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## A Note on the Peierls Force

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A simple theory of the Peierls force in covalent crystals was developed. The calculated Peierls forces were 460 kg/mm<sup>2</sup> in silicon and 253 kg/mm<sup>2</sup> in germanium. If there were an internal friction peak due to Seeger's mechanism in germanium, it might be observed at 1300°K for 40 kc/s. The internal friction peak observed at 380°C for 40 kc/s by Kessler was suggested to be due to the motion of kinks dragging vacancies. The low temperature internal friction peaks in some crystals with high Peierls force may be due to the same origin.

### 1. Introduction

Since Seeger<sup>1)</sup> and his co-workers<sup>2)</sup> have developed the theory of the Bordoni peak relating to the Peierls force, many works on this phenomenon appeared to obtain informations about the Peierls force. Peierls forces derived from the measurements of the Bordoni peaks in Al<sub>2</sub>O<sub>3</sub><sup>3)</sup>, MgO<sup>3),5)</sup> and LiF<sup>4),6),7)</sup> are almost equal to that of copper or less than it. This situation is very difficult to understand from the known mechanical properties of these crystals, and it may raise a doubt about the Seeger theory of the Bordoni peak.

The most valuable test of the Seeger theory of the Bordoni peak may be the exact calculation of the Peierls force and comparison with the low temperature internal friction. Now it might be possible to calculate the Peierls force at a reasonable degree of approximation by the help of high speed computing machine in typical metals such as copper, and in typical ionic crystals such as NaCl, KCl. The calculation of the Peierls force, however,

seems to be carried out more easily in covalent crystals because of its high value, and very recently the present author discussed fully the Peierls force in covalent crystals.

In this note a brief account of the calculation of the Peierls force was given and the relation between the Peierls force and the internal friction in germanium measured by Kessler<sup>8)</sup> was discussed.

### 2. The Peierls Force in Covalent Crystals

The perturbation in the atomic configuration around a dislocation is too large to apply any standard approximation to the evaluation of the electronic structure. We are, however, concerned only with the cohesive energy, so the simplest tight binding approximation used by Leman and Friedel<sup>9)</sup> may provide a plausible method to treat the energy change during the motion of a dislocation in the covalent crystal.

In Leman and Friedel's approximation the energies of the valence electrons are shown

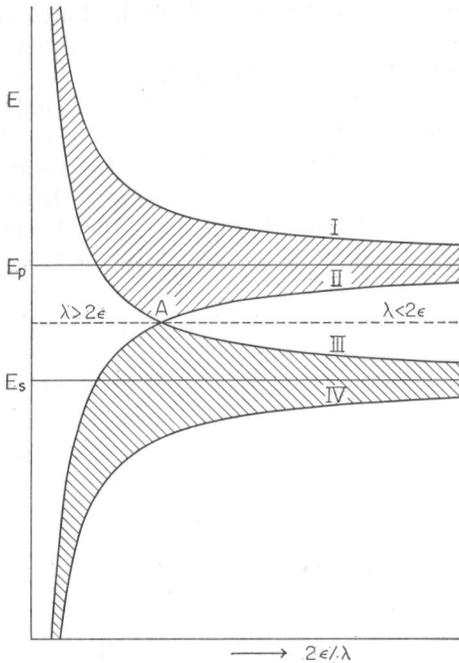


Fig. 1 Variation of  $E$  as a function of  $2\epsilon/\lambda$ : the shaded area corresponds to the allowed energy value.

by Fig. 1, where the abscissa is  $2\epsilon/\lambda$ . Here  $4\epsilon$  is the promotion energy between  $\varphi_s$  and  $\varphi_p$  atomic states, of energy  $E_s$  and  $E_p$ :

$$4\epsilon = E_p - E_s \quad (1)$$

and  $\lambda$  is the overlap integral given by

$$\int \phi_{jm} V_j \phi'_{kn} d\tau = \int \phi_{jm} V'_k \phi'_{kn} = -\lambda \quad (2)$$

where  $\phi_{jm}$  and  $\phi_{kn}'$  are the  $sp$  hybridized atomic orbitals which point along  $n$ -th bond. The band structure is quite different on either side of the intersection point A, where  $\lambda = 2\epsilon$ : a)  $\lambda > 2\epsilon$ : Both the lower and upper bands are made up of two broad subbands and a flat subband which is at the top of each band. Both the lower and the upper bands have 4 electronic states per atom. Both bands have a width  $4\epsilon$ , and the energy gap between them is

$$E_g = 2\lambda - 4\epsilon \quad (3)$$

b)  $\lambda < 2\epsilon$ : The flat subband previously at the top of the lower band, is now at the bottom of the upper band. The lower band is made up of two broad subband, thus contains two electrons per atom. The lower and the upper bands have both a width equal to  $2\lambda$ , and the energy gap has the value  $4\epsilon - 2\lambda$ .

