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Studies on the Statistical Problems of the
Solid Solution Hardening

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Abstract

This report deals with statistical problems of hardening of a solid solution by computer simulation.   In a dilute solid solution, several studies clarified that the yield stress was proportional to $C^{1/2}$, where C was the concentration of solute atoms.   In a concentrated solid solution, however, many statistical problems remain unsolved.

Labusch has shown that the behaviour of the dislocaion is controlled largely by the dimensionless parameter β defined $\beta = f_m/4TCW^2$, and has also shown that within the limit of $\beta \gg 1$, the yield stress is proportional to $C^{2/3}$.

We calculated the yield stress, varying the line tension, over a wide range of concentration (0.01 at. % $\cdots$ 10.0 at. %) and found that Labusch's parameter, β is still insufficient to explain the statistics of solid solution hardening.

1. Introduction

Generally the yield stress of a crystal increases in proportion as the concentration of the solute atoms increases.   This phenomenon, known as solution hardening, is one of the strengthening methods in crystals and is due to the interaction between solute atoms and dislocations.   If solute atoms are dissolving radomly in the matrix lattices statistical treatment may be adopted for the hardening effect.

It is clear that the parameters on which the hardening of a crystal by solute atoms depends are, the range and strength of the interaction potential field between solute atoms and a dislocation, the concentration of solute atoms, the line tension of dislocation and etc..   In spite of all efforts to explain the statistics of hardening with these parameters many problems remain unsolued.

For example, the theoretical studies by Friedel[1] and Foreman- Makin's[2] computer simulation explained the concentration dependency of the yield stress in the case of low concentrations where they assumed only a single kind of strength of point obstacles, but these can not be applied directly to the case of high concentrations.   Labusch's method of distribution function[3,4] would be a more unified theoretical treatment as it treats the range and broad strength spectrum of the

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interaction potential field between solute atoms and a dislocation.

In this report, by using the method of computer simulation devised by Saka-moto et al.,[5] some statistical problems of hardening, especially the concentration dependency of the yield stress, are presented and compared against Labusch's results.

2. Procedure of Computer Simulation

Sakamoto et al.[5] modified the method of Foreman and Makin's computer simulation to obtain the dislocation motion in a highly concentrated KCl–KBr solid solution, and their procedure is followed in the present simulation.

In the string model[6]~[8] the motion of dislocation is given by following equation:

$$m\frac{\partial^2 y}{\partial t^2} = b(\tau_i + \tau_a) - B\frac{\partial y}{\partial t} + \Gamma\frac{\partial^2 y}{\partial x^2} \tag{1}$$

where y is the displacement of the dislocation under an influence of effective applied stress, m the effective mass of dislocation line per unit length, B the viscous-damp-ing constant, Γ the force per unit length due to the effective tension for a bowed out dislocation, τ_a the external applied stress, τ_i the internal stress, b the magnitude of burgers vector and x is a coordinate along the dislocation line.   As the frictions due to conduction electrons or phonon damping, and a high speed dislocation motion are not dealt with in this work, the inertial term is neglected and eq. (1) is trans-formed to the next equation:

$$\Gamma\frac{\partial^2 y}{\partial x^2} + b\Big(\tau_i(x, y) + \tau_a\Big) = 0 \tag{2}$$

Mathematically the yield stress is the upper limit of τ_a and above such stress the solution of eq. (2) is impossible for a given function $\tau_i(x, y)$ and material constants b and Γ.   In eq. (2) it is very difficult to estimate the internal stress spectrum $\tau_i(x, y)$ correctly and solve it analytically.   This problem is solved by the numerical solution method as follows.

2.1 Model Crystal

The model crystal in a computer memory space is shown in Fig. 1.   For simplicity crystal structure is assumed to be a simple cubic and solute atoms con-sidered here are limited to a substitutional type.

The total number of atoms is 43,200 and the internal stress at a given posi-tion (x, y, z) is determined by considering the solute atoms within $-2b \leqq x, y, z \leqq 2b$. The positions of the solute atoms are determined by random numbers.   To generate random numbers* by the computer FACOM 230–75 installed in the Computer Center of Hokkaido University the algorithm of "SEQUENTIAL RANDOM INTEGERS GENERATOR" devised by Kuo et al.[9] was modified.

