bar{P}$  is about 15%.

It is clear from these results that the mechanical state of a material may be conveniently described by the three parameters P,  $\epsilon$  and  $\sigma$ . To check whether  $\sigma \equiv \sigma \{P, \epsilon\}$  and the implication #4 tests were conducted in which P value was abruptly changed from a higher value to a lower one and vice versa at a certain strain (0.04). Fig. 2 (a) re-



presents the stress-strain curves and the effect of the change in the parameter from 7260 to 3577 °K while in Fig. 2(b) the stress-strain curves and the effect of parameter-change from 3577 to 5080°K are shown. It is clear from these that the mechanical equation of state failed and  $\sigma \{P, \epsilon\}$  is not uniquely defined. As will be shown later, the effective stress is independent of the work-hardened state of the material, and varies only with the temperature and the strain-rate. Therefore the failure of the mechanical equation of state as depicted in Fig. 2 may be explained through the change in the magnitude of the athermal stress ( $\sigma_G$ ).

During the deformation up to  $\epsilon_0$  (0.04) recovery may take place at different rates depending upon the test temperature, and the strain-rate, so that the athermal stress level at  $\epsilon_0$  becomes different for the two specimens, (tested at  $P_1$  and  $P_2 \rightarrow P_1$ ). In the temperature range employed here, however, the rate of recovery is too low to substantially affect the athermal stress level. In addition, if recovery in fact contributes to the deformation process, then the rate of work-hardening after the change in  $P$  will be different from that tested all the way from the start at the new  $P$  value. As a consequence the stress-strain curves beyond  $\epsilon_0$  would not be parallel [2], contrary to the present observations (Fig. 2), and the earlier findings in copper by Bullen and Hutchison [9]. Moreover it is to be noted that the effective stresses corresponding to the different  $P$  values are different. Consequently dislocation mobilities will be different, and local obstacles of different strength will be surmounted resulting thereby in different quasi-equilibrium dislocation substructures. As a result, the athermal stress ( $\sigma_G$ ) levels at  $\epsilon_0$  will be different for the specimens tested at  $P_1$  and  $P_2$ . This explains the

failure of the equality of the flow stress after the change in the parameter.

Thus the reasonable explanation for the failure of the mechanical equation of state is that the parameter and hence the effective stress play major role in inducing significant changes in the dislocation substructure. The resulting substructure dictates the level of the back stress, thereby contributing to the failure of the mechanical equation of state even in the absence of any recovery. Thus a complete description of the flow stress still needs an unknown parameter  $s$  (in addition to  $P$  and  $\epsilon$ ) so that

$$\begin{aligned}\sigma &= \sigma^* \{T, \dot{\gamma}\} + \sigma_G \{\epsilon, s\} \\ &\equiv \sigma \{P, \epsilon, s\}\end{aligned}\tag{7}$$

where  $s$  includes the thermo-mechanical history of the material.

In the present case one can uniquely define the rate of strain hardening, given the parameter and strain and thus

$$\frac{d\sigma}{d\epsilon} = \frac{d\sigma^*}{d\epsilon} + \frac{d\sigma_G}{d\epsilon} = \frac{d\sigma_G}{d\epsilon} \{P, \epsilon\}\tag{8}$$

It is to be noted, however, that earlier observations by Dorn et al [2] on polycrystalline Al disagree with this result. Some process of recovery may be responsible for their findings.

Hart in his attempts to develop a phenomenological theory [4] for plastic deformation stated that the mechanical state of a material may be described by:

$$\sigma = \sigma \{Z, \dot{\epsilon}, T\} \quad \text{and}\tag{9a}$$

$$\frac{dZ}{d\epsilon} = f \{\dot{\epsilon}, Z, T\}\tag{9b}$$

where  $Z$  is some dimension of the dislocation structure. A comparison of this with the present work brings out the equivalence of  $S$  in equation (7) with  $Z$ . If a recovery process takes place during deformation, however,  $Z$  depends on  $\sigma$ ,  $\epsilon$ ,  $T$ ,  $\dot{\epsilon}$  and other factors, and cannot be treated as a well defined state variable. In this case no simple integrating factor can be used for equation (9b) to define the mechanical state of a material as suggested by Hart.

