

# Theory of Plasticity I : Correlation between Lattice Transformation and Plastic Gliding in Metals

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# Theory of Plasticity I.

## Correlation between Lattice Transformation and Plastic Gliding in Metals

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### Synopsis

Two fundamental relations, which are essential to express the resistance against the plastic gliding in terms of the thermodynamic function were derived, by considering the structure of dislocation. One is a relation which connects the free energy difference  $\Delta G$  dissipated during the lattice transformation with the mechanical energy  $f \cdot \Delta L$  required for the plastic gliding and it has been assumed in the previous report. Here  $f$  is the resistance against the plastic gliding and  $\Delta L$  the amount of deformation in the process of lattice transformation, its numerical value being 0.306. Another relation gives a method to obtain the free energy difference  $\Delta G$  for a crystal in which the lattice transformation cannot take place under the usual condition.

### I. Introduction and the condition of lattice transformation

It is well known that attempts to derive the mechanical properties of crystals by means of the lattice theory have failed as yet<sup>(1)</sup>; the tensile strength, for example, estimated in this way, is about one hundred times larger than the observed values<sup>(2)</sup>. The lack of success in these attempts has led many physicists to believe that real crystals should include various types of imperfection such as small holes or cracks, etc., which could considerably diminish their strength, consequently attempts on using various models for the imperfection in crystals have been performed so far<sup>(3)</sup>. Of these, the dislocation model<sup>(4)</sup> has been accepted as the most appropriate one. It is generally supposed that the plastic gliding in crystals takes place through the propagation of dislocations along slip planes.

Peierls<sup>(5)</sup> has proved that, when dislocations exist in crystal, the plastic gliding proceeds under such a small stress found in actual observations. Though considerable rough approximations were used in his calculation, the essential feature of the propagation

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\* The 554th Report from the Research Institute for Iron, Steel and Other Metals.

- (1) M. Born; *Atomtheorie des festen Zustandes*, Berlin (1923), F. Zwicky; *Phys. Z.*, 24 (1923) 131; M. Born and R. Fürth; *Proc. Camb. Phil. Soc.*, 36 (1940) 454.
- (2) M. Born and R. Fürth; *Proc. Camb. Phil. Soc.* 36 (1940), 454.
- (3) A. Smekal; *International Conference on Physics II*, London (1935), 93, A. A. Griffith; *Phil. Trans. Roy. Soc., A* 221 (1921), 163.
- (4) G. I. Taylor; *Proc. Roy. Soc. A* 145 (1934), 362.
- (5) R. Peierls; *Proc. Phys. Soc. London*, 52 (1940), 34.

of dislocation was described correctly for the crystal which contains only one dislocation as the imperfection. But further considerations are required to calculate the resistance against motion of the dislocation in cases as follows: when the crystal includes atomic defects such as vacant lattice sites and different sorts of constituent atoms, etc., or when effects of thermal vibration should be in question, these are practically conceivable figures of natural substances. The dynamical theory of this problem should fail on account of mathematical complexity of the many body problems. We can only expect to avoid the difficulties on calculation by means of statistical treatment, and it will be the first step towards this direction to express the resistance against gliding in terms of thermodynamic function.

In the previous paper<sup>(6)</sup>, starting from the fact that the lattice transformation which occurs in the supercooled  $\gamma$  phase of carbon steels or iron-nickel alloys resembles the plastic gliding in their crystallographic mechanisms, we have assumed a relation which connects the conditions for occurrence of the plastic gliding with that of the lattice transformation. This relation is expressed as

$$\Delta G = f\Delta L,$$

and

$$\Delta L = 0.306,$$

where  $\Delta G$  is the free energy irreversibly dissipated in the process of the lattice transformation per unit volume,  $f$  the resistance against gliding per unit area and  $\Delta L$  the amount of deformation accompanied by the lattice transformation.

As one of the authors has already shown<sup>(7)</sup>, the lattice transformation in such alloys neither takes place at the temperature at which both crystal phases  $\alpha$  and  $\gamma$  are in equilibrium with each other nor at the temperature at which the free energies of them having the same concentration are equal, but it takes place, on cooling, at the lower limiting temperature in the coexisting region of two phases in which both crystal phases are in equilibrium, and on heating, at the upper limit. The free energies of both states are shown schematically in Fig. 1 in connection with the phase diagram of the alloy. When the lattice transformation  $\gamma \rightarrow \alpha$  occurs on cooling, the  $\gamma$  phase must be in a state of excessive free energy compared with the  $\alpha$  state by a certain amount  $PQ$ , which is represented as the free energy difference between both states when a tangent, drawn for the free energy curve of  $\alpha$  state at the concentration  $x_1$  in consideration, comes to the common tangent for the free energy curves of both states. In this way, a definite amount of free energy is irreversibly dissipated in the process of lattice transformation. The resistance against gliding, therefore, can be expressed in terms of thermodynamic function by applying the thermodynamic condition of the lattice transformation.

