北海道大学工学部研究報告
第 140 号（昭和 63 年）

Bulletin of the Faculty of Engineering,
Hokkaido University. No. 140 (1988)

A Unified Study of Thermally Activated Dislocations Motion with the Dynamic Effect in a Random Distribution of Point Obstacles

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(Recieved December 26, 1988)

Abstract

In order to investigate dislocations behavior at cryogenic temperature, a unified study is attempted to incorporate the thermal activation process, the string model of Granato, Friedel statistics of hardening and Sumino's concept of steady state deformation into a single equation. The deterministic nature of the string model is compromised with the thermal activation process by following Suzuki's concept which considers the average effect during the decay time of a vibrating dislocation. The calculated results not only reproduced experimental tendencies at moderate temperatures but also revealed the peculiar nature caused by the dynamic effect at cryogenic temperatures.

1. Introuduction

Theoretical studies of solid solution hardening which have been advanced so far may be most conveniently classified into the following three categories: 1. elementary interaction force between a single dislocation and an obstacle, 2. statistical problem arising from a single dislocation glide on a slip plane where obstacles are scattered, and 3. collective behavior of multiple dislocations.

The physical origins of interaction force responsible for various hardening mechanisms have been elucidated in the first category. The calculations of the elastic interaction force between stress field of a dislocation and strain field of a solute atom, which was first performed by Cottrell [1], is a typical example that falls into this category. Other examples in this category are found in electric interaction proposed by Cottrell, Hunter, Nabarro et al. [2], and in Suzuki's chemical interaction or the solute segregation effect [3]. These provided the most fundamental mechanisms of solid solution hardening. In addition to these static equilibrium studies, recent development of cryogenic technologies have revealed some anomalies of plastic deformation which were hardly expected in a high temperature region. Among them are the sudden change of flow stress due to the transition between super-conducting and normal states [4], and non-monotonical behavior of the temperature dependency of yield stress below about 100 K [5]. Those anomalies have been extensively investigated and the basic mechanisms underlying the phenomena have been partly elucidated. Mainly the dynamic effect of a moving dislocation line such as inertia effect and

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damping effect play a significant role. This dynamic effect should also be accounted for in the first category.

The critical resolved shear stress (hereafter abbreviated as c. r. s. s.), however, cannot be estimated only by the knowledge of elementary interaction force, which raises the following second category. In general, the c. r. s. s. is not given by the simple sum of elementary interaction forces caused by each type of obstacles, but is a complicated function of a concentration, strength and distribution of obstacles, or line tension of a dislocation etc. This problem known as the statistical aspect of hardening has been extensively studied in 1970s both theoretically and by means of a computer simulation technique set forth by Foreman and Makin. [6] The body of the work centered on finding the power law relationship between c. r. s. s. and various parameters described above, and the dependencies have been clarified in a simple analytical form. [7, 8]

Finally, the last category is as follows. A common structual material usually contains dislocations of which density is nearly 10^6(cm/cm^3) to 10^{12}(cm/cm^3). A macroscopic deformation process is largely dominated by the multiple behavior of these dislocations. The central concern of this category is, then, to establish the thermodynamical principle which dominates the multiple dislocation motion. The analysis of the collective behavior of dislocations was originally performed by Gilman and Johnston [9] more than twenty years ago on the LiF crystal and recently succeeded by Alexander and Haasen [10] for Ge and Si crystals. More recently, Suezawa et al. [11] proposed the concept of steady state deformation which was further solidified by nonequilibrium thermodynamics. [12]

Those categories have been discussed and analyzed as separate items in most theoretical studies. Although the qualitative feature of deformation process may be revealed by the outcome of each category, no quantitatively reliable results comparable to experimental measurements can be expected. One of the most important objects studied in this report is to unify those three categories into a single theoretical framework. In particular, our basic concern in this study is the deformation process at cryogenic temperatures in which the dynamic effects of dislocations become significant as mentioned previously.

It should be recognized that the thermal activation process is quite important even in such a low temperature region. Then the unification of dynamic effect with the thermally activation process is indispensable for proper treatment. This is, however, not an easy task, since one is a quite deterministic process while the other is a stochastic process, and the rigorous unification of these two processes demands the basic concepts of statistical physics, which is beyond the scope of this work. What was tried in this study as an alternative is the introduction of some averaging process with respect to time [15], as will be discussed below.