To test the validity of the fact that the effective stress is independent of the work hardened state of the material, a series of samples were prestrained to a certain stress ( $6.4 \times 10^8$  dynes/cm<sup>2</sup>) in the athermal region (550°K), and then were tested at various temperatures at a constant value of the strain-rate ( $4.5 \times 10^{-5}$  sec<sup>-1</sup>). Fig. 3 shows the temperature variation of the flow stress for these prestrained samples, in addition to that obtained on annealed samples as well as the earlier data of Lau et al [10] obtained on samples prestrained to  $3.1 \times 10^8$  dynes/cm<sup>2</sup> at 550° K. As is obvious from the figure, the effective stress and its temperature variation turned out to be identical in all the three cases thereby providing an experimental verification of the independence of  $\sigma^*$  on the initial structure. This in addition proves that  $A$  is a material constant as expected when the Peierls mechanism operates [6,7]. These findings substantiate the present results in Table I, where  $A$  was determined to be  $(1.45 \pm \frac{3.34}{0.32}) \times 10^6$  sec<sup>-1</sup>. Similar observations were reported earlier by Wynblatt et al [11] on Fe-Mn alloy, and by Spitzig and Keh [8] in single crystals of iron.

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TABLE I

P values obtained from equivalent combinations of temperatures and strain-rates.

