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# Interaction between dislocation and defects induced by X-irradiation in alkali halide crystals

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# Abstract

Interaction between dislocation and defect induced by X-irradiation has been investigated in NaCl and KCl single crystals by strain rate cycling tests under superimposition of ultrasonic oscillation during plastic deformation. The interaction energy between dislocation and radiation-induced defect has been obtained by fitting Barnett model to experimental results, assuming that the defect is tetragonal. The interaction energies between dislocation and defect were determined to be 0.39 and 0.87eV for NaCl and KCl, respectively. The larger interaction energy for KCl presents its larger tetragonality of defect induced by X-irradiation than NaCl.

Keywords: X-irradiation; Alkali halide; Dislocation; Interaction

# 1. Introduction

It is well known that radiation hardens crystals because dislocation motion is obstructed by defects induced by irradiation (Sibley et al., 1963; Nadeau, 1964; Reppich, 1971; Tanimura et al., 1978). The interaction between dislocation and the defect is not yet clear. Recently, it has been reported that the interaction energy between dislocation and impurity in alkali halide crystals can be obtained from the relation between stress and activation volume. The relation is given by the measurement of the stress decrement due to application of ultrasonic oscillatory stress and the strain rate sensitivity of flow stress under superimposition of ultrasonic oscillation during plastic deformation (Ohgaku et al., 2003, 2005, 2009). We report the interaction between dislocation and

defect induced by X-irradiation in NaCl and KCl.

# 2. Experimental procedure

Samples were prepared by cleaving NaCl and KCl single crystals, which were grown from the melt of superfine reagent powder by the Kyropoulos method in air, in size of  $5x5x15mm^3$  and annealing just below each melting point for 24 hours. The samples were exposed to x-ray (W-target, 30kV, 20mA) for three hours on each of the pair wide surfaces at room temperature. The total exposure time is six hours. Fig.1 shows the absorption spectrum of the X-irradiated NaCl and KCl measured with a Hitachi U-2000 spectrophotometer. Seitz (1946, 1954) has reported the color center of alkali hahide. The peaks of F- (2.7eV) and F<sub>2</sub>-band (1.7eV) are seen in the spectra of X-irradiated NaCl, and there seems to be the peak of V<sub>2</sub>- (5.6eV) band. The peak of 6.7eV is attributed to OH<sup>-</sup> (Klein e al., 1968). In the spectra of the X-irradiated KCl, the peak of F- (2.2eV) band is seen and the peak of 5.8-6.0eV is attributed to V<sub>3</sub>-band and OH<sup>-</sup> (Christy, 1961). The average concentration of F-center is 22.3x10<sup>16</sup> and 2.81x10<sup>16</sup> cm<sup>-3</sup> for NaCl and for KCl, respectively. The F-center concentration in NaCl is ten times larger than in KCl.

A schematic illustration of the apparatus is shown in Fig. 2(a). A resonator composed of a vibrator and a horn with the resonant frequency of 20kHz was attached to an Instron 4465 testing machine. The samples were compressed in the <100> direction along the longest axis of a crystal at the base strain rate  $\dot{\varepsilon}_1$  of  $1.1 \times 10^{-5} \text{s}^{-1}$  for the crosshead speed of  $10 \,\mu$  m min<sup>-1</sup>. When ultrasonic oscillation is applied to the samples in the same direction as the compression, flow stress  $\tau_a$  decreases by  $\Delta \tau$ , as shown in Fig. 2(b). When strain rate changes from  $\dot{\varepsilon}_1$  to  $\dot{\varepsilon}_2$ ,  $\tau_a$  increase by  $\Delta \tau'$ . The procedure was intermittently repeated between the crosshead speeds of 10 and 50  $\mu$  m min<sup>-1</sup> under superimposition of oscillation with various stress amplitude. The stress amplitude  $\tau_v$  was observed with a piezoelectric transducer and was kept constant during a strain rate cycling. The oscillatory strain of a specimen is considered to be homogeneous because the wavelength is about 15 times as long as the length of a specimen.  $\Delta \tau'$  gives strain rate sensitivity  $\lambda (=\Delta \tau'/\Delta \ln \dot{\varepsilon} = \Delta \tau'/\ln(\dot{\varepsilon}_2/\dot{\varepsilon}_1))$ . The tests were carried out in the temperature range between 77 K and room temperature.

