Study on the interaction between a dislocation and impurities in KCl : Sr^{2+} single crystals by the Blaha effect

Part II *Interaction between a dislocation and aggregates for various force-distance relations between a dislocation and an impurity*

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A strain-rate cycling test during the Blaha effect measurement was carried out at 83–239 K for the purpose of studying the force-distance relation between a dislocation and the aggregate for KCl : Sr^{2+} (0.05 mol% in the melt) single crystals. On the basis of the dependence of strain-rate sensitivity due to the aggregates on temperature, it was found that the interaction between a dislocation and the aggregate in the specimen can not be approximated to the Fleischer's model taking account of the Friedel relation within the temperature. The square force-distance relation between a dislocation and an impurity seemed to be the most suitable model among the three: a square force-distance relation, a parabolic one and a triangular one, taking account of the Friedel relation for the specimen. In addition, the values of enthalpy and Gibbs free energy of activation for overcoming of the aggregate by a dislocation were obtained for the three force-distance relations.

1. Introduction

We have reported the information on the interaction between a moving dislocation and the impurities for KCl doped with divalent impurities [1–3] or monovalent ones [4, 5] so far. This is studied on the basis of the relative curve of strain-rate sensitivity and stress decrement. The curve is obtained by the strain-rate cycling test during the Blaha effect measurement and is considered to reflect the influence of ultrasonic oscillation on the dislocation motion on the slip plane containing many impurities and a few forest dislocations [1, 4].

In earlier paper [2], we have described the influence of heat treatment on the relation between temperature and the effective stress, τ_{p1}, due to the divalent impurities. Further, the critical temperature, T_C, at which the effective stress becomes zero and the activation enthalpy, ΔH, for the breakaway of the dislocation from the impurity were also examined for KCl : Sr^{2+} (0.05 mol% in the melt) single crystal. In this paper, we investigate the various force-distance relations between a dislocation and an aggregate in the specimen. The aggregates form at least trimers by heat treatment [6]. In addition, the enthalpy and Gibbs free energy of activation for overcoming of the aggregate by a dislocation are examined for the various force-distance relations.

2. Experimental procedure

2.1. Preparation of specimens

The single crystal of KCl : Sr^{2+} (0.05 mol% in the melt) was cut to the size of about $5 \times 5 \times 15$ mm^3 by cleaving technic. The specimens were kept at 973 K for 24 h and were cooled to room temperature at a rate of 40 Kh^{-1} in order to reduce dislocation density. Furthermore, the specimens were held at 673 K for 30 min and were cooled by water quenching in order to disperse the impurities. Finally, the specimens were prepared by keeping the quenched specimens at 370 K for 500 h and gradually cooling in the furnace for the purpose of aggregating the impurities [6].

2.2. Compression test

The specimens were deformed at temperature range of 83–239 K by compression along the ⟨100⟩ axis and the ultrasonic oscillatory stress was applied by a resonator in the same direction as the compression during the strain-rate cycling test. The stress change due to the strain-rate cycling is $\Delta\tau'$, when the strain-rate cycling is carried out keeping the stress amplitude constant. The strain-rate sensitivity was obtained on the basis of the $\Delta\tau'$. The strain-rate cycling test during the oscillation has been described in detail in the previous papers [1, 5].

3. Discussion for the force-distance relation between a dislocation and the aggregate

It was suggested in the foregoing paper [2] that the force-distance relation between a dislocation and the aggregate for KCl : Sr^{2+} (0.05 mol% in the melt) could not be approximated by the Fleischer's model [7] from the proportionality of ΔH and the temperature, $\Delta H(T)$, when the I-V dipoles turn into the aggregates by the heat treatment. In this paper, various force-distance relations between a dislocation and an impurity are investigated for the same specimens as described in the previous paper [2] on the basis of the dependence of strain-rate sensitivity due to impurities on temperature as follows. Firstly, we assume that the interaction between a dislocation and the aggregate for the specimen can be approximated to the Fleischer's model taking account of the Friedel relation [8]. The model is named the F-F in this paper. Then, the relative formula of τ_{p1} and temperature, which will reveal the force-distance relation between a dislocation and an impurity [1], is given by [9]