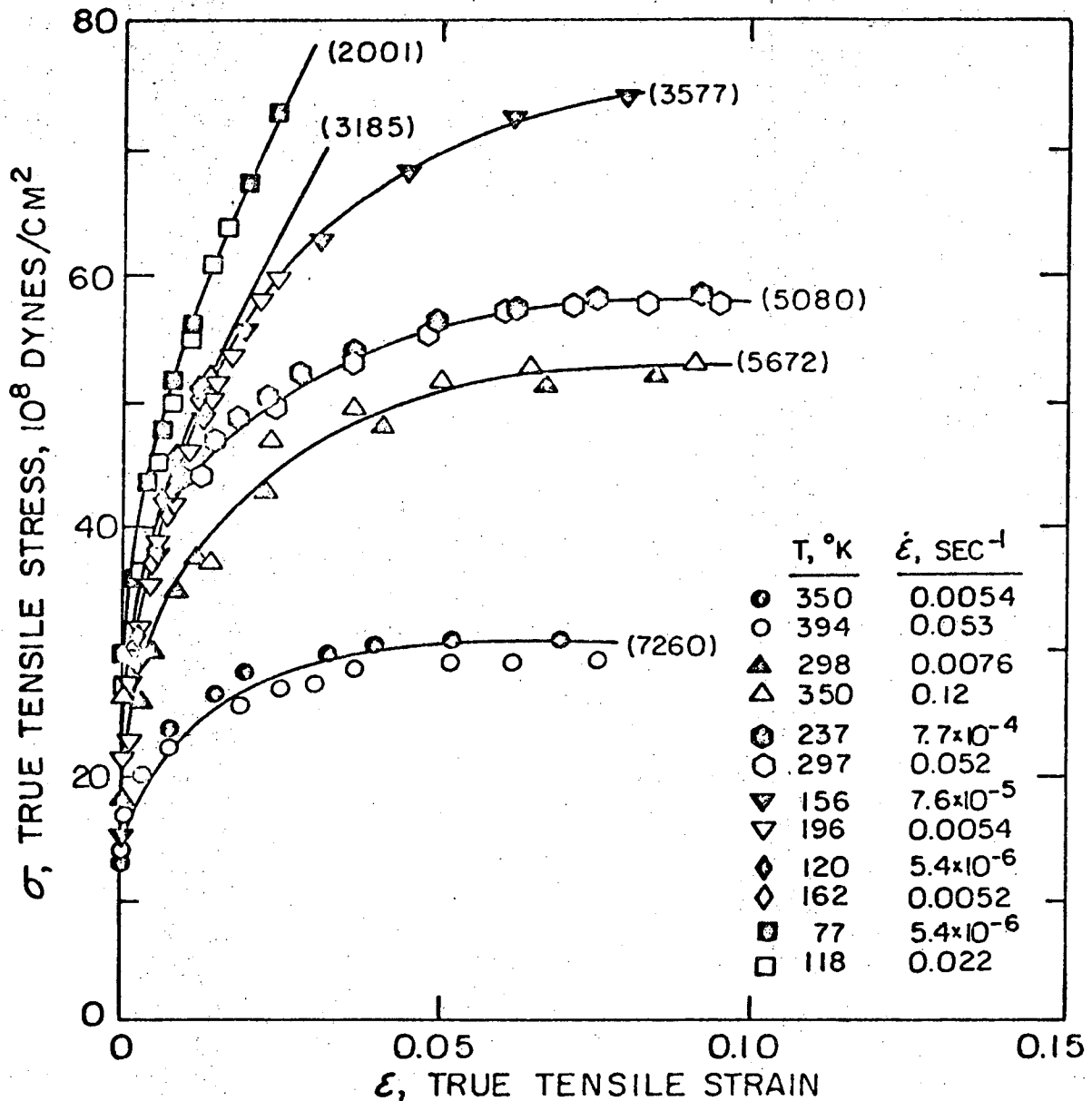
T °K	$\dot{\epsilon}$ sec <sup>-1</sup>	A sec <sup>-1</sup>	P °K	$\bar{P}^*$ °K	$\langle P \rangle^\dagger$ °K
77	$5.4 \times 10^{-6}$	$1.35 \times 10^5$	1842	2160	$2001 \pm 159$
118	$2.2 \times 10^{-2}$				
120	$5.4 \times 10^{-6}$	$1.82 \times 10^6$	3180	3190	$3185 \pm 5$
162	$5.2 \times 10^{-3}$				
156	$7.6 \times 10^{-5}$	$1.34 \times 10^5$	3320	3835	$3577 \pm 257$
195	$5.4 \times 10^{-3}$				
237	$7.7 \times 10^{-4}$	$8.90 \times 10^5$	4960	5200	$5080 \pm 120$
297	$5.2 \times 10^{-2}$				
298	$7.6 \times 10^{-3}$	$8.91 \times 10^5$	5535	5810	$5672 \pm 137$
350	$1.2 \times 10^{-1}$				
350	$5.4 \times 10^{-3}$	$4.79 \times 10^6$	7630	6890	$7260 \pm 370$
394	$5.3 \times 10^{-2}$				

\*Obtained using  $A = 1.45 \times 10^6 \text{ sec}^{-1}$ .