(6) S. Takeuchi and H. Suzuki; Rep. RITU. 2 (1950), 43.

(7) S. Takeuchi; Sci. Rep. RITU. 1 (1949), 43.

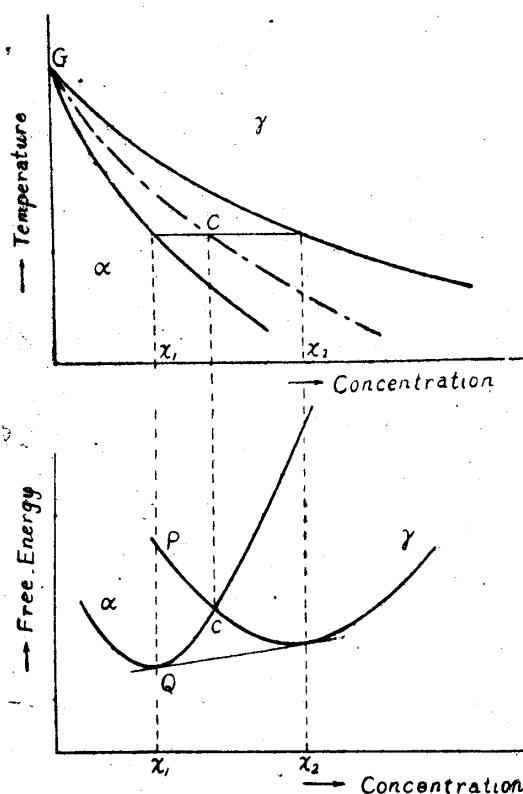


Fig. 1. Condition of the lattice transformation

In the following sections, by detailed considerations on the structure of the dislocation centre, we will justify the relation assumed in the previous paper and discuss a method to obtain the free energy difference  $\Delta G$  for a crystal in which the lattice transformation can not take place under usual conditions.

## II. Dislocation model (the first relation)

In the dislocation theory developed by Orowan<sup>(8)</sup> and Taylor<sup>(4)</sup>, detailed discussions concerning the center of dislocation have been omitted because the distortion of lattice around it is beyond any argument of the theory of elasticity and it was considered that the propagation of dislocation could be obstructed only by the mutual interference of elastic strain around the dislocation. However, we must suppose that the motion of dislocation should be mainly governed by conditions for the motion of its

center, being not determined only by the interference of elastic strain around it, because the energy of dislocation is to be stored as the energy of lattice defects in its centre much more than as the elastic energy in its surrounding. Since the atomic arrangement in the strongly distorted region in the neighborhood of dislocation centre depends upon the type of crystal system, we will confine ourselves to the discussion on the case of a crystal system having face centred cubic lattice.

In this case the plastic gliding takes place to the direction  $[110]$  along the slip plane  $(111)$ , on which the atomic arrangement is indicated in Fig. 2 by marks  $\bullet$  representing the relative positions of atoms on the plane I neighboring to the plane II where atoms are in positions shown by marks  $\circ$ . Though the plastic gliding proceeds by relative displacement of atoms  $\bullet$  of the upper plane I to atoms  $\circ$  of the neighbouring plane II through the motion of dislocation, there is no reason to believe that each atom on the plane I should move on straight towards the  $[110]$  direction. It is rather natural to consider that respective atom moves along the courses of the lowest energy, which are most remote from atoms on the neighbouring atomic plane. We can suppose that these courses are along the direction  $[211]$ , but zigzag as shown by broken lines in Fig. 2 and

(8) E. Orowan; Z. Phys. 89 (1934), 634

they must be parallel to the  $[110]$  direction in average. In this case, of course, it is unnecessary to consider that the atomic plane II is fixed and atoms on the plane I alone move on the zigzag path, we should suppose that atoms on both planes displace relatively so as to pass through the configuration as shown in the figure.