Therefore, the present study provides a method to treat the thermally activatied dislocations behavior with dynamic effect in a randomly distributed obstacle field.

The organization of this paper is as follows. In the next section, the framework of our theoretical model is constructed. The main results are presented and discussed in the third section. A brief summary is provided in the last section.

2. Theoretical Model

We assume that moving dislocations of which density is Nm (cm/cm^3) in a slip plane where a single type of point obstacles of concentration $\bar{C}$ are scattered. The dislocation segment trapped by an obstacle whose strength is represented by interaction energy, G_0, overcomes the barrier by external stress, with the aid of the dynamic effect and the thermal activation process. The released segment is again trapped whenever other obstacles are encountered and the same overcoming process is repeated. The average area swept by the segment is, therefore, equal to the one occupied by an obstacle, which is exactly the assumption adopted by Friedel [13] in his statistical study of hardening. This is schematically described in Figs. 1 and 2. Since the obstacle is point-like and the interaction barrier is localized, the flight time between one obstacle and the next one is negligiblly small as compared with capture time at an obstacle. The rate controlling process is, therefore, the overcoming process of the dislocation segment at an obstacle.

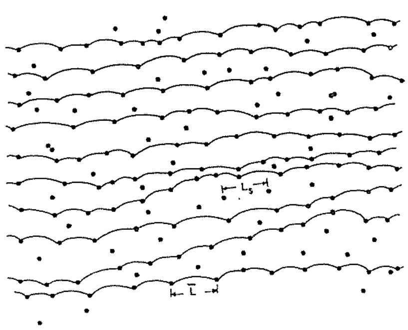

Fig. 1 Schematic view of dislocations motion through a randomly distributed obstacle field. L_s is defined as the average distance between obstacles, while $\bar{L}$ is the average distance between two adjacent obstacles along a dislocation line.

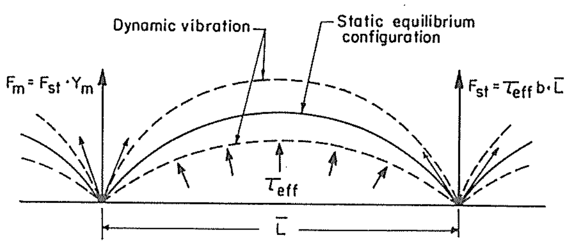

Fig. 2 Vibrating dislocation segment between two adjacent obstacles under the influence of effective stress.

2-1 Strain rate

The total number of obstacles, P, interacting with dislocations is given by

$$P = \frac{Nm}{\bar{L}} \tag{1}$$

where $\bar{L}$ is the average distance between the obstacles along a dislocation line. Since the area swept by a dislocation segment before encountering the next obstacle can be given by Ls^2, where Ls is the average distance between obstacles in the slip plane and is related to the concentration of obstacles by $\sqrt{b^2/\bar{C}}$, the strain, $\Delta\varepsilon$, introduced during the time, Δt, is given as

$$\Delta\varepsilon = \Delta P (Ls)^2 b \tag{2}$$

where ΔP is the number of obstacles which are overcome during the time Δt. Then the strain rate, $\dot{\varepsilon}$, is given by

$$\dot{\varepsilon}=\lim_{\Delta t\to 0}\frac{\Delta\varepsilon}{\Delta t}$$

$$=\frac{\Delta P}{\Delta t}(Ls)^2 b$$

$$=\dot{P}^{+}(Ls)^2 b \tag{3}$$

In the above eq. (3), $\dot{P}^{+}$ is, what is called, activation frequency and is alternatively expessed as

$$\dot{P}^{+}=\frac{P}{t_W} \tag{4}$$

where t_w is the waiting time at an obstacle which is related to activation energy, ΔG^*, by

$$\frac{1}{t_w}=\nu \exp\left(-\frac{\Delta G^*}{kT}\right) \tag{5}$$

where ν the trial frequency, k the Boltzman constant and T is the temperature. Substitution of eqs. (1), (4) and (5) into eq. (3) yields the following expression for a strain rate

$$\dot{\varepsilon}=\frac{Nm}{\bar{L}}\nu \exp\left(-\frac{\Delta G^*}{kT}\right)(Ls)^2 b \tag{6}$$