†Mean of P and  $\bar{P}$

FIGURE CAPTIONS

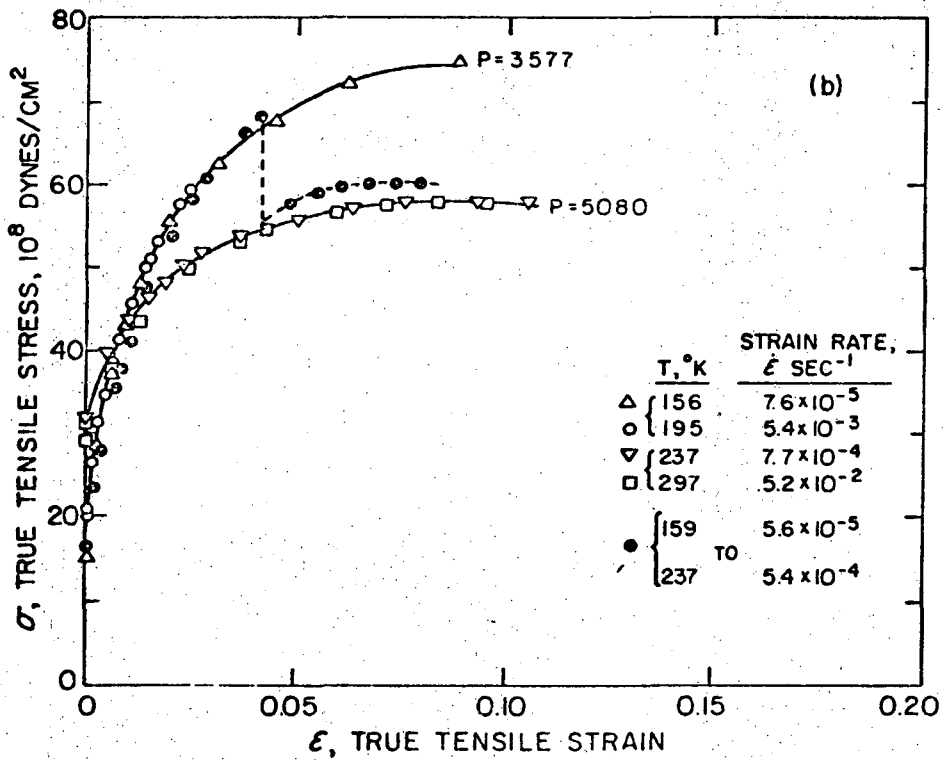
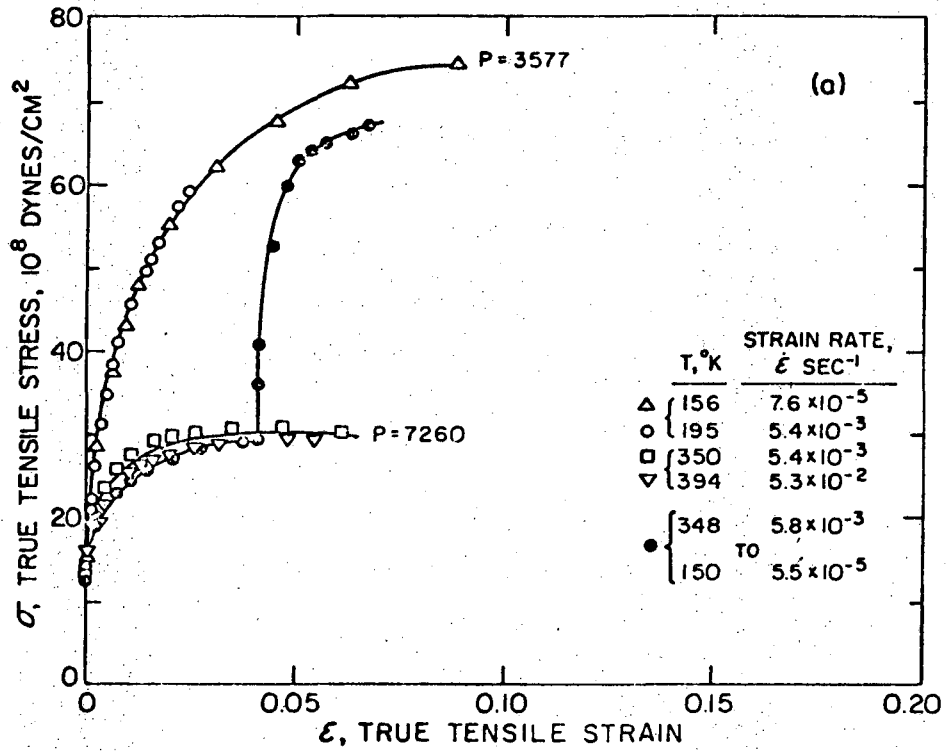
1. Effect of strain rate and temperature on stress-strain curve. P values are indicated in parentheses.
2. Stress-strain curves and the effect of change in P indicating the failure of the mechanical equation of state. P value was changed from a higher to lower value (fig. a) and vice versa (fig. b).
3. Flow stress vs Temperature.