$$(\tau_{p1}/\tau_{p0})^{1/3} = 1 - (T/T_C)^{1/2} \quad (1)$$

The result of Equation 1 is shown in Fig. 1. The values of T_C and τ_{p0} obtained from Fig. 1 are given in Table I. The τ_{p0} is obtained by extraporating the line to 0 K and is considered the effective stress due to the aggregates without thermal activation [1]. The relative curve of temperature and the strain-rate sensitivity due to the aggregates for the F-F is represented as a solid line in Fig. 2. The strain-rate sensitivity is calculated from the following equation [9]:

$$\partial\tau/\partial \ln\dot{\varepsilon} = \{(3\tau_{p0}T)/(2T_C)\}(T_C/T)^{1/2} \times \left\{1 - (T/T_C)^{1/2}\right\}^2 \Big/ \alpha \quad (2)$$

where α is an arbitrary constant. The open circles represent the $(\Delta\tau'/\Delta \ln\dot{\varepsilon})_p$ which is given by the difference between strain-rate sensitivity at first plateau region and at second one on the relative curve of strain-rate sensitivity and stress decrement [2, 3, 5]. The open circles seem to be distant from the solid line below 150 K. Therefore, it is difficult to approximate the interaction between a dislocation and the aggregate in the specimen to the F-F. Secondly, we examine the three models [10]: a square force-distance relation, a parabolic one and a triangular one, which are termed the SQ, the PA and the TR respectively in this paper, in the similar way. The three force-distance relations are also taken account of the Friedel relative [8]. The relative formula of τ_{p1} and temperature for the SQ is given by

$$(\tau_{p1}/\tau_{p0})^{2/3} = 1 - (T/T_C) \quad (3)$$

The PA gives

$$(\tau_{p1}/\tau_{p0})^{2/3} = 1 - (T/T_C)^{2/3} \quad (4)$$

and the TR gives

$$(\tau_{p1}/\tau_{p0})^{2/3} = 1 - (T/T_C)^{1/2} \quad (5)$$

The results of Equations 3–5 are shown in Fig. 3a–c for the specimen. The slopes of straight lines are determined by the method of least squares. Further, the strain-rate sensitivity due to the aggregates for the SQ is obtained as

$$\partial\tau/\partial \ln\dot{\varepsilon} = \{3\tau_{p0}/(2T_C)\}\{1 - (T/T_C)\}^{1/2}T/\alpha \quad (6)$$

TABLE I Values of T_C and τ_{p0} for various force-distance relations between a dislocation and the aggregate in the specimen

The force-distance relation	T_C (K)	τ_{p0} (MPa)
F-F	322	10.30
SQ	220	2.17
PA	225	3.28
TR	228	4.53

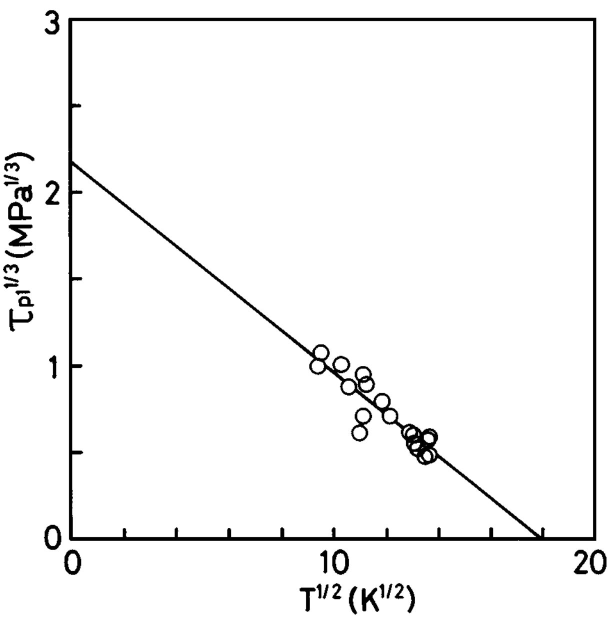


Figure 1 Linear plots of the effective shear stress and the temperature for the specimen at the F-F.