2-2 Thermal Activation Process with the aid of the Dynamic Effect

According to the string model of Teutonico et al. [14], the motion equation of a moving dislocation is given by

$$m\frac{\partial^2 y}{\partial t^2}+B\frac{\partial y}{\partial t}-\Gamma\frac{\partial^2 y}{\partial x^2}=(\tau_{app}-\tau_i(x,y))b \tag{7}$$

where m is mass of a dislocation per unit length, y the coordinate of moving direction of a dislocation, t the time, B the damping constant, Γ the line tension per unit length, x the stretching direction of a dislocation line, b the Burgers vector and the right hand side of the above equation represents the effective stress, τ_{eff}, acting on a dislocation which is the difference between applied stress, τ_{app}, and the internal stress τ_i (x, y). The solution of the above differential equation for the following boundary conditions

$$y=0 \text{ at } x=0 \text{ and } \bar{L} \tag{8-1}$$

and initial condition

$$\dot{y}=v_0 \text{ at } t=0 \tag{8-2}$$

where v_0 is the initial velocity which is assumed to be negligibly smaller than the transversal sound velocity, v_s, is given by

$$y=\frac{\tau_{eff}}{2\Gamma}(\bar{L}-x)x-\frac{4\tau_{eff}b\bar{L}^2}{\pi^3\Gamma}\exp(-\gamma t)\sin\left(\frac{\pi x}{\bar{L}}\right)\cos\left\{\omega_0\left(1-\frac{\gamma^2}{\omega_0^2}\right)^{\frac{1}{2}}t\right\} \tag{9}$$

where

$$\gamma=\frac{B}{2m} \tag{10}$$

and

$$\omega_0=\frac{\pi}{\bar{L}}\left(\frac{\Gamma}{m}\right)^{\frac{1}{2}} \sim \pi\frac{v_s}{\bar{L}} \tag{11}$$

Then the tension force of the dislocation line exerted on an obstacle is obtained as

$$F=\left| 2\Gamma \left(\frac{dy}{dx}\right) / \sqrt{1+\left(\frac{dy}{dx}\right)^2} \right|_{x=0}$$

$$\sim 2\Gamma \left(\frac{dy}{dx}\right)_{x=0} \tag{12}$$

The force F approaches a static equilibrium value either asymptonically (overdamping) or in an oscillating manner (underdamping) with time.

The thermal activation process is essentially a stochastic process as was mentioned in the introduction and can not be incorporated into the motion equation (7) which represents the deterministic process in a simple manner. This should be settled by returning to basic statistical physics, which is beyond the scope of this report. In order to avoid this fundamental trouble, we, then, followed Suzuki's prescription [15] and calculated the average amplitude with respect to decay time $1/\gamma^*$ and introduced the dynamic effect as an average effect in the following manner.

$$\frac{1}{1/\gamma^*}\int_0^{\frac{1}{\gamma^*}} F(t)\,dt=\tau_{eff}\,\bar{L}b\overline{Ym} \tag{13}$$

$\overline{Ym}$ in eq. (13) indicates the magnitude of the dynamic effect and is given by

$$\overline{Ym}=1+\frac{e^{-z*}}{1/\gamma^*}\int_0^{\frac{1}{\gamma^*}} e^{-z^*t}\,dt$$

$$\sim 1+0.6\,e^{-z^*} \tag{14}$$

with

$$z^*=\frac{\pi\gamma}{\omega_0} \tag{15}$$

The activation energy which should be provided by thermal energy is, therefore, given by the following equation which incorporates the averaged dynamic effect in a quasi-static manner

$$\Delta G^*=G_0-\tau_{eff}\,\bar{L}bd\overline{Ym} \tag{16}$$

where d is the width of an obstacle.

To obtain the average separation of obstacles along a dislocation line $\bar{L}$ has been the central concern of statistical problem of hardening. $\bar{L}$ is generally a complicated function of strength and the concentration of obstacles, extension of interaction field, line tension of a dislocation etc. Friedel [13] first discussed this problem for localized and weak obstacles and was able to derive an analytical expression. Recently, the problem has been revived and numerous computer simulation works as well as analytical studies have been performed in order to investigate more general cases. [7] All studies, however, have been devoted to the static equilibrium case and no explorations have been done on the dynamic problem, the one studied in this report. The extension of static studies towards a dynamic case would raise another difficulty and we avoided this complication by merely introducing the Friedel statistics and by examining the results critically. This is discussed in a later section again. In order to follow Friedel statistics, it should be noted that the strength of obstacle G_0 is small and the obstacle is limited to point-like one. Consequently, we put the magnitude of Burgers vector, b, to d in the eq. (16) in the present analysis. According to the Friedel statistics, $\bar{L}$ is given by

$$\bar{L}=\left(\frac{2b\Gamma}{C}\right)^{\frac{1}{3}}\tau_{eff}^{-\frac{1}{3}} \tag{17}$$