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* The program "KUNIRN" which was devised at Kyoto University was partly used in our original generator.
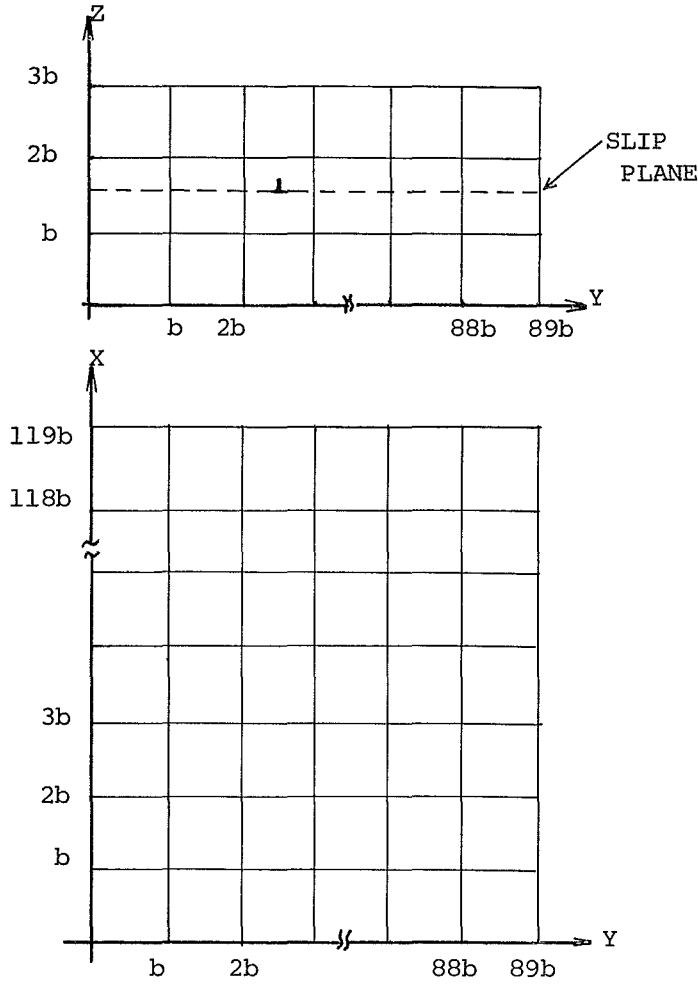
Fig. 1. Model lattice in a memory space (120×90×4)

2.2 Internal Stress Spectrum

Various kinds of interaction between solute atoms and a dislocation, for example, elastic interaction, chemical interaction and electrical interaction are known, but in this work elastic interaction alone due to the size effect is considered.

In the stress tensor due to the size effect of a solute atom, the effective component, which refers to the slip motion of the disolcation on the slip plane is given by the equation[5] (3):

$$\tau_{x,y} = (\text{Material Factor}) \cdot (\text{Geometrical Factor}) \qquad (3)$$

$$\text{Material Factor} = -\frac{2}{3}\frac{1+\nu}{1-\nu}\,\mu\,(r_s^3 - r_0^3)$$

$$\text{Geometrical Factor}\,;\; G(x,y,z) = \frac{(y-y_s)\cdot z_s}{((x-x_s)^2 + z_s^2 + (y-y_s)^2 + C)^{5/2}}$$

where (x, y, z) is the Cartesian coordinate in the crystal, (x_s, y_s, z_s) is that of a solute atom, μ the rigidity of a crystal, ν the Poisson's ratio, r_s the radius of the solute atom, r_0 is that of the host atom and C is the correction term, which is kept at $0.25b^2$ throughout this simulation. The spectrum of internal stress on a slip plane is determined by superimposing the effect of all solute atoms within $-2b \leqq x, y, z \leqq 2b$. The internal stress is calculated at intervals of b in x direction and of $0.5b$ in y direction. Moreover in y direction, to estimate the internal stress between the fixed points mentioned above, a given function; $G(x, y, z)$ is expanded into a Taylor's series and three terms are considered.