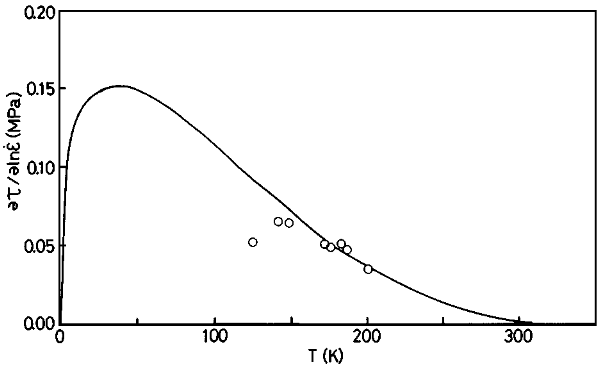
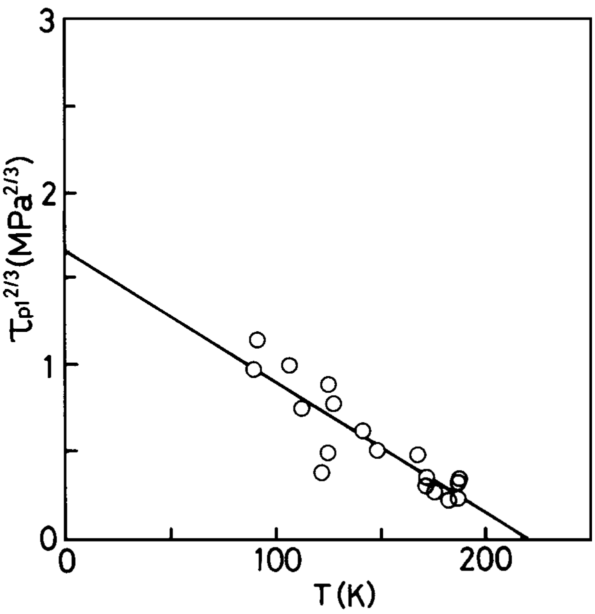
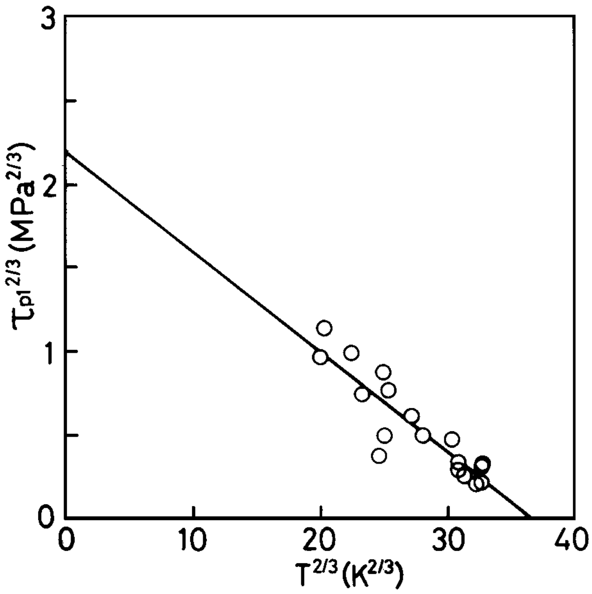


Figure 2 Relationship between the strain-rate sensitivity due to the aggregates and temperature for the specimen. (—) corresponds to the dependence of temperature and the strain-rate sensitivity for the F-F. (○): $(\Delta\tau'/\Delta \ln\dot{\varepsilon})_p$ for the specimen.



(a)



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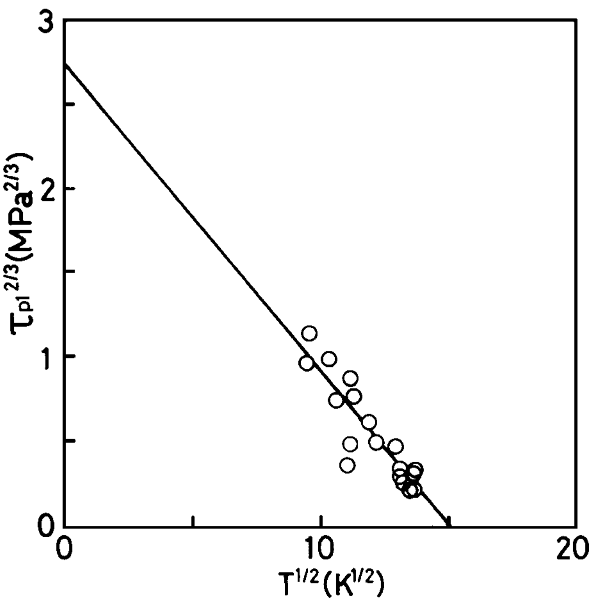


(c)

Figure 3 Linear plots of the effective shear stress and the temperature for the specimen at various models: (a) the SQ, (b) the PA and (c) the TR.