In Fig. 2, 1 represents the configuration of the face centred cubic lattice in the initial state, and when the atom in 1 arrives at position 2 the relative displacement comes to 0.353, consequently it will not be regarded as an elastic deformation but rather resembles the displacement of atoms in the lattice transformation of f.c.c. lattice  $\rightarrow$  b.c.c. lattice. In the

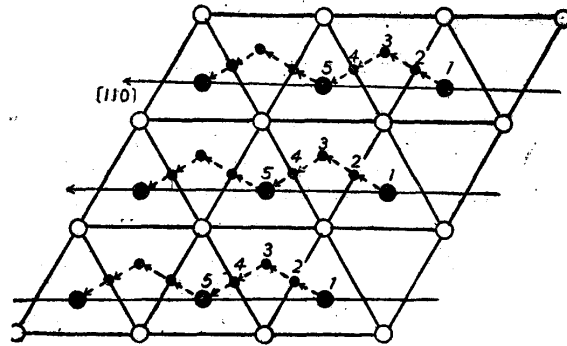


Fig. 2. Path of atoms on the  $(111)$  plane in the process of gliding

Nishiyama's mechanism, for example, (see Fig. 3) lattice points in (a) which constitute the f.c. lattice turn into the sites which are shown in (b) after the transformation to the b.c.c. lattice. This process is equivalent to the displacement of atoms from the position 1 to 2 in Fig. 2. The displacement  $2 \rightarrow 3$  corresponds to the reverse transformation b.c.c.  $\rightarrow$  f.c.c. The configuration in the position 3 represents a state of twin to the initial state 1 of f.c.c. lattice. In the same way, the displacements  $3 \rightarrow 4$  and  $4 \rightarrow 5$  are equivalent to the lattice transformation f.c.c.  $\rightarrow$  b.c.c. and b.c.c.  $\rightarrow$  f.c.c. respectively. When the relative positions of atoms change in this way, some amounts of expansion and contraction in lattice spacing responding to this change are added.

The potential energy curve plotted against the amounts of displacement of the neighbouring two atomic planes in the direction of gliding, even in a schematic consideration, will not be approximated by a sinus curve with the period of one atomic distance, but, in addition, a potential with the period of  $1/4$  atomic distance will be superposed on it. Then the usual picture on the extension of dislocation will be modified more or less. But we shall omit further discussions on the form of

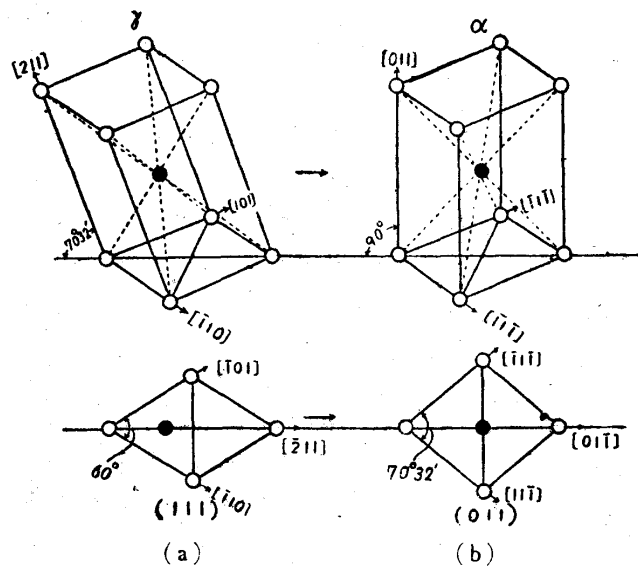
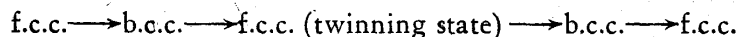


Fig. 3. Nishiyama's mechanism in the lattice transformation

of potential, for it has little relation to the following discussion concerning the resistance against gliding.

Thus, it can be considered that the plastic gliding of one atomic distance along the slip plane (111) to the direction [110] in face centred cubic lattice consists of the process of four repetitions of lattice transformation as follows:



where the free energy dissipated on each of such transformations has the same value of  $\Delta G$ . Consequently, we may conclude that the energy to be dissipated irreversibly by the plastic gliding of one atomic distance is equal to the free energy to be required for the transformation repeated four times.

Let  $f$  be the resistance against gliding,  $\Delta G$  the free energy per mole to be dissipated in the process of the lattice transformation and  $V$  the volume occupied by a mole of the crystal, we have

$$4\Delta G = V \cdot f \cdot l,$$

where  $l$  is the amount of gliding in the direction [110] corresponding to the displacement of one atomic distance, so that

$$l/4 = 0.306.$$

Rewriting the above relation, we have

$$\left. \begin{aligned} \Delta G &= V \cdot f \cdot \Delta L \\ \Delta L &= 0.306 \end{aligned} \right\} \quad (1)$$

This is the first relation which connects the resistance against gliding with the free energy of the lattice transformation and it has been assumed in the previous paper<sup>(6)</sup>.

