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The determination of the activation energies of dislocation motion in solid solution single crystals

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The shape of experimental curves CRSS–T (critical resolved shear stress versus temperature) in solid solution crystals is compared with that deduced by Kratochvíl *et al.* [3] and it is shown that at low temperatures agreement is obtained for a certain value of the activation energy U_1. So it is possible to find the value of the activation energy of dislocation motion U_1 at low temperatures from the CRSS–T dependences.

1. Introduction

Recent studies on the solid solution hardening [1–3] have shown that it is necessary to take into account the effects not only in the plateau region, but also at very low temperatures, ~ 4 K or even lower. The event of overcoming the solute atoms by dislocation is thermally activable. Kratochvíl *et al.* [3] were able to explain qualitatively the observed temperature dependence of CRSS on the basis of the simplified model. This took into account the fact that even in relatively dilute solid solutions the impurities are present not only as monomers (i.e. isolated atoms) but also as dimers, etc. Therefore, a single type of impurity atoms can form a spectrum of obstacles for the dislocation motion.

In the analysis below the concept of "the effective obstacle" is used. One assumes that: (i) a specific CRSS–T dependence corresponds to each type of the obstacle characterized by a certain activation energy; (ii) at any temperature the measured value of τ is given by that type of the obstacle, which is effective at the given temperature.

If there exist n types of effective obstacles, the resulting CRSS–T dependence might consist of n parts, corresponding to the n-types of effective obstacles each being determining in a certain temperature interval $\langle T_{i-1}, T_i\rangle$.

It is the purpose of the present paper to correlate this view point with the experimental data available in the literature.

2. Basic equations and the use of the experimental data

It is assumed that the flow stress component corresponding to the presence of solute atoms is thermally activable. Hence the flow stress $\tau = \tau_\mathrm{H} + \tau_\mathrm{R}$, where τ_R is the flow stress in the crystal without obstacles due to the presence of foreign atoms in the lattice and τ_H is the flow stress component corresponding to the presence of solute atoms in random distribution.

It was shown [3] that

$$\tau_\mathrm{H} = \tau_\mathrm{OH}\left[2\exp\left(-\frac{kT}{U}\ln 2\ln\frac{\dot{a}_0}{\dot{a}}\right)-1\right] \quad (1)$$

Equation 1 was deduced on the assumption that both the experimental relations for the activation volume,

$$v_\mathrm{ex} = \frac{\mathrm{K}_1}{\mathrm{K}_2+\tau}$$

and the relation

$$v = -\left(\frac{\partial U}{\partial \tau}\right)_T$$

are valid, where K_1 and K_2 are arbitrary constants, T is the temperature, U is the activation energy for the motion of the dislocations over the

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array of effective obstacles, $\dot{a}$ is the strain rate, and $\dot{a}_0$ is a constant to be discussed below.

τ_{OH} in Equation 1, according to Labusch [1], is given by

$$\tau_{OH} = \frac{c^{2/3}K^{4/3}w^{1/3}}{2r^{4/3}4E^{1/3}b} \tag{2}$$

where c is the volume concentration of obstacles, K is the interaction force between the obstacle and the dislocation, w is the range of the interaction, E is the dislocation line tension, r is the size of the obstacle and b is Burgers vector. Index zero denotes $T = 0\,\mathrm{K}$.

From Equation 1 we may obtain "the reduced flow stress"

$$\tau' = \frac{\tau_H}{\tau_{OH}} = 2\exp\left(-\frac{kT}{U}\ln 2\ln\frac{\dot{a}_0}{\dot{a}}\right) \tag{3}$$

where $\dot{a}_0$ is a constant depending on geometry and is proportional to the Debye frequency of the material. The values used for $\dot{a}_0$ are always very different. It is very difficult to determine its value experimentally as it depends on the value of the characteristics of the supposed activation process. Here the value 15 was used for $\ln(\dot{a}_0/\dot{a})$. It should be noted that the change of $\ln(\dot{a}_0/\dot{a})$ by two orders of magnitude does not influence the determination of the activation energy U by more than 30%. The plots of τ' are given in Fig. 1 for several values of the activation energy U. In Equation 3 negative values of τ' are allowed for each specific type of the obstacle, namely for $T > T_c$, where

$$T_c = \frac{U}{k\ln(\dot{a}_0/\dot{a})}$$

Before this occurs another type of obstacle is responsible for τ' as T_c is proportional to U.