#### 3. Results

Fig.3(a) for KCl at 123K shows that  $\Delta \tau$  increases with increasing stress amplitude. Fig.3(b) shows that  $\lambda$  increases with strain and decreases with stress amplitude. The variation of  $\lambda$  with stress amplitude seems to be small at low and high amplitudes. In order to obtain the relation between  $\Delta \tau$  and  $\lambda$  for the given internal structure, their values at the same strain are read from Fig.3 and are plotted at the strain of 10, 12 and 14 % in Fig.4. The variation of  $\lambda$  with  $\Delta \tau$  is stair-like. There are three regions. In the first plateau region at low  $\Delta \tau$ ,  $\lambda$  is constant. As  $\Delta \tau$  increases further, the curve bends and  $\lambda$  decreases with  $\Delta \tau$  in the second region. The curve bends again and the second plateau region appears at large  $\Delta \tau$ . The absolute values of  $\lambda$  tend to be larger as the value of strain increases. The value of  $\Delta \tau$  at the first bending point is referred to as  $\tau_p$  and the difference between  $\lambda$  in the first plateau region and that in the second one to as  $\lambda_p$ , as shown in the figure. The phenomena mentioned above are the same as that described in the previous papers (Ohgaku et al., 2003, 2005, 2009) although obstacle to dislocation motion in this study is neither monovalent nor divalent impurity.

### 4. Discussion

It is reported in the previous papers (Ohgaku et al., 2003, 2005, 2009) that  $\tau_p$  and  $\lambda_p$  defined in Fig.4 are attributed to the interaction between dislocation and point defects.  $\tau_p$  is the stress that is needed when the dislocation overcomes defects with the aid of thermal activation. And  $\lambda_p$  is regarded as a component of strain rate sensitivity due to point defects that is proportional to the reciprocal of average spacing of the defects on dislocation. Then,  $\lambda_p$  gives the activation volume for the thermally activated dislocation motion. The dependence of  $\tau_p$  and  $\lambda_p$  on temperature reflects the interaction between dislocation and defects.

Fig.5 shows the dependence of  $\tau_p$  on temperature. The value of  $\tau_p$  decreases with increasing temperature and appears to be zero at the critical temperature  $T_c$  near room temperature. Fig.6 shows the dependence of  $\lambda_p$  on temperature. Fig.7 shows the relation between  $\tau_p$  and the activation volume that is given by  $\lambda_p$ . The relation reflects the interaction between dislocation and defects.

Barnett et al. (1973) reported the force-distance profile between screw dislocation

and tetragonal defects. Vacancy or F-center has the weak interaction with dislocation and does not act as obstacle to dislocation motion (Zakrevskii et al.). Hole center such as  $V_2$ - or  $V_3$ -center is not isotropic but is considered to be tetragonal. Therefore, they act as strong obstacle to dislocation motion. We assume the force-distance profile given by Barnett et al. for the interaction between dislocation and X-ray induced defects for NaCl and KCl. The solid curves in Fig.5, Fig.6 and Fig.7 were obtained taking account of the Friedel relation (Friedel,1964). The profile is expressed by

$$f = f_0 \alpha^{3/2} \frac{\alpha \xi^2 + 2\sqrt{2}\xi - 1}{(\alpha \xi^2 + 1)^2}$$
$$f_0 = \Omega \Delta \varepsilon C_{44} / 4\pi b ,$$

where  $\alpha$ =1.42 for NaCl and 3.53 for KCl,  $\xi$  is the distance from the position of defect on the slip plane *b* away from it in units of *b*,  $\Omega = 2\sqrt{2}b^3$ ,  $\Delta \varepsilon$  the difference between longitudinal and transverse strains of the distortion around defect, i.e. the tetragonality,  $C_{44}$  the shear elastic modulus and *b* the magnitude of Burgers vector. Calculation was performed using the least square method. Each of the curves agrees with the corresponding data. The parameters used for calculation are listed in Table 1.  $\tau_0$  and  $G_0$ are the value of  $\tau_p$  and the interaction energy between dislocation and defect at absolute zero, respectively. The value  $G_0$  is larger for KCl than for NaCl although the errors are a little large. This means that the tetragonality of defect induced by X-irradiation in KCl is larger than in NaCl. This may be because the obstacle to dislocation motion is V<sub>2</sub>-center in NaCl but V<sub>3</sub>-center in KCl although the effect of OH ion is not clear.