### III. The second relation

The resistance against the plastic gliding, the critical shear stress,  $f$ , of various metals or alloys can easily be estimated by means of the relation (1) when their free energies  $\Delta G$  for the lattice transformation are known. However, the lattice transformation can not always take place in metals and alloys, so we must find a method to determine  $\Delta G$  for any metal or alloy to calculate the resistance against gliding by means of (1). In the dislocation model described in II, we have considered that the transformation takes place in the neighbourhood of the dislocation centre even in cases of metals or alloys having no transformation under ordinary condition. If the metals and alloys were put under the same condition as at the circumference of the dislocation centre, the condition for occurrence of transformation is satisfied, and  $\Delta G$  is calculated in accordance with the theory of lattice transformation. The reason why the transformation can occur around the dislocation centre is in the fact that in its circumference there exists so far larger stress that the lattice around the dislocation centre is forced to deform far beyond the ordinary limit of elastic strain of the crystal, changing it to the other type of lattice as a result.

In order to carry out the thermodynamic treatment of this process, let us suppose the following ideal process: The whole system consists of a rigid holder  $F$ , on which the face centred cubic crystal  $C$  in consideration is set up, a spring of strength  $X$  giving an external stress to the crystal and a rigid wall  $E$  by which further deformation of the crystal beyond  $\Delta L$  are prevented (see Fig. 4). The crystal is stuck on the flat holder with non-viscous paste at the plane  $AD$  parallel to the plane (111) and fixed only at the point  $A$  rigidly on the holder, so that the crystal does no work by the expansion or contraction, which should be accompanied in the process of the lattice transformation. The spring has no weight and a sufficiently large length that its strength is always kept parallel to the glide direction in the crystal even if the transformation takes place.

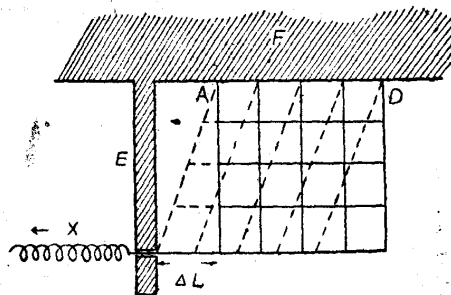


Fig. 4. Imaginary transformation

Since the crystal in this ideal process corresponds to a very small part around the dislocation, its deformation may always be uniform except for the instants when the crystal lattice is in the course of displacement. The potential energy due to the uniform shearing deformation of the crystal has the same feature as that in the case of relative displacement of the neighbouring two atomic planes. According to the argument in II, the potential energy on account of the relative displacement of the neighbouring two atomic planes, even for a schematic consideration, will not be represented by a sinus curve with the period of one atomic distance, but, in addition, a potential with the period of  $\frac{1}{4}$  atomic distance will be superposed on it. Hence the potential curve has two inflection points in the interval of deformation 0 to  $\frac{1}{4}$  atomic distance. In this ideal process, owing to the rigid wall  $E$ , the crystal can not deform beyond  $\Delta L$ , namely, the potential energy will be represented as Fig. 5, where the full line corresponds to the case of stress free, and the broken line corresponds to the case of stress  $X$ . As easily seen in this figure, the amount of deformation of crystal is either less than that corresponding to the first inflection point on the potential curve which is one nearer to the initial state or just  $\Delta L$ , which is the amount of deformation in the process of lattice transformation and is equal to the relative displacement of  $\frac{1}{4}$  atomic distance between the neighbouring two atomic planes. We consider, in the ideal process, that the state of crystal deformed uniformly by  $\Delta L$  is nothing but the state transformed to the imaginary crystal phase, which is taken as a body centred crystal state.

We have assumed the uniform deformation only in the state of rest, but not in the course of motion. It is rather natural to suppose the deformation as being non-uniform when the crystal lattice is in the course of displacement, because the crystal contains sufficiently many degrees of freedom and the potential energy will be diminished in the case of non-uniform deformation compared with the uniform one. Therefore, it is not necessary to consider that in order to transform the crystal the strength of the spring

should exceed a certain value to be required to pass over the steepest region of the potential curve, namely, the first inflection point in Fig. 5.