This expression for the energy was obtained

as in usual treatment without destroying the crystal symmetry of the diamond lattice. Leman and Friedel, however, have shown that the valence band in the diamond structure has a nearly pure bonding character in the semiconductive or insulating material, where hybridization has necessarily occurred, and, therefore, the spatial electronic density differs very little from what a mere superposition of independent covalent bonds would give. This expression, therefore, may be applicable to the displacement around a dislocation, where the states of four bonds around an atom are not the same with each other.

Let us consider the energy change during the shear deformation along (111) atomic plane in [110] direction as shown in Fig. 2. It is easily seen that the major part of the shear

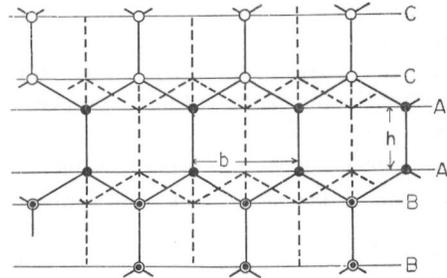


Fig. 2 Shear displacement along (111) plane in [110] direction in the diamond lattice.

displacement takes place between the same-type atomic planes, namely, between AA, BB and CC, but not between AB, BC, CA. It is, therefore, assumed that the shear takes place only between the same type atomic planes. Then the change in the cohesive energy per bond during the displacement may be given by the Leman-Friedel model as follows.

For  $2\epsilon < \lambda$

$$\begin{aligned} E_b/2 &= (E_s + E_p) - [E_{III} + 1/2(E_{III} + E_{IV})] \\ E_{III} &= E_p - \lambda, \quad E_{IV} = E_s - \lambda \\ E_b/2 &= E_s - E_p + 2\lambda. \end{aligned} \quad (4)$$

For  $2\epsilon > \lambda$

$$\begin{aligned} E_b/2 &= (E_s + E_p) - [E_{II} + 1/2(E_{III} + E_{IV})] \\ E_{II} &= E_p - \lambda, \quad E_{III} = E_s + \lambda, \quad E_{IV} = E_s - \lambda \\ E_b/2 &= \lambda. \end{aligned} \quad (5)$$

From (4) and (5) we can see that the restoring force for the displacement decreases abruptly to the half of the previous value when the strain energy of each bond exceeds  $E_p$ , where  $2\epsilon = \lambda$ . Meanwhile, as far as the displacement is small, the deformation obeys Hooke's law

and we have

$$U = \frac{1}{2} \mu \left( \frac{2}{3} \frac{u}{h} \right)^2 \left( \frac{(3/2)h}{n} \right)^2 = \frac{3}{4\sqrt{2}} \mu b^3 \left( \frac{u}{b} \right)^2, \quad (6)$$

where  $U$  is the strain energy of each bond,  $\mu$  the shear modulus in (111) plane,  $u$  the translational displacement of the atomic plane relative to the neighbouring same type atomic plane,  $h$  the distance between the neighbouring same type atomic planes,  $n$  the number of bonds crossing the slip plane,  $b$  the magnitude of the Burgers vector of a perfect dislocation. This relation should hold in the region  $2\varepsilon < \lambda$ , where the strain energy of each bond is less than  $E_g$ . The potential energy in the region where  $2\varepsilon > \lambda$  can not be evaluated, but it may be approximated by a smooth curve provided that the tangent at the point  $2\varepsilon + \delta = \lambda$  is a half of that at the point  $2\varepsilon - \delta = \lambda$ , where  $\delta$  is an infinitesimal positive quantity. The potential energy for the displacement is then represented by the curve in Fig. 3(b).

The displacement  $u_c$  corresponding to the

Table I. Range of elastic deformation

Material	$E_g$ (eV)	$\mu$ ( $10^{12}$ dynes/cm <sup>2</sup> )	$b$ ( $10^{-8}$ cm)	$u_c/b$
C	7	5.04	2.523	0.51
Si	1.19	0.583	3.838	0.330
Ge	0.77	0.433	4.005	0.290

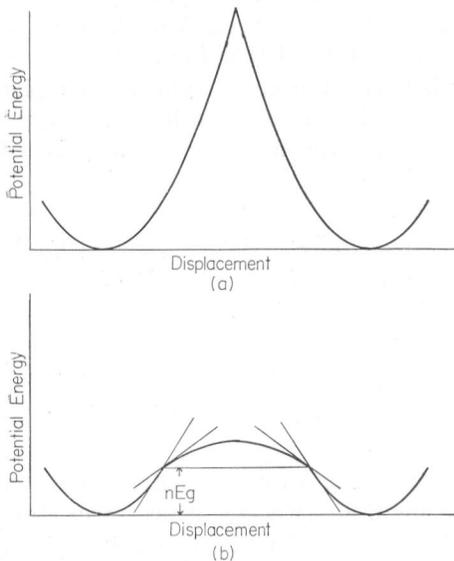


Fig. 3 Schematic representation of the potential energy for the shear displacement: (a) diamond, (b) silicon and germanium.

point  $2\varepsilon = \lambda$ , is shown in Table I. Since  $u_c$  in diamond exceeds  $b/2$ , the potential energy may be denoted as Fig. 3(a).