The trial frequency ν of a dislocation segment is, now, expressed as [18]

$$\nu=\frac{b}{2\bar{L}}\nu_D \tag{18}$$

where ν_D is the Debye frequency. By substituting eqs. (16), (17) and (18) into the eq. (6), one can attain the final expression for the strain rate

$$\dot{\varepsilon}=Nm\frac{\nu_D}{2}\frac{b^4}{C}\left(\frac{2b\Gamma}{C}\right)^{-\frac{2}{3}}\tau_{eff}^{\frac{2}{3}}\exp\left[-\frac{G_0-b^2\left(\frac{2b\Gamma}{C}\right)^{\frac{1}{3}}\tau_{eff}^{\frac{2}{3}}\overline{Ym}}{kT}\right] \tag{19}$$

2-3 Collective Behavior and Mobile Dislocation Density

Generally, a tremendous amount of dislocations participate in macroscopic deformation process. Those dislocations do not move around in a random manner but a physical principle does exist behind the phenomenon. As was mentioned in the introduction section, the pioneering work which studied the multiple behavior of dislocations should be attributed to Gilman and Johnston [9] who succeeded to reproduce the stress-strain curve of LiF crystal as functions of deformation temperature, applied stress, strain rate etc. This traditional work, however, is essentially semi-empirical and the physical principle behind the phenomenon were somewhat ambiguous. Moreover, one serious drawback is the fact that the dislocation density increases linearly with strain, which is by no means acceptable. This point is recently modified by Alexander and Haasen [10] by taking account of the back stress field originated from the long range stress field of multiple dislocations. The theory well reproduced the experimental stress-strain behavior for materials like Si and Ge which are characterized by high Peierls Potential. Suezawa et al. [11] further expanded this phenomenological treatment and developed the concept of steady state deformation based on their ample experimental data. According to their analysis, the stage of the steady state deformation in which the effective stress takes a constant value with respect to strain is realized by adjusting the mobile dislocations density so that the stress acting on moving dislocations is minimized. This can be expressed as:

$$\left(\frac{\partial(\tau_{eff}+\tau_i^0)}{\partial Nm}\right)_{\dot{\varepsilon}}=0 \tag{20}$$

where τ_i^0 is the interaction force acting among moving dislocations and is related to mobile dislocation density Nm as

$$\tau_i^0=A\sqrt{Nm} \tag{21}$$

where A is a proportional constant which is a function of rigidity G and b. The criterion of steady state deformation was further examined and consolidated based on non-equilibrium thermodynamics. [12]

Again, the treatment described above was originally derived for the static dislocations and the direct application to moving dislocations with dynamic effect may not be fully guaranteed. An emission of phonon by moving dislocations, for instance, may violate the simple equality of eq. (21). But our problem has been virtually transformed to the static case as was demonstrated in the previous section, and the complication arising from the fundamental natures of moving dislocation could be safely avoided.

Thus, by solving the simultaneous equations (19) and (20), we analyzed the dislocations behavior which are under a thermal activation process with the aid of a dynamic effect.

3. Results and Discussion

Prior to the analysis, in order to reduce the number of parameters and to simplify the analysis, the following dimensionless parameters are introduced: $\tau^* = \tau_{eff}/G$, $Q = G_0/d_1 Gb^3$, $\varepsilon^* = 2\dot{\varepsilon}/\nu_D$, and $N^* = Nmb^2$, where G is rigidity. The concentration is kept at a constant value of 1at. % throughout the investigation. This is because, as was described previously, the Friedel statistics is assumed, then the present calculation is rationalysed only in the low concentration regime.