2.3 Configuration of Dislocation

To solve the differential equation (2) by a numerical method using $\tau_i(x, y)$ calculated in section 2.2, the boundary condition, eq (4), is introduced:

$$(dy/dx)_{x=0} = (dy/dx)_{x=119b} = 0 \qquad (4)$$

under the consideration that the dislocation is met at right angles by image forces at each side of the crystal. The dislocation line is approximated by 120 coordinates Y_k, and differential eq. (2) is transformed to the difference eq. (5):

$$Y_{k-1} - 2Y_k + Y_{k+1} + \frac{b^3}{\Gamma}\left(\tau_i(Y_k) + \tau_a\right) = 0 \qquad (5)$$

$$k = 2, 3, \cdots, 121, \qquad Y_1 = Y_3, \qquad Y_{120} = Y_{122}$$

To find the equilibrium configurations the Succesive Over-Relaxation Method[10] is used, therefore eq. (5) is transformed to eq. (6):

$$Y_{k,m+1} = Y_{k,m} + \omega\left(\left(Y_{k-1,m+1} + Y_{k+1,m} + \frac{b^3}{\Gamma}\left(\tau_i(Y_{k,m}) + \tau_a\right)\right)/2 - Y_{k,m}\right) \qquad (6)$$

$$k = 2, 3, \cdots, 121, \qquad Y_{1,m} = Y_{3,m}, \qquad Y_{122,m} = Y_{120,m}$$

where m is the number of iteration for a convergence to a true value, ω is a relaxation coefficient and the value $\omega = 1.3$ is the optimum for this internal stress spectrum. The maximum iteration number is 5000.

3. Results and Discussion

3.1 Internal Stress Spectrum and Configuration of Dislocation

Three patterns of the internal stress spectrum for three levels of solute concentration are shown in Figs. 2 and 3. Here only $G(x, y, z)$ is considered and Material Factor is kept at 1.0 in all cases.

Although in many computer simulations, not to speak of the famous Foreman-Makin's simulation, point obstacles are treated. From the Fig. 2 and 3 it is clear that even in the case of low concentration the stress field is not localized but diffused*, hence the assumption of point obstacles is considered to be over simplified.