## 5. Conclusion

The interaction between dislocation and X-ray induced defect in NaCl and KCl single crystals has been investigated using strain rate cycling tests under superimposition of ultrasonic oscillatory stress during plastic deformation. The interaction energy is 0.39 and 0.87 eV for NaCl and for KCl, respectively.

The relation between  $\tau_p$  and the activation volume reflects the interaction between dislocation and defects induced by X-irradiation. The tetragonality of defect induced by X-irradiation in KCl is larger than in NaCl.

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## Figure captions

Fig 1. Absorption spectrum of X-irradiated NaCl and KCl.

Fig.2. Schematics of apparatus (a) and stress variation (b) during compression test.

Fig.3. Dependence of (a) the stress decrement  $\Delta \tau$  due to superimposition of oscillation and (b) the strain rate sensitivity  $\lambda$  of flow stress given by strain rate cycling on strain at 123K and various stress amplitudes for X-irradiated KCl. The stress amplitude is monitored by the output voltage from the piezoelectric transducer, which is beside each symbol.

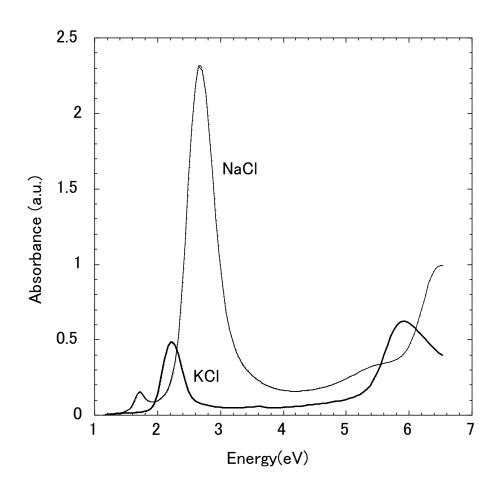
Fig.4. Relation between  $\lambda$  and  $\Delta \tau$  at the strain of 10 (circle), 12 (triangle), 14% (square). The plotted points are obtained from figure 3. The relation is stair-like and has three regions, i.e. two plateaus and a decreasing region between them.  $\tau_p$  and  $\lambda_p$  are defined in the figure. These values give us information about the interaction between dislocation and defect induced by X-irradiation.

Fig.5. Dependence of  $\tau_p$  on temperature for X-irradiated NaCl and KCl. The solid curves are given by numerical calculation.

Fig.6. Dependence of  $\lambda_p$  on temperature for X-irradiated NaCl and KCl. The solid curves are given by numerical calculation.

Fig.7. Relation between  $\tau_p$  and activation volume for X-irradiated NaCl and KCl. The solid curves are given by numerical calculation.

Table 1. Parameters used for calculation.