At any rate, in thermodynamics all considerations concern only the stationary states, in other words, all considerations do not depend on the process of transition with a finite rate. As the strength of the spring increases with an infinitesimal small rate, the deformation

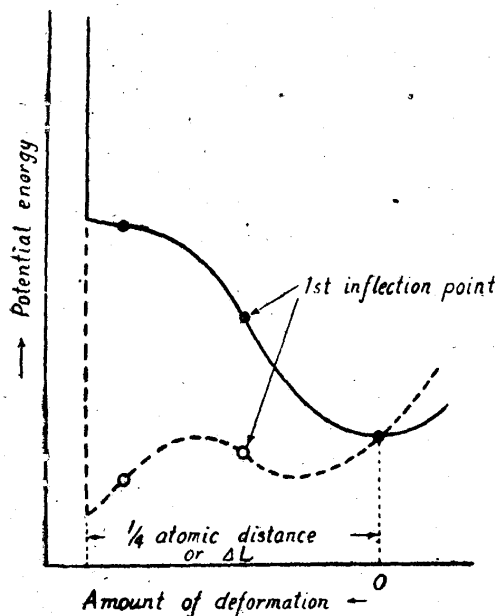


Fig. 5. Potential energy in the imaginary transformation

of crystal proceeds with an infinitesimal small rate satisfying the relation represented by the potential curve in Fig. 5. When the deformation takes place with a finite rate under the force  $X$ , it should continue until it becomes  $\Delta L$ , because, if the crystal is at rest, the spring should be balance with the potential force in Fig. 5, but according to the argument about the potential curve this condition can not hold except for the case of transformed state, or the reversibly deformed state at the instant after when the deformation immediately takes place with a finite rate.

The strength  $X$ , at which the deformation takes place with a finite rate, is nothing but the strength which causes the

imaginary transformation in this ideal process. Under this stress the crystal is either in the reversibly deformed state or in the transformed and the free energies of these two states should satisfy the condition of lattice transformation. When the crystal is deformed reversibly, the Gibbs' free energy of this system can be expressed as the summation of the following terms, if the energy zero is referred to the state of spring at the time when the crystal under the stress of spring deforms reversibly up to the limiting value, beyond which it deforms immediately with a finite rate: Helmholtz's free energy of the crystal in stress free state...  $F^r$ ,

and increase of the internal energy by the reversible strain...  $V \int_0^{\delta L} P dl$ .

The Gibbs' free energy  $G^r$  is, then,

$$G^r = F^r + V \int_0^{\delta L} P dl$$

where  $V$  is the volume occupied by a mole of the crystal,  $\delta L$  the amount of reversible deformation under the force  $X$ , and  $l$  an amount of strain under a shearing stress  $P$ . Of course the above integral satisfies the relation

$$X\delta L > \int_0^{\delta L} P dl \geq \frac{X\delta L}{2}$$



therefore,

$$\left. \begin{aligned} G^r &= F^r + V \cdot \alpha \cdot X \cdot \delta L, \\ 1 > \alpha &\geq \frac{1}{2} \end{aligned} \right\} \quad (2)$$

The Gibbs' free energy for the transformed state is given similarly: Helmholtz's free energy of the crystal in stress free state..... $F^i$ , and decrease of the potential energy of spring..... $V \cdot X(\Delta L - \delta L)$ .

The Gibbs' free energy  $G^i$  is, then,

$$G^i = F^i - V \cdot X(\Delta L - \delta L)$$

Consequently the condition of lattice transformation is satisfied when the quantities  $G^r$  and  $G^i$  change by  $\alpha \cdot V \cdot X \cdot \delta L$  and  $V \cdot X(\Delta L - \delta L)$  respectively under the stress  $X$ , where  $1 > \alpha \geq 1/2$  and  $\delta L < \Delta L$ . Namely, by the ideal process, we can consider that the crystal is able to transform into the other crystal lattice which is unstable and can not exist under ordinary circumstances.