The Peierls force in a covalent crystal can now be calculated by means of the procedure used by Peierls<sup>(10)</sup> and Nabarro<sup>(11)</sup>. Here we notice only the difference in force between the potential shown in Fig. 3 and the sinusoidal potential. Since the potentials in Fig. 3 deviate from the sinusoidal one only in the region of high energy, the displacement around the dislocation may be approximated by the solution for the sinusoidal potential. The displacement of the upper atomic plane, just above the slip plane, relatively to the neighbouring atomic plane, just below the slip plane, may be given by the relations

$$u - \frac{b}{2} = \frac{b}{\pi} \tan^{-1} \left[ \frac{4}{3} (1-\nu)(x-\xi)/h \right] \quad (7)$$

for an edge dislocation, and

$$u - \frac{b}{2} = \frac{b}{\pi} \tan^{-1} \left[ \frac{4}{3} (x-\xi)/h \right] \quad (8)$$

for a screw dislocation, where  $\nu$  is the Poisson ratio,  $\xi$  the position of the dislocation.

Denoting the force acting between  $i$ -th atom in the upper atomic plane and atoms in the lower atomic plane by  $f_i$ , the relation

$$\sum_i f_i \delta u_i = \sigma \delta \xi, \quad (9)$$

should hold for a small distance motion of the dislocation, where  $u_i$  is the displacement of the  $i$ -th atom,  $\sigma$  is the force acting on the dislocation. If the potential energy for the displacement was sinusoidal curve, (9) should give a nearly same result with that by Peierls and Nabarro. The deviation from the case of sinusoidal curve may be denoted in terms of the atomic bond strained beyond  $E_g$ . The deviation in the force on an atom may be the maximum when the atom in the broken bond form a new bond with the next atom as shown in Fig. 4 (b). The force deviated from the sinusoidal potential energy is then a half of the elastic force at  $u = u_c$ . Since the Peierls-Nabarro force may be negligible for the sinusoidal potential in comparison with the force due to the deviation, the Peierls force for the potential of Fig. 3 (b) is given by

$$\sigma_0 = \left( \frac{\partial u}{\partial \xi} \right)_{u_c} = \frac{1}{\sqrt{2}} \sqrt{\frac{\mu E_g}{b^3}}. \quad (10)$$

The above mentioned approximation may be useful for silicon and germanium, but in

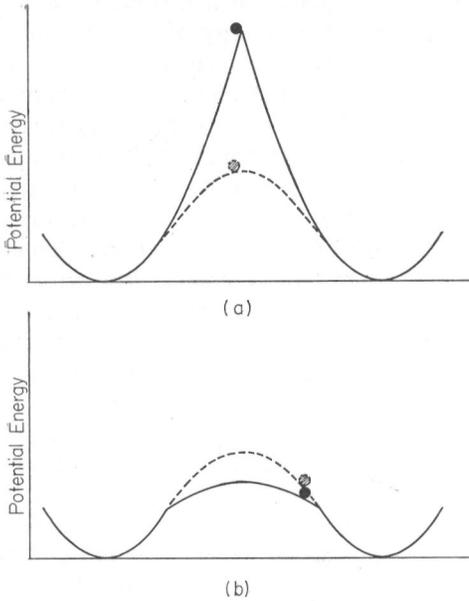


Fig. 4. Difference between the potential in Fig. 3 and the sinusoidal potential: (a) diamond, (b) silicon and germanium.

the case of diamond the energy gap is so large as the potential is given only by the elastic deformation of each bond. The deviation from the sinusoidal potential is denoted as Fig. 4(a). The highest resisting force against the motion of a dislocation corresponds to the case that the bond is sheared by  $b/2$ . The force required to move the dislocation is then

$$\sigma_0 = \left( \frac{\partial u}{\partial \xi} \right)_{u=b/2} \cdot \frac{\mu b}{2h} \quad (11)$$

If the energy gap is less than 0.1 eV, the Peierls force cannot be calculated so simply as above, because the number of bonds strained beyond  $u_0$  is then two or more than two. It may be safe, however, to say that even in such cases the Peierls force should be higher for the potential in Fig. 3(b), which is discontinuous in its derivative, than for the smooth sinusoidal potential.