That for the PA is expressed by

$$\partial\tau/\partial \ln\dot{\varepsilon} = (\tau_{p0}/T_C)\{(T_C/T)^{2/3} - 1\}^{1/2}T/\alpha \qquad (7)$$

and also that for the TR is expressed by

$$\partial\tau/\partial \ln\dot{\varepsilon} = \left\{3\tau_{p0}/(4T_C)\right\}\{(T_C/T) - (T_C/T)^{1/2}\right\}^{1/2}T/\alpha \qquad (8)$$

The values of T_C and τ_{p0}, which are obtained from Fig. 3a–c, are given in Table I. The process of leading Equations 6–8 is already described in the previous paper [5]. Fig. 4 shows the strain-rate sensitivity due to the aggregates for the specimen. The curves for the SQ, the PA and the TR are derived from the calculations of Equations 6–8. The open circles correspond to the $(\Delta\tau'/\Delta \ln\dot{\varepsilon})_p$ for the specimen. As can be seen from Fig. 4, the interaction between a dislocation and the aggregate in the specimen may be approximated to the SQ within the temperature. If the $(\Delta\tau'/\Delta \ln\dot{\varepsilon})_p$ for the specimen can be obtained below about 100 K, the most suitable force-distance relation between a dislocation and the aggregate will be distinctly selected among the three from Fig. 4. However, the values below 100 K could not be unfortunately obtained.

We attempt to investigate the relation between the temperature and the ΔH for the interaction between a dislocation and the aggregate in the specimen. The ΔH for the SQ is calculated from the following relation [5]

$$\Delta H = kT^2(\Delta \ln\dot{\varepsilon}/\Delta\tau')_p\{3(1 - T/T_C)^{1/2}\tau_{p0}/(2T_C)\} \qquad (9)$$

where k is Boltzmann's constant. The ΔH for the PA is expressed by [5]

$$\Delta H = kT^2(\Delta \ln\dot{\varepsilon}/\Delta\tau')_p\left[\left\{(T_C/T)^{2/3} - 1\right\}^{1/2}\tau_{p0}/T_C\right] \qquad (10)$$

and also, that for the TR is expressed by [5]

$$\Delta H = kT^2(\Delta \ln\dot{\varepsilon}/\Delta\tau')_p\left[3\left\{(T_C/T) - (T_C/T)^{1/2}\right\}^{1/2}\tau_{p0}/(4T_C)\right] \qquad (11)$$

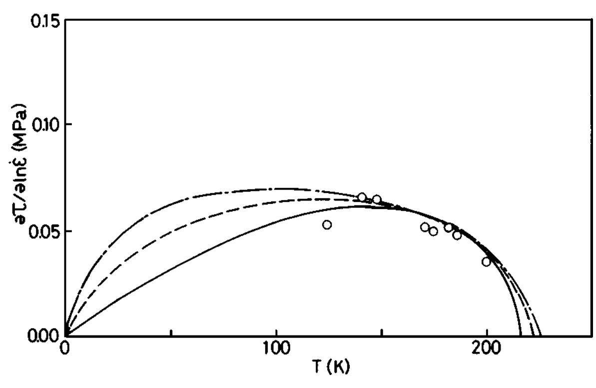


Figure 4 Relationship between the strain-rate sensitivity due to the aggregates and temperature for the specimen. (—) corresponds to the dependence of temperature and the strain-rate sensitivity for the SQ, (– – –) does that for the PA and (– - –) does that for the TR. (○): $(\Delta\tau'/\Delta \ln\dot{\varepsilon})_p$ for the specimen.

TABLE II Values of $\Delta H(T_C)$ for various force-distance relations between a dislocation and the aggregate in the specimen

The force-distance relation	$\Delta H(T_C)$ (eV)
SQ	0.43
PA	0.41
TR	0.41

The results of calculations for $\Delta H(T)$ are shown in Fig. 5a at the SQ, Fig. 5b at the PA and Fig. 5c at the TR respectively. The lines of $\Delta H(T)$ are determined by the method of least squares. However, it is difficult to select the most suitable force-distance relation among the three from the proportionality of $\Delta H(T)$ within the temperature as shown in Fig. 5a–c. The value of $\Delta H(T_C)$ obtained from these figures is given in Table II. The value of $\Delta H(T_C)$ is almost the same for the three force-distance relations from Table II.

