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EFFECTS OF ORDER ON DISPERSION STRENGTHENING AT HIGH TEMPERATURES: A FIRST MODEL

E. Arzt and E. Göhring
Max-Planck-Institut für Metallforschung and
Institut für Metallkunde der Universität, Stuttgart, Germany

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Introduction

The creep strength of metallic materials can be improved significantly by the introduction of fine, non-shearable dispersoid particles (see e.g. /1-3/). Over the last decade the theoretical understanding of this technologically important effect has been improved considerably; the results of these studies can be summarized as follows:

i) During the passage of a dislocation through an array of particles at high temperatures the Orowan stress is not reached because dislocation climb occurs /4,5/. At high homologous temperatures however climb is much too rapid to allow an explanation of the creep rates based on this mechanism alone. Only the assumption of "local" climb /5/ leads to correct order-of-magnitude in strength; the necessary dislocation configuration is however very unlikely /6,7/.

ii) A more natural explanation for the effect is based on TEM observations /8,9/ which suggest an attractive particle-dislocation interaction. Such a mechanism can be rationalized as being due to rapid diffusional relaxation in the particle-matrix interface /10/. A model which simulates the attractive force by assigning a lower line energy to the dislocation segment in the interface shows that only a small relaxation is necessary for dislocation detachment from the dispersoid to become the strength-determining event /11/.

iii) A more complete model /11,12/, which also considers the possibility of thermally activated dislocation detachment, results in a creep equation that has been successfully applied to several dispersion-strengthened materials:

$$\dot{\varepsilon} = \frac{6\cdot\lambda\cdot\rho\cdot D_v}{b}\cdot\exp\left(-\frac{Gb^2r\cdot\left[(1-k)\left(1-\frac{\sigma}{\sigma_d}\right)\right]^{3/2}}{k_BT}\right) \quad (1).$$

where $\dot{\varepsilon}$ is the creep rate, 2 λ the particle spacing, ρ the density of mobile dislocations, D_v the volume diffusivity, b the Burgers vector, G the shear modulus, 2 r the dispersoid diameter, k the relaxation parameter, k_B the Boltzmann's constant and σ_d the athermal detachment stress.

Both the otherwise "abnormal" stress sensitivities and the activation energies can in many cases be explained naturally with this equation /12/.

iv) The model of detachment-controlled creep leads to several new consequences for optimum alloy design /1/.

While this kind of modelling has up to now been carried out for <u>disordered</u> matrix materials, there is presently considerable interest in raising the strength of <u>ordered</u> matrix materials by dispersion strengthening. The reason lies in the fact that the creep strengths of monolithic intermetallic compounds are generally inferior, by a large margin, to those of advanced superalloys. This weakness may preclude the application of some otherwise attractive compounds in certain areas.

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In this paper we explore the effects which are introduced into the model as it stands by atomic order in the matrix. It is shown that, depending on the APB energy, certain intermetallic compounds may be more amenable to dispersion strengthening than others. The new model also leads to first conclusions concerning optimum alloy design, in particular whith respect to obtaining an optimum dispersoid size.

Effects of Order on Dispersoid-Dislocation Interaction

Consider an ordered matrix material with a low volume fraction of non-shearable dispersoid particles, such as Y_2O_3 in NiAl for example. In comparison with disordered materials, at least two separate phenomena peculiar to intermetallics must be taken into account: First, the diffusivity (which enters in all creep models, including equation 1) often exhibits a complicated dependence on the stoichiometry of the compound (e.g. /13/); constitutional vacancies, for example, provide a possible explanation for the reduced creep strength of off-stoichiometric compositions (e.g. /14/). If the diffusivity is known as a function of composition, this effect can readily be incorporated in equation 1.

Secondly, an ordered matrix is known to affect the structure of lattice dislocations: complete dislocations in the disordered lattice become incomplete in the ordered matrix and hence superdislocations form, e.g. /15/. When treating the process by which a dislocation surmounts a dispersoid particle, the interaction of the superpartials must now be considered (figure 1). The present paper will focus on this effect.