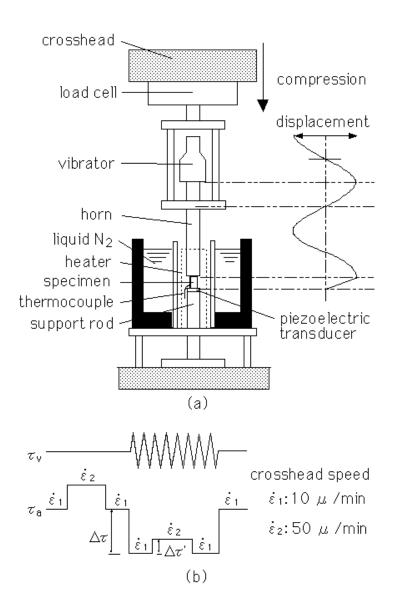


Fig.2

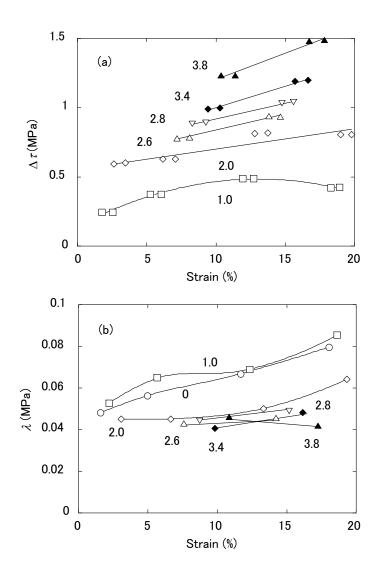
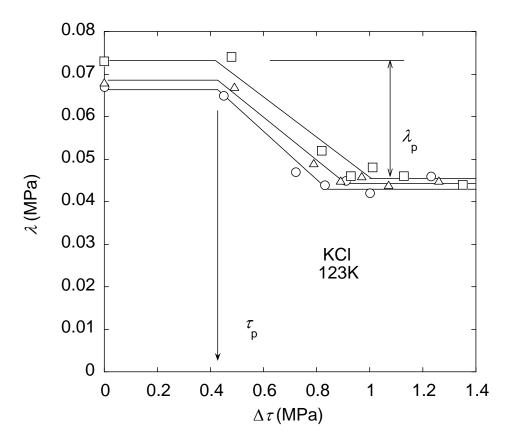


Fig.3



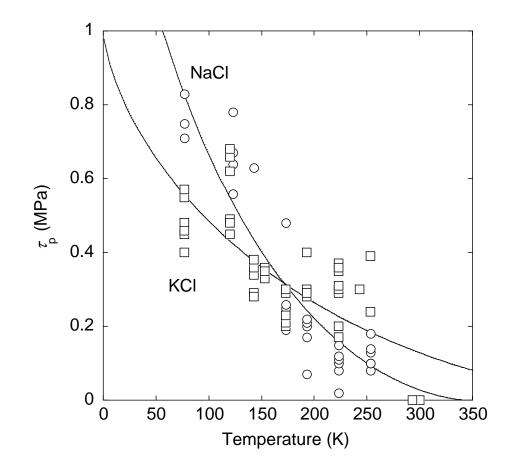
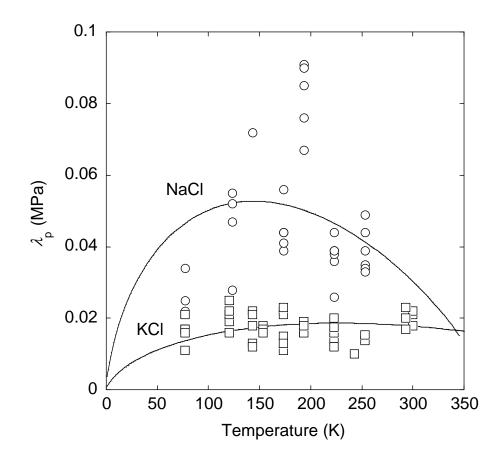
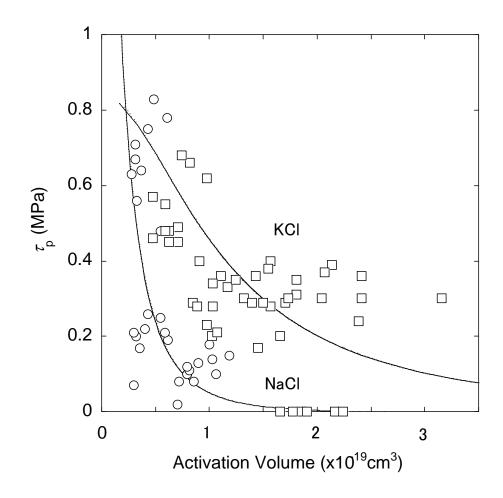


Fig.5





specimen	$ au_{0}$ (MPa)	<i>T</i> <sub>c</sub> (K)	$G_{0}(eV)$
NaCl	1.94	346	$0.39 \pm 0.09$
KCl	1.00	528	$0.87 \pm 0.19$

Table 1.