The Peierls force calculated by the relation

Table II. Peierls forces in covalent crystals at 0°K

Material	$f$ ( $10^{10}$ dynes/cm <sup>2</sup> )	$\left( \frac{\partial u}{\partial \xi} \right)_{u_0}$	$\sigma_s$ ( $10^{10}$ dynes/cm <sup>2</sup> )	$\sigma_e$ ( $10^{10}$ dynes/cm <sup>2</sup> )
C	206	0.78	161	107
Si	11.78	0.574	6.77	4.51
Ge	7.66	0.486	3.72	2.48

(10) for silicon and germanium and by (11) for diamond are shown in Table II. It is seen from the table that the Peierls force for diamond is exclusively larger than the other materials, and it may be impossible to reach this stress level under the usual condition. The Peierls forces in germanium and silicon, however, are not so large and they may be realized under some conditions. For example, Johnston, Stokes and Li<sup>(2)</sup> have shown an unusually high fracture strength of about 300 kg/mm<sup>2</sup>, and obtained definite evidence of generation and motion of dislocations by bending germanium crystals in CP-4 solution.

Table III. Formation energy of a kink pair (eV)

Material	C	Si	Ge
Energy	9.7	2.30	1.67

The Peierls potential for the motion of dislocations in a covalent crystal has some different characters from those in Peierls-Nabarro's approximation. The potential energy for the motion of a dislocation increases steeply near the top and is given approximately by the relation

$$V = \alpha(x-na)^2, \quad (12)$$

where  $\alpha$  is a constant,  $x$  the position of the dislocation,  $a$  the distance between the neighbouring potential valley, and  $n=0, \pm 1, \pm 2, \pm 3, \dots$  satisfying the relation

$$|x-na| \leq \frac{a}{2}.$$

The activation energy required to move a dislocation forming a kink pair is then obtained by the usual method and we have

$$2W_k = a \sqrt{\frac{ab\sigma_0 T}{2}} \left( 1 - y + \frac{1}{2} y \log y \right), \quad (13)$$

where  $\sigma_0$  is the Peierls force,  $T$  the line tension of the dislocation and  $y = \sigma/\sigma_0$ .

### 3. Comparison with the Internal Friction Measurements

The discussion in the previous section showed that the deformed germanium crystal will have an internal friction peak with the activation energy of about 1.7 eV due to the mechanism proposed by Seeger. The internal friction peak due to the Seeger mechanism should appear around 1300°K for 40 kc/s, where germanium melts. Kessler<sup>(3)</sup>, however, meas-

ured another internal friction peak around 380°C and also exponential increase of internal friction above 500°C with an activation energy of about 1 eV. The peak at 380°C decreases by the deformation of the crystal, while the exponential growth increases. Kessler concluded that the internal friction is due to the motion of dislocations dragging vacancies around them. This means that dislocations can easily move at these temperatures. Meanwhile, the discussions in the previous section indicate that the motions of dislocations are prohibited at these temperatures for the frequencies of 40 kc/s. Meanwhile, the motion of kinks seems to require far less activation energy than the formation of kinks. The internal friction observed by Kessler seems to be due to the rearrangement of vacancies around the dislocation by the one atomic distance migration of dislocation through the kink motion. The amplitude of dislocation migration in Kessler's estimation was about  $5 \times 10^{-9}$  cm, and this distance does not seem to induce the rearrangement of vacancies.

The above discussions suggest that there may be other internal friction peak due to the motion of kinks dragging point imperfections than that due to Seeger's mechanism. Interstitial atoms seem to be created during cold work and form an atmosphere around dislocations. In some cases interstitial atoms can be absorbed into dislocations but in other cases such as extended dislocations or interstitial atoms in ionic crystals may be hindered to be absorbed into the dislocations. These interstitial atoms may be the origin of the internal friction as the vacancies in 380°C peak in germanium.

Suda and Suzuki have measured recently the creep in KCl crystals over a wide temperature range and found that the creep was almost completely inhibited between 0°C and 200°C, while conspicuous creep was observed at low temperatures. This observation suggests that dislocations in KCl deformed at room temperature are locked by the cloud

point defects. Johnston and Gilman<sup>13)</sup> showed that the activation energy of the motion of a dislocation in LiF was almost constant and was about 0.7 eV at the temperatures between 200 and 300°K, but decreased considerably if the measurement at liquid nitrogen temperature was included. The activation energy of 0.7 eV is almost the same as that of the migration of lithium ion vacancy. Thus it may be suggested in comparison with germanium that the velocity of dislocations in LiF crystal is determined by the vacancy dragging motion. Since the migration energy of the interstitial atoms in ionic crystals may be smaller than the vacancies, the interstitial dragging motion of kink may take place at lower temperatures.

Of course, the internal friction caused by the above mentioned mechanism is significant at low temperatures only in crystals with high Peierls force. The apparent smallness of the Peierls force in applying Seeger's theory to the low temperature internal friction peak might arise from the neglect of such kink motions dragging point imperfections.

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