One of the main purposes of the present study is to clarify the influence of the dynamic effect. Shown in Fig. 3 are the temperature dependeny of effective stress at 1at. % both for the dynamic case and for the static case which was obtained by putting unity to $\overline{Ym}$ in the eq. (19). The prescribed values of ε^* and Q are obtained by putting $\dot{\varepsilon} = 5\times10^{-6}\,\mathrm{sec}^{-1}$, $\nu_D = 4.43\times10^{12}\,\mathrm{sec}^{-1}$, $G_0 = 0.2$ eV, $d_1 = 1$, $G = 2.8\times10^{11}$ dyne/cm^2 and $b = 2.8\times10^{-8}$ cm which simulate Al matrix.

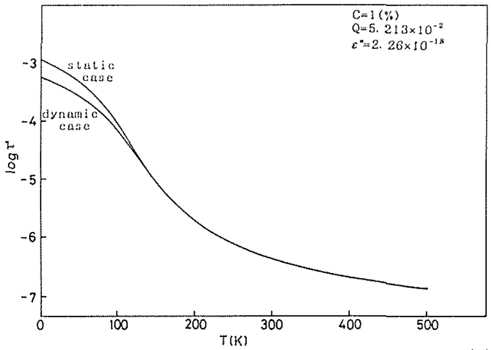

Fig. 3 Temperature dependency of effective stress for both static and dynamic case. Note that the effective stress are normalized. The concentration and strength of the obstacle as well as the strain rate are given in the figure.

The overall dependency for both cases demonstrates typical thermal activation behavior. However, at around T=50 K, a single curve in the higher temperature starts to split into two branches. This lift of degeneracy clearly indicates the influence of the dynamic effect which becomes notable at lower temperatures where thermal activation is less significant. The dynamic effect can be further discussed from a different point of view by examining the $\overline{Ym}$ value which was defined by eq. (14). Shown in Fig. 4 are the temperature dependency of $\overline{Ym}$ for various strengths of obstacles at the constant strain rate $\varepsilon^* = 2.26\times10^{-18}$ (solid line) and for various strain rates (broken line) at constant strength of an obstacle $Q = 5.213\times10^{-2}$. As may easily understood from the eq. (14), the bigger dynamic effect is indicated by larger $\overline{Ym}$ value, while at unity, a completely static situation is realized. The figure indicates that, at a constant temperature, a larger dynamic effect is required both for the stronger obstacles in order to maintain a given strain rate, and for the higher strain rate at a constant strength of an obstacle. Both for the constant values of Q and ε^* on the other hand, $\overline{Ym}$ decreases with the increase in temperature. This is because the aid of the dynamic effect is less required under sufficient supply of thermal energy. One can see that the

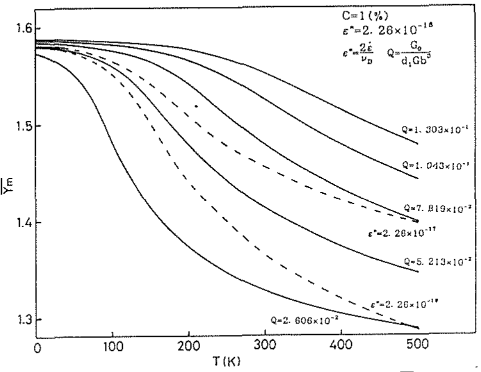

Fig. 4 Temperature dependency of $\overline{Y}$m for various strength of obstacles (solid line) at a constant strain rate and for various strain rates (broken line) at constant strength of an obstacle.

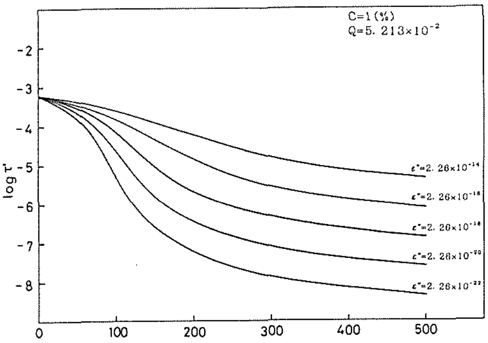

Fig. 5 Temperature dependency of normalized effective stress for various values of strain rate.

thermal activation and the dynamic effect are complementary to each other.