The thermodynamic condition for lattice transformation is represented by the condition of common tangent for the free energy *vs.* concentration curves of both phases before and after the transformation as described in I. Therefore, when the Gibbs' free energies obtained as above are plotted against the concentration of the alloy, a tangent drawn for the  $G^i$  *vs.* concentration curve of transformed state at the given concentration  $x_1$  must be the common tangent for the curves of both  $G^i$  and  $G^r$  to satisfy the condition of lattice transformation. The  $G^i$  *vs.* concentration curve is obtained by making to shift the  $F^i$  *vs.* concentration curve downward vertically to the axis of concentration as far as the constant amount  $V \cdot X \cdot (\Delta L - \delta L)$  and the  $G^r$  curve by making to shift the  $F^r$  curve upward as far as  $V \cdot \alpha \cdot X \cdot \delta L$ . The quantities  $V \cdot X \cdot (\Delta L - \delta L)$ ,  $V \cdot \alpha \cdot X \cdot \delta L$  and the strength  $X$  depend upon the concentration  $x_1$  of crystal in consideration

Let us illustrate the above description graphically in Fig. 6, in which the free energy *vs.* concentration curves for the actual crystal state and for the imaginary state produced by the transformation are drawn by full lines for the states free from stress. When the external stress  $X$  is applied by the spring to the given crystal these curves shift vertically to the concentration axis, maintaining the same shape, as far as the positions indicated by broken lines respectively, so that the condition of the transformation is satisfied at  $x_1$ .

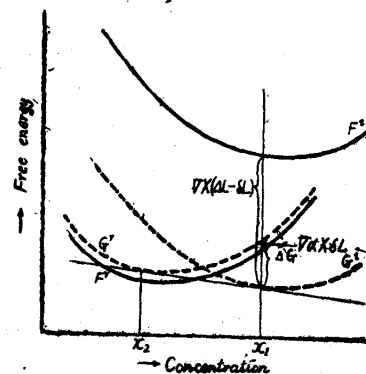


Fig. 6. Schematic diagram showing the change of free energy in the ideal process

The free energy of the imaginary phase, which is unstable under ordinary conditions,

is always higher than that of the real crystal phase, so that we have

$$F^i > F^r.$$

But when the both phases satisfy the condition of lattice transformation as a result of imposing the stress in the ideal process:

$$V \cdot f \cdot \Delta L = \Delta G = G^r - G^i = F^r - F^i + V \cdot a \cdot X \cdot \delta L + V \cdot X (\Delta L - \delta L).$$

$$\therefore V \cdot f \cdot \Delta L > V \cdot X \cdot \Delta L - V \cdot X \cdot \delta L (1 - a).$$

All quantities in this expression are positive, so it follows

$$f > X,$$

and also the quantity  $(1 - a) \cdot V \cdot X \cdot \delta L$  is sufficiently small compared with  $V \cdot X \cdot \Delta L$  as shown in the following calculations. This inequality tells us that the stress required for the forced transformation around the dislocation centre should be always greater than the resistance against gliding, and this is nothing but the characteristic feature concerning the dislocation.

Thus the second relation is expressed as follows: In order to suppose the transformation for the crystals which could not transform under ordinary condition, it is necessary and sufficient to reduce the free energy of the imaginary phase which could be obtained after the transformation until the condition of the lattice transformation, which is the free energy *vs.* concentration curves for real and imaginary phase to be in contact with the common tangent, is satisfied. In this operation the free energy *vs.* concentration curves shift without changing their shape.

#### IV. Summary

Two fundamental relations, which are essential to express the resistance against plastic gliding in terms of the thermodynamic function were set up, by considering the structure of dislocation centre.

(I) Let  $\Delta G$  be the free energy difference, per mole, dissipated in the process of latticet transformation,  $f$  the resistance against gliding and  $V$  the volume occupied by a mole of the crystal, we have

$$\Delta G = V \cdot f \cdot \Delta L \quad (\Delta L = 0.306).$$

(II) In order to suppose the transformation for the crystals which could not transform under ordinary condition, it is necessary and sufficient to diminish the free energy of the imaginary phase which would be obtained by means of the transformation, until the free energy *vs.* concentration curves for real and imaginary phase come in contact with the common tangent.

The relation (I) was derived by considerations on the displacement of atoms in slip planes of crystals, in which it was shown that a gliding displacement of one atomic distance through the motion of dislocation is equivalent to repeating the lattice transformation four times.

The lattice of small region around the dislocation centre is distorted far beyond the elastic strain of crystal under the strong field of force around the centre. When such deformed lattice is regarded as a state of the other type of lattice, thermodynamic conditions of lattice transformation for the crystal, in which the transformation can not occur under usual circumstances, should be satisfied. We obtained the relation (II) by means of an ideal process concerning the deformation of crystal under a strong field of stress, namely, under the stress field around the dislocation centre.

Now, we can calculate the resistance against gliding for any crystals, whose thermodynamic functions are known, by using these two relations.