4. The Gibbs free energy for overcoming of the aggregate by dislocation

The thermally activated deformation rate, $\dot{\varepsilon}$, is expressed by an Arrhenius equation

$$\dot{\varepsilon} = \dot{\varepsilon}_0 \exp(-\Delta G/kT) \tag{12}$$

where $\dot{\varepsilon}_0$ is a frequency factor, ΔG is the change in Gibbs free energy of activation for overcoming of local barriers by dislocations. The change in Gibbs free energy is expressed for square force-distance relation between a dislocation and an impurity as follows

$$\Delta G = \Delta G_0 - \tau L b d \tag{13}$$

where τ is the effective shear stress, L is the length of dislocation, b is the magnitude of the Burgers vector and d is an activation distance. From the Friedel relation [8], the average spacing, L, of impurities along the dislocation is

$$L = \left\{2L_0^2 E/(\tau b)\right\}^{1/3} \tag{14}$$

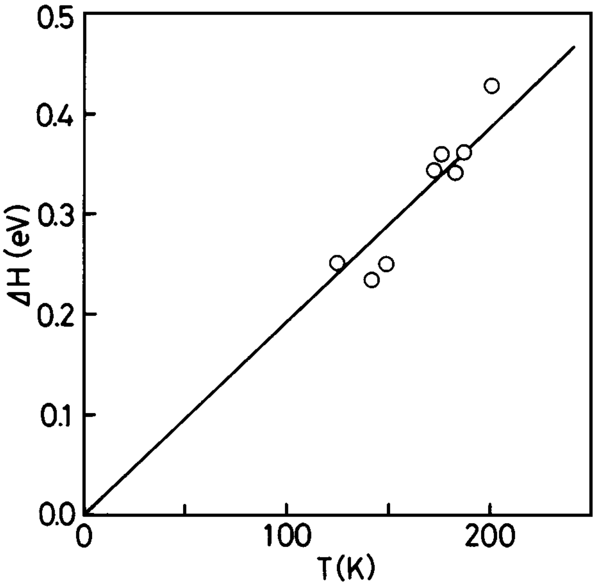
where L_0 is the average spacing of impurities on the slip plane, E is the line tension of the dislocations. Substituting of Equation 14 in Equation 13, the Gibbs free energy for the SQ is given by

$$\Delta G = \Delta G_0 - \beta\tau^{2/3}$$
$$\left(\beta = \left(2\mu b^4 d^3 L_0^2\right)^{1/3}\right) \tag{15}$$

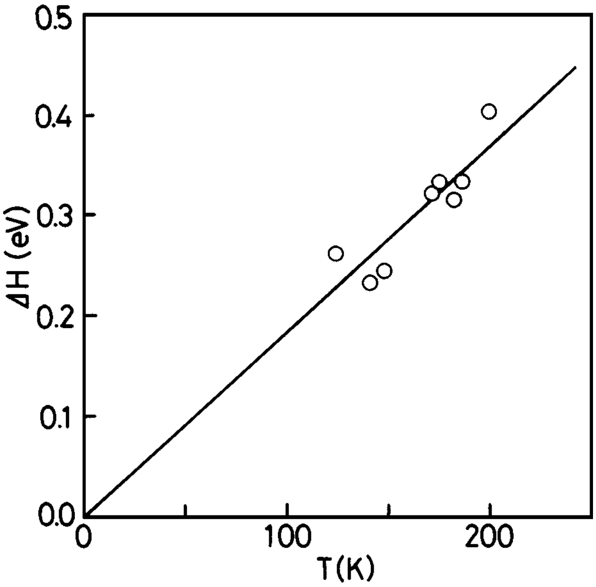
where μ is the shear modulus. Differentiating the substitutional equation of Equation 15 in Equation 12 with respect to the shear stress, we find

$$\tau_{p1}(\partial \ln\dot{\varepsilon}/\partial\tau) = \{2\Delta G_0/(3kT)\} + (2/3)\ln(\dot{\varepsilon}/\dot{\varepsilon}_0) \tag{16}$$