The following information can be obtained from the experiment: (i) τ_H, by subtracting τ_R from the CRSS of a certain solid solution at any given temperature. (ii) The experimental value of τ', later called τ'_{ex}:

$$\tau'_{ex} = \frac{\tau_H(T)}{\tau_{OH}}.$$

For τ_{OH} we used τ_H (4.2 K). Then a proper U_1 in Equation 3 is to be found to fit the experimental curve for the interval $\langle 0, T_1\rangle$. U_1 is the activation energy for the motion of dislocations over effective obstacles due to the presence of solute atoms (not necessarily isolated solute atoms) for the interval $\langle 0, T_1\rangle$.* The result of the typical proce-

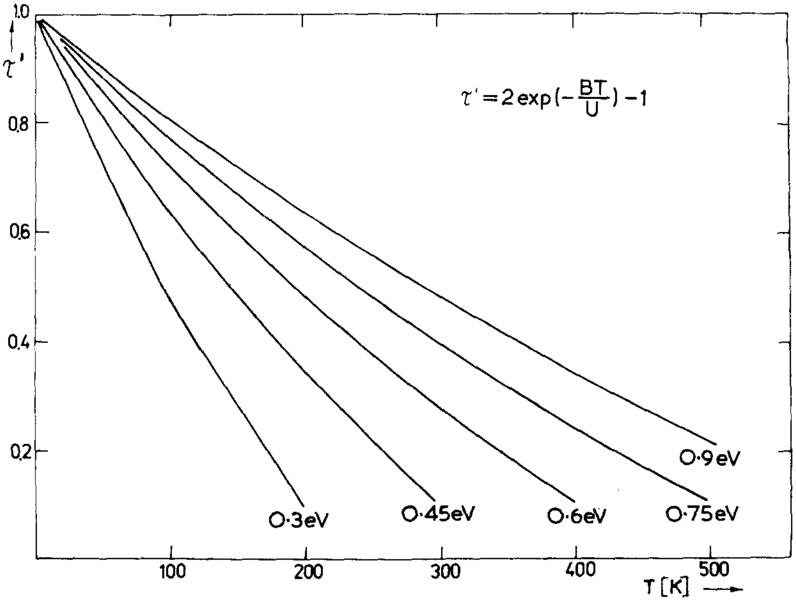

Figure 1 The dependence of the calculated reduced flow stress τ' on temperature for several values of the activation energy U. $\ln \dot{a}_0/\dot{a}$ is kept constant equal to 15.

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* Let us assume that from T_1 to T_2 the activation process with energy U_2 is the prevailing one, etc. The ith part of $\tau'_{(i)ex}-T$ curve is described by

$$\tau'_{(i)ex} = \frac{\tau_{Hi}}{\tau_{OH1}}\left[2\exp\left(-\frac{BT}{U_i}\right)-1\right]. \tag{3a}$$

The determination of U_i is very difficult because of the error in the extrapolation of τ'_{ex} from the interval $\langle T_{i-1}, T_i\rangle$ to 0 K. For the determination of U_i Equation 3a must be again transformed so as to obtain $\tau' = 1$ for $T = 0$ K. This proceeds by multiplying $\tau'_{(i)ex}$ by τ_{OH1}/τ_{Hi}, which is the reciprocal value of Equation 3a for $T = 0$ K.

dure is shown in Fig. 2a and b for Mg–In and Cu–Al respectively. The experimental data suitable for the analysis given above are, nevertheless, very few. This is because of the lack of flow stress data at very low temperatures. The data gathered from [4–9] are summarized in Table I, where the values of U_1, together with solubility limits, are given for all evaluable results in different binary solid solution systems. At low temperatures, the experimental decrease $d\tau'_{ex}/dT$ can be described by a curve of the type given by Equation 3. The activation energy U_1 for a given binary system A–B sometimes depends on the solute concentration.

If we use the measurements with the lowest temperature being 77 K, more experimental data will be available. An example of such date is given in the review paper by Ahlers [9]. Nevertheless, the extrapolation to 0 K brings a lot of inaccuracy in the determination of U_1.