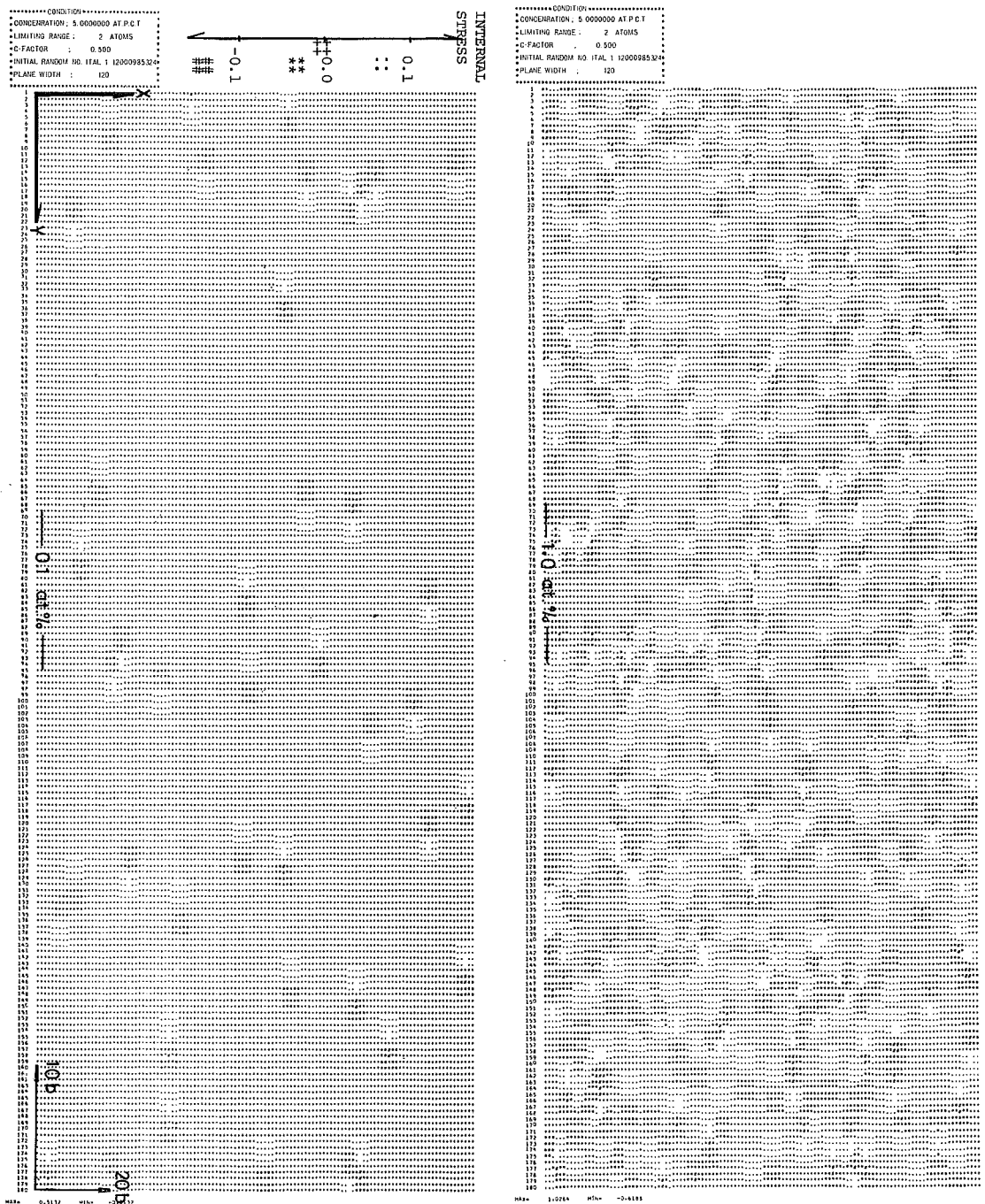* From these figures the width of the potential field is about $5b \times 5b$.
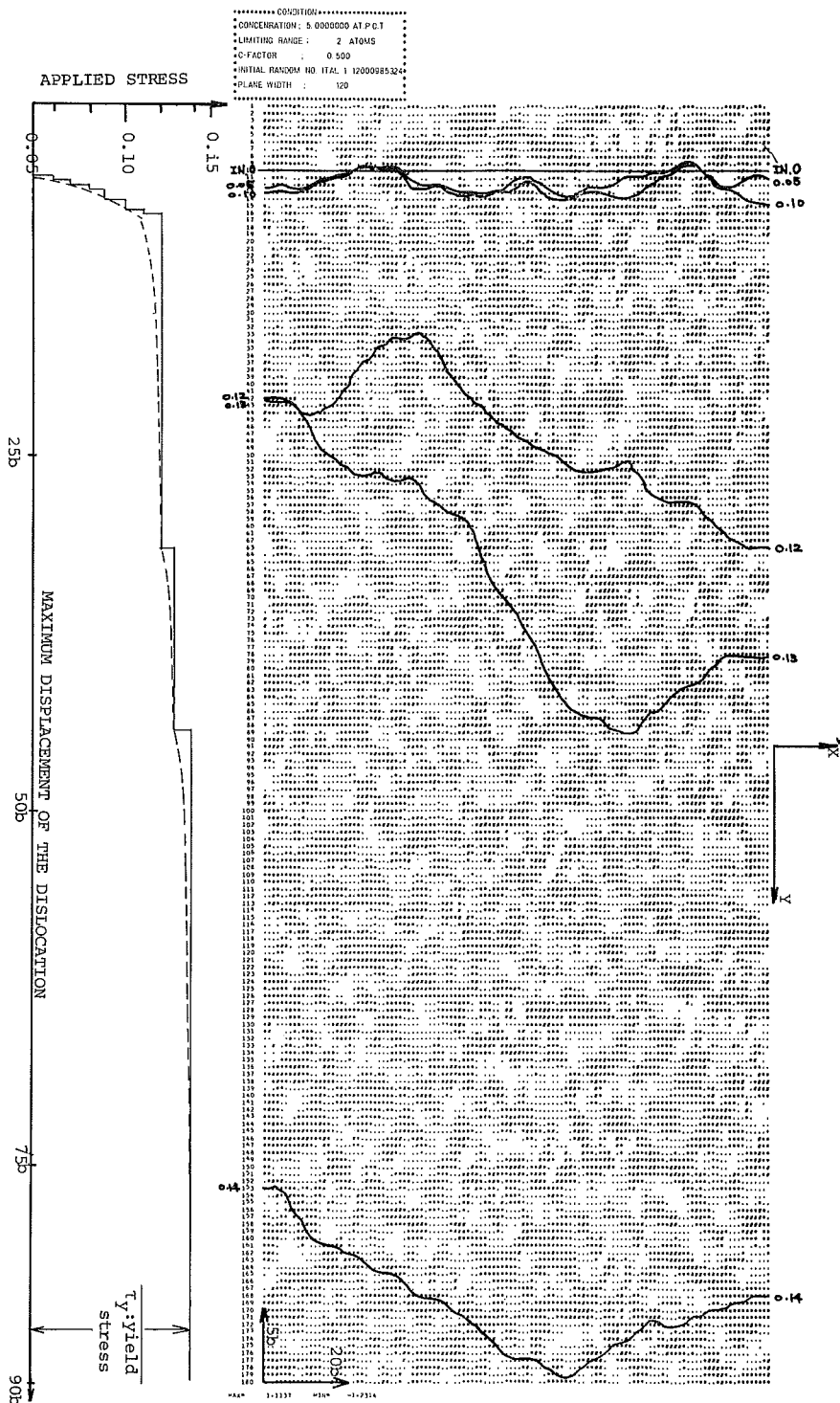
Fig. 2. Spectrum of internal stress.