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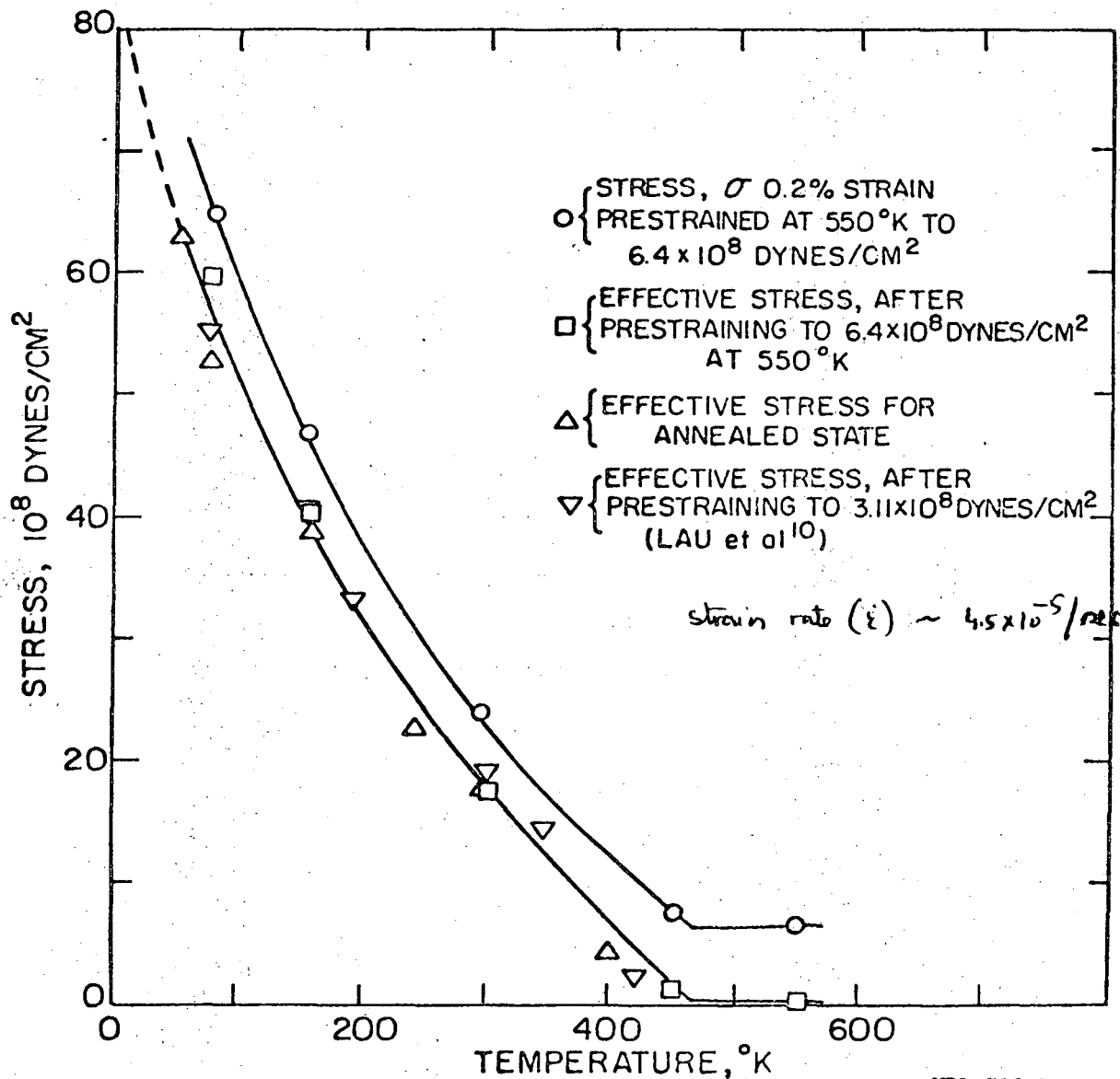
Fig. 1





XBL 718-7138

Fig. 2



XBL 718-7135

Fig. 3

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