3. Discussion

It is questionable whether the described procedure is applicable to any τ–T dependence in the ma-

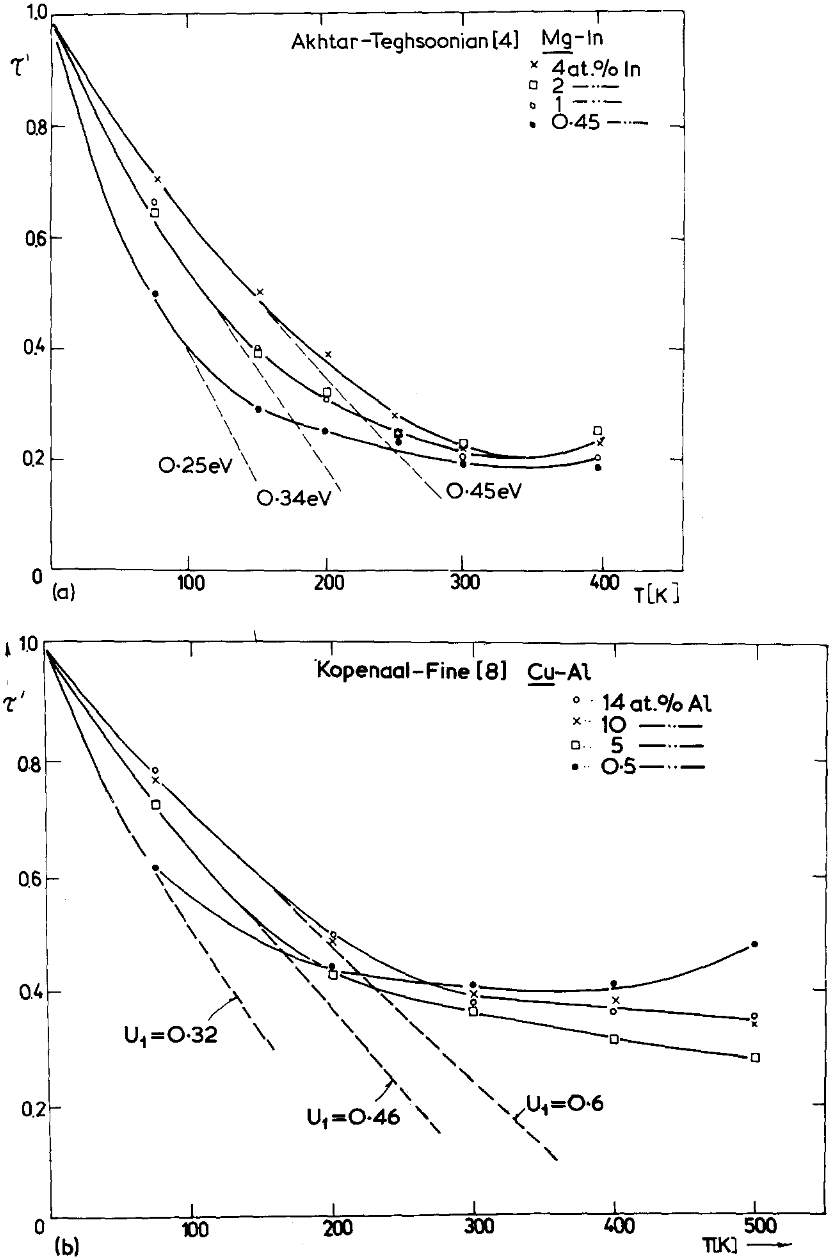

Figure 2(a) The experimental reduced flow stresses τ'_{ex} as a function of temperature for Mg–In (data from [4]). (b) The experimental reduced flow stresses τ'_{ex} as a function of temperature for Cu–Al (data from [8]).