Fig. 3.

Because the types of obstacle are categorized for four extreme ones[4] and these slip planes in our case include them, the simulation on the slip planes may give a more general solution than any other former treatment[11] of statistics of hardening. Furthermore broad spectrum of strength of interaction forces is considered.

In the case of 5.0 at. % and $b^2/\Gamma = 1.0$, several equilibrium configurations related to applied stress are shown in Fig. 3, and the relation between applied stress and maximum displacement are also shown on the right hand side of the figure. In this figure, we realize that until the applied stress increases to a certain critical stress level a dislocation can not start to slide significantly and fluctuates repeatedly around the initial position. As soon as the applied stress attains a critical level a catastrophic motion of dislocation occurs. We may call this critical stress as yield stress. (In this simulation the increment of applied stress is 0.01. If $\Delta\tau_a \to 0$, a solid line will approach the broken line asymptotically.)

3.2 Concentration Dependency of the Yield Stress

Prior to determining the concentration dependency of the yield stress, in order to check up on the influence of the width of the slip plane, yield stresses are calculated for various kinds of width from $10b$ to $120b$ at a constant concentration, 1.0 at. %. The result is shown in Fig. 4. From this figure the yield stress reaches almost constant at $120b$, and in the latter discussions the influence of the width of the slip plane can be neglected.

Using the same procedure as in the case of 5 at. % the yield stresses are calculated at several levels of concentration from 0.01 at. % to 10.0 at. %. In these calculations, Γ/b^2 (which is abbreviated to LT here after) is maintained at 1.0.

Fig. 5 shows that in the "dilute solid solution", lower than 1.0 at. %, the yield stress is nearly constant and does not depend on concentration, which is inconsistent with the prediction of Friedel or the results of Foreman-Makin's simulation.

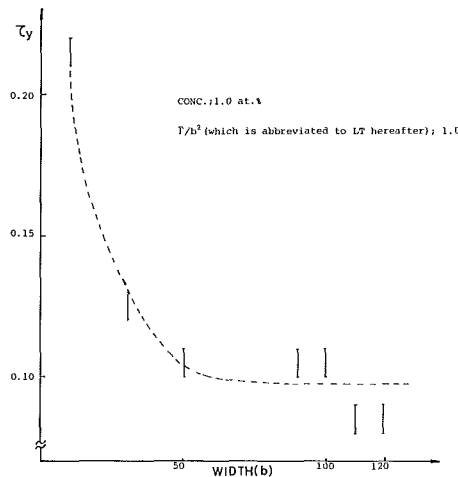Fig. 6 shows the relation between $\log \tau_y$ and $\log C$ in the "concentrated solid