Next, we examined the dependency of the effective stress and mobile dislocation density on the deformation temperature, strength of obstacles and strain rate. Fig. 5 shows the dependency of effective stress on temperature for various values of strain rate at 1at, %. With the increase of both temperature (under constant strain rate) and strain rate (under constant temperature), the effective stress decreases, which is quite generally observed in a conventional deformation test. Fig. 6 shows the dependency of effective stress on temperature for various values of obstacle strength at a given strain rate. One should notice in Fig. 5 that, at T=0, the τ^*'s converge on the constant value, while not in the Fig. 6. This can be understood from the following argument. At the limiting case of T=0, the exponent in the eq. (19) diverges on negative infinite and the strain rate is reduced to zero for any effective stress. This is the natural consequence of the thermal activation process governed by the rate equation (19). On the other hand, once a strain rate $\dot{\varepsilon}$ is prescribed at T=0, the only way to maintain the strain rate is to supply the applied stress which cancels the numerator of the exponent,

$$G_0 - b^2 \left(\frac{2b\Gamma}{C}\right)^{\frac{1}{3}} \tau_{eff}^{\frac{2}{3}} \overline{Ym} = 0 \tag{22}$$

This equation uniquely determines the effective stress at T=0 which certainly depends on the strength of obstacles as is shown in the Fig. 6. This, however, generates the uncertainty for the resulting values of $\dot{\varepsilon}$. In other words, for any effective stress which satisfies eq. (22), the strain rate is not uniquely determined, which is the case of Fig. 5.

Since we assumed the Friedel statistics in the quite natural consequence, it should be noted that a violent dynamic effect can not be dealt within the present framework.

Shown in Fig. 7 is the dependency of the mobile dislocation density on the concentration of obstacles for various values of strength of obstacles at 100 K. The behavior can be explained in the following manner. In order to maintain a constant strain rate, the mobile dislocations participating in the deformation should increase, since the mobility of a single dislocation is retarded by increasing the strength of an obstacle or concentration. This is essentially reflected in the result.

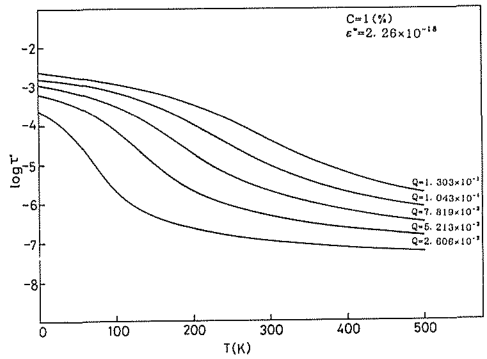

Fig. 6 Temperature dependency of normalized effective stress for various strength of obstacles.

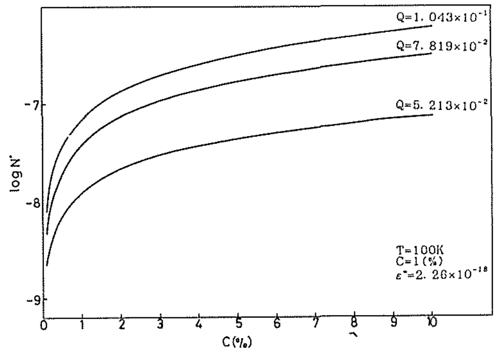

Fig. 7 Concentration dependency of normalized mobile dislocation density at 100 K.

4. Conclusion

Based on the string model, we constructed the theoretical framework which describes a thermally activated dislocation motion with the aid of the dynamic effect in a random distribution of point obstacles. In order to compromise the stochastic process (thermal activation) with the deterministic process (dynamic effect), the averaged dynamic effect with respect to decay time is introduced. Furthermore, the collective behavior of multiple dislocations is considered by introducing the idea of steady state deformation initially proposed by Sumino.

The present study well reproduced the generally observed tendency between stress and temperature, strain rate, and concentration and strength of obstacles. This confirms the reliability of the model. The significance of the dynamic effect is also indicated in the cryogenic temperature range.

Furthermore modification of the present model is due to the introduction of temperature dependency of damping constant B and rigidity G. In fact, the several anomalies described in the introduction section may be resolved by introducing such additional factors, which will be the subject of the forthcoming paper.

Finally, we should point out that our preliminary comparison with the available experimental data of Al-Mg system shows a quite reasonable agreement in the temperature dependency of c. r. s. s. A critical experimental confirmation would seem in order.

5. Acknowledgement

This work was supported in part by a Grant-in-Aid for Coorperative Research from the Japanese Ministry of Education, Science and Culture.

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