The stress-distance profile for the disordered case

When a single dislocation climbs over a spherical particle, it will encounter two distinct "obstacles" which result from an increase in total line energy /11/: as the dislocation climbs up, it has to increase its length: this effect leads to a "climb barrier". On the other hand, when the dislocation leaves the energetically favorable particle-matrix interface, additional specific line energy has to be supplied: this is the origin of the "detachment barrier". As before /11/, the attractive interaction is modelled by assigning a line energy $k \cdot T_M$ to the dislocation segment in the interface, where k lies in the theoretical range 0 to 1, and T_M is the line energy remote from the particle. Thus k = 1 denotes the case of no attractive interaction, the magnitude of which increases as k falls further below 1.

The shear stress τ necessary for the dislocation motion over the particle to continue at any position x, i.e. the "back stress", has been evaluated as a function of position x /11/:

$$\frac{\tau}{\tau_0} = \frac{\frac{\lambda}{r}-1}{\frac{\lambda}{r}-\frac{a}{r}} \cdot \frac{\frac{x}{a}}{1+\left(\frac{x}{a}\right)^2} \cdot \left\{ -\frac{k}{\sqrt{1-\left(\frac{a}{r}\right)^2}} + \sqrt{1+\left(\frac{x}{a}\right)^2 \left[1-\frac{k^2}{1-\left(\frac{a}{r}\right)^2}\right]} \right\} \tag{2}$$

where τ_0 is the Orowan stress in shear and $a = \sqrt{r^2 - h^2 - x^2}$ with h as the distance of the glide plane from the equator of the particle.

Figure 2 shows a plot of this stress profile in normalized form. It is seen, as expected, that the climb barrier decreases with increasing relaxation (smaller k), while the detachment barrier shows the opposite dependence. It has been shown /11/ that the climb threshold is given by

$$\frac{\tau_c}{\tau_0} = \left(k - \frac{h}{r}\right)^{3/2} \tag{3a}$$

where h is the distance of the glide plane from the equator of the particle. When averaged over all possible glide plane/particle configurations, this becomes:

$$\frac{\tau_{c,\,ave}}{\tau_0} = 0.4\,k^{5/2} \tag{3b}$$

The detachment threshold has the following dependence on k:

$$\frac{\tau_d}{\tau_0} = (1 - k^2)^{1/2} \tag{3c}$$

Equation 3c gives the athermal detachment stress without consideration of thermally activated detachment. The present paper will be restricted to this case.

Effect of superpartials on the detachment stress

Now consider the case of a superdislocation consisting of two partials with equal Burgers vector b. We assume that the spacing w between the partials is fixed by the APB energy γ_0 and is unaffected by the external stress; this is a reasonable simplification for $\gamma_0/b >> \tau$, which is usually the case. The dispersoid spacing along both partials is considered to be identical and independent of the bowing out distance. Finally, we restrict ourselves to the case of low volume fractions, e.g. below 10%, such that the change, with dislocation position, in APB area (figure 1) and in the extent of the fault in the interface can to a first order be neglected.

As one dislocation moves forward by an increment δx, virtual work is done against the back stress at the position of the dislocation considered. The total energy balance is composed of the work done by the external shear stress, the work done by the mutually repulsive stress on the partials and the change in APB area. For the leading dislocation (1) at $x = x_1$ we get:

$$\tau \cdot b \cdot L \cdot \delta x + \frac{\alpha}{w} \cdot L \cdot \delta x - \gamma_0 \cdot L \cdot \delta x = \tau(x_1) \cdot b \cdot L \cdot \delta x \tag{4a}$$

where τ is the external shear stress, L the dispersoid spacing, $\alpha = Gb^2/2\pi\kappa$ with the shear modulus G and $\kappa = 1$ for screw and $\kappa = 1 - \nu$ for edge dislocations, ν is Poisson's ratio, and $\tau(x_1)$ the back stress on dislocation (1) due to the particle, as given by equation 2.

Similarly we get for the trailing dislocation (2) at $x = x_2$

$$\tau \cdot b \cdot L \cdot \delta x - \frac{\alpha}{w} \cdot L \cdot \delta x + \gamma_0 \cdot L \cdot \delta x = \tau(x_2) \cdot b \cdot L