TABLE I

Alloy	Reference	U_1	Solubility limit [13]
Mg–0.45 at. % In	[4]	0.25 eV	19.4 at. % at 484° C
Mg–1.0 at. % In	[4]	0.34	18.7 at. % at 327° C
Mg–2.0 at. % In	[4]	0.34	13.9 at. % at 200° C
Mg–4.0 at. % In	[4]	0.45	
Mg–0.24 at. % Al	[4]	0.28	11.6 at. % at 437° C
Mg–0.59 at. % Al	[4]	0.42	2.6 at. % at 200° C
Mg–0.89 at. % Al	[4]	0.42	1.3 at. % at 100° C
Mg–1.63 at. % Al	[4]	0.42	
Cd–0.2 at. % Zn	[5, 12]	0.95	5.0 at. % at 266° C
Cd–0.05 at. % Zn	[5, 12]	0.60	
Au–1.0 at. % Ag	[6]	0.81*	unlimited
Au–3.0 at. % Ag	[6]	0.81	
Au–5.0 at. % Ag	[6]	0.81	
Ag–1.0 at. % Au	[6]	0.80*	unlimited
Ag–3.0 at. % Au	[6]	0.74	
Ag–5.0 at. % Au	[6]	0.74	
Ag–1.0 at. % Al	[7]	0.41	20 at. % at 500° C
Ag–2.0 at. % Al	[7]	0.64	8.75 at. % at 200° C
Ag–3.0 at. % Al	[7]	0.64	
Ag–4.0 at. % Al	[7]	0.64	
Cu– 0.5 at. % Al	[8]	0.32	19.6 at. % at 200–565° C
Cu– 5.0 at. % Al	[8]	0.46	
Cu–10.0 at. % Al	[8]	0.60	
Cu–14.0 at. % Al	[8]	0.60	
Cu– 1.6 at. % Ni	[11]	0.69	11 at. % at 574° C 1.2 at. % at 300° C

* Compare with the values estimated in [6] by a different method: 0.58 ± 0.10 eV and 0.51 ± 0.12 eV for Au–Ag and Ag–Au respectively.

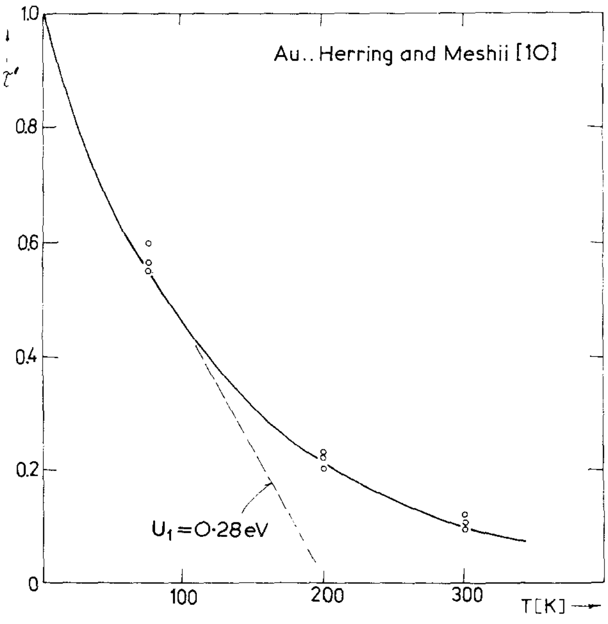

Figure 3 The experimental reduced flow stresses τ'_{ex} as a function of temperature for gold single crystals pre-deformed to different strains (data from [10]).

terial with arbitrary obstacles. We suppose, that this is true if τ is τ_H of Equation 1, i.e. if only the thermally activable part of τ is taken into account. Herring and Meshii [10] had measured the effective stress of the pre-deformed gold single crystals as a function of temperature. Analysing these results we obtain Fig. 3. The amount of prestrain has no effect on U_1 which means that the activation process has the same activation energy at low temperatures in all crystals (pre-deformed to different strains), which is a very reasonable result.

The accuracy of describing the first part of the $\tau'-T$ dependence by a certain value of U_1 depends on the experimental error in the determination of τ. The error in U_1 is, therefore always smaller than ±0.05 eV.

The activation energy is obviously more or less dependent on the value of the concentration relative to the solvus line. The values of U_1 probably do reflect the nature of the obstacles and their configurations at very low temperatures. This is justified by the fact that in dilute alloys U_1 is very near to the expected values for the interaction energy between a single solute atom and a dislocation (see e.g. [14, 15]). U_1 often increases with increasing concentration of impurities. This might be due to the presence of solute atom groups.

Quantum theory may be used to estimate the interaction energy between a group of solute atoms and a dislocation.

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