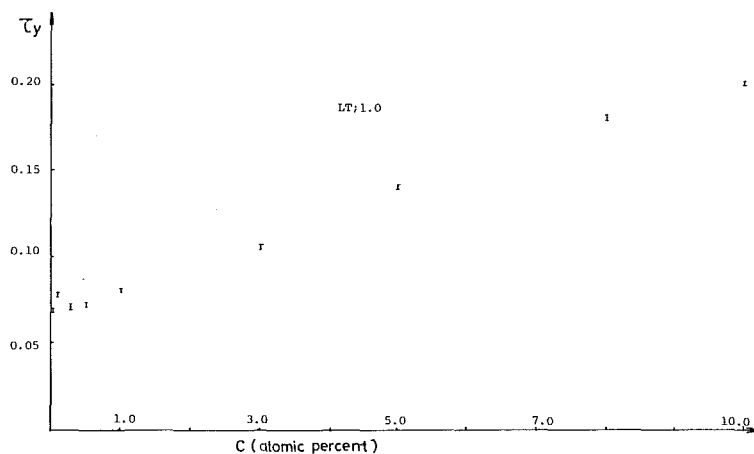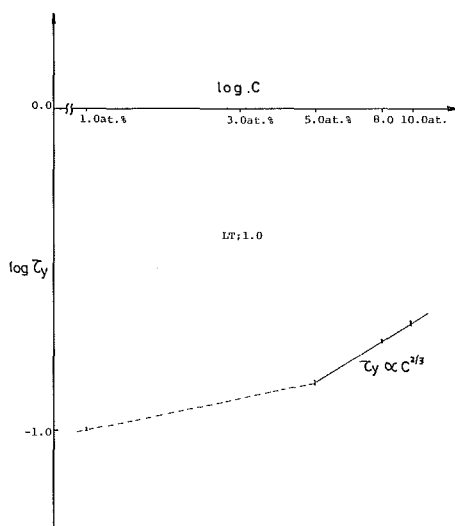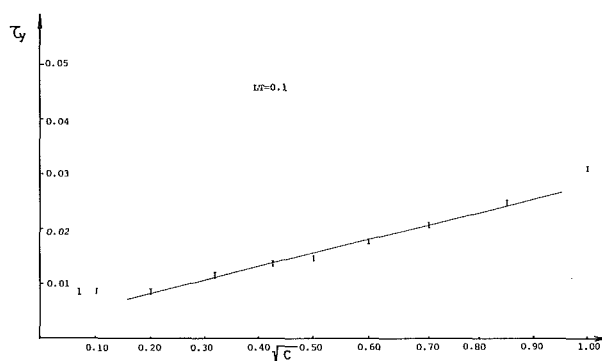**Fig. 4.** Influence of the width of the slip plane on the yield stress.

Fig. 5.   Concentration dependency of the yield stress.

Fig. 6. $\log \tau_y - \log C$ in the range high conc.

Fig. 7.   Relation between $\sqrt{C}$ and τ_y in the range of low conc.

solutions" higher than 1.0 at. %. At concentrations higher than 5.0 at.%, the relation $\tau_y \propto C^{2/3}$, which was predicted by Labusch, appears.

In order to check upon the influence of line tension LT is changed to 0.1 and the yield stresses are calculated in the "dilute solid dolution". The results are shown in Fig. 7. From this figure we realize that in lower concentrations less than 0.04 at. %, the yield has no dependency on concentration but above such a concentration level, the yield stress is proportional to $C^{1/2}$. This dependency in the "dilute solid solution" is in accordance with the Friedel's prediction.

From these results we can easily understand when W, the range of interaction potential field, is kept constant, the yield stress depends not only on concentration but also on line tension sensitively.

In the discussion of the statistical problem of hardening, the parameter β defined by $\beta = f_m/4TCW^2$ is often used, where f_m is the maximum interaction force, T the line tension, C the concentration of solute atoms and W is the range of interaction potential field. According to the Labusch's method of distribution functions, in the limit of $\beta \gg 1$

$$\tau_y b \propto C^{2/3} f_m^{4/3} W^{1/3}/T^{1/3} \qquad (7)$$

It is clear that although the present case treats the limit of $\beta \gg 1$, because $W \sim 5b$, the concentration dependency of yield stress is not always in accordance with eq. (7). Even within the limit of $\beta \gg 1$, the yield stress shows no dependency on concentration or is proportional to $C^{1/2}$ and etc. as shown in Figs. 5, 6 and 7.

These results may indicate not only the assumption of a single kind of strength of point obstacles but also the physical meaning of β in the slip plane which includes a diffusive and broad strength spectrum of potential field must be re-examined. Moreover from Fig. 1 it is clear that in our slip plane the distribution function, $\rho(x, y)$, of the Labusch's theory is zero. So Labusch's method can not be applied to the present case without modifications.

Acknowledgements

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