Two other models, namely the PA and the TR, will be examined. The force, F, acted on the dislocation as a function of the distance, x, until the obstacle on the slip



(a)



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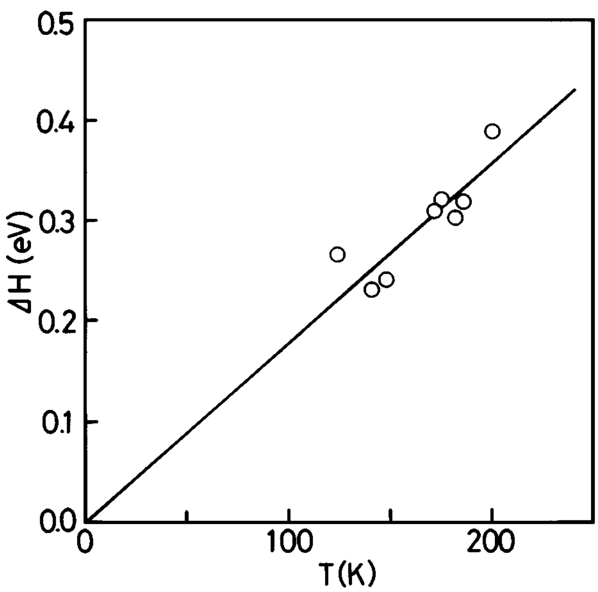

(c)

Figure 5 Proportional relationship between the temperature and the activation enthalpy for the interaction between a dislocation and the aggregate in the specimen at various models: (a) the SQ, (b) the PA and (c) the TR.

plane is

$$F(x) = F_0(1 - |x|^n/a^n), \quad |x| < a$$
$$(F(\pm a) = 0, \quad F(0) = F_0) \tag{17}$$

where triangular $F(x)$ is for the case of $n = 1$ and parabolic $F(x)$ for $n = 2$ [10]. Integrating Equation 17 with respect to x, the Gibbs free energy is given by

$$\Delta G = 2F_0 a\{n/(n+1)\}\{1 - (F/F_0)\}^{(n+1)/n} \tag{18}$$

The Gibbs free energy for the PA obtained from Equations 14 and 18 is expressed by

$$\Delta G = \Delta G_0\left\{1 - (\tau_{\mathrm{p1}}/\tau_{\mathrm{p0}})^{2/3}\right\}^{3/2} \tag{19}$$

Differentiating the substitutional equation of Equation 19 in Equation 12 with respect to the shear stress, we find

$$\partial\ \ln\dot{\varepsilon}/\partial\tau = (\Delta G_0/\mathrm{k})\left\{\left(\tau_{\mathrm{p0}}^2\tau_{\mathrm{p1}}\right)^{-2/3} - \tau_{\mathrm{p0}}^{-2}\right\}^{1/2}\Big/T + (\partial\ \ln\dot{\varepsilon}_0/\partial\tau) \tag{20}$$

From Equations 14 and 18, the Gibbs free energy for the TR yields

$$\Delta G = (\beta/8)\left(\tau_{\mathrm{p0}}^{2/3} - 2\tau_{\mathrm{p1}}^{2/3} + \tau_{\mathrm{p0}}^{-2/3}\tau_{\mathrm{p1}}^{4/3}\right) \tag{21}$$

Similarly from Equations 12 and 21, we find

$$\partial\ \ln\dot{\varepsilon}/\partial\tau = \{4\Delta G_0/(3\mathrm{k})\}\left\{\left(\tau_{\mathrm{p0}}^2\tau_{\mathrm{p1}}\right)^{-1/3} - \left(\tau_{\mathrm{p0}}^{-4}\tau_{\mathrm{p1}}\right)^{1/3}\right\}\Big/T + (\partial\ \ln\dot{\varepsilon}_0/\partial\tau) \tag{22}$$

The results of calculations for Equations 16, 20 and 22 are shown as the open circles in Fig. 6a, b and c respectively. The Gibbs free energy for the interaction between a dislocation and the aggregate in the specimen, which is obtained from the slopes of straight lines in Fig. 6a–c, is given in Table III.

Because the SQ seems to be the most suitable force-distance relation among the three from Fig. 4, we attempt to investigate the width of force-distance curve for the SQ without applied stress from the following equation:

$$d = \{\Delta G_0/(\tau_{\mathrm{p0}}b)\}\left\{\tau_{\mathrm{p0}}b\Big/\left(2L_0^2E\right)\right\}^{1/3} \tag{23}$$

where the line tension of the dislocations is calculated by μb^2. The shear modulus, μ, for [110] direction is

TABLE III Values of ΔG_0 for various force-distance relations between a dislocation and the aggregate in the specimen

The force-distance relation	ΔG_0 (eV)
SQ	0.26
PA	0.18
TR	0.17

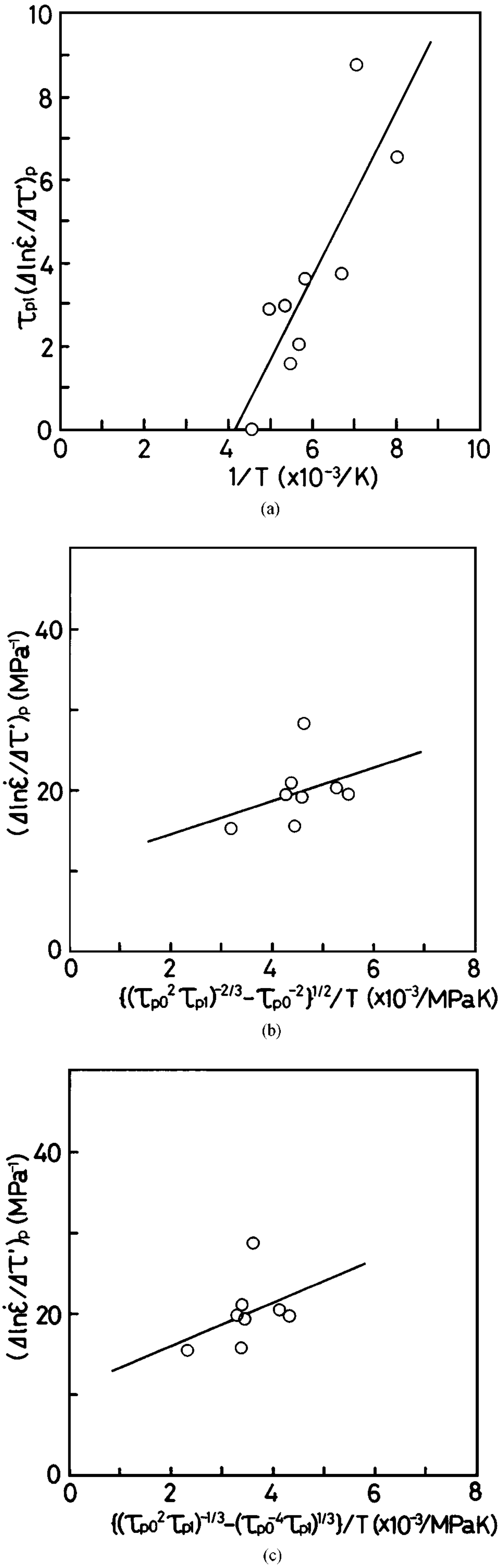

Figure 6 Linear plots of (a) Equation 16 for the SQ, (b) Equation 20 for the PA and (c) Equation 22 for the TR in the specimen.

assumed to be 1.01×10^{10} Pa at 0 K [11]. The average spacing of the aggregates on the slip plane is given by

$$L_0 = b/c^{1/2} \tag{24}$$

where the concentration of the aggregates, c, is 32.1 ppm from atomic absorption method. As a result, the width of the force-distance curve was found to be 1.5 Å less than the magnitude of the Burgers vector.

5. Conclusion

The following results can be found on the basis of the dependence of strain-rate sensitivity due to the aggregates on temperature. The interaction between a dislocation and the aggregate for the specimen can not be approximated to the F-F. The SQ seems to be the most suitable model among the three which are the SQ, the PA and the TR. However, the most suitable model can not be selected among the three from the proportionality of $\Delta H(T)$ within the temperature.

The values of $\Delta H(T_C)$ and ΔG_0 obtained from Figs 5a–c and 6a–c are given in Tables II and III for the SQ, the PA and the TR. The $\Delta H(T_C)$ is almost the same for the three force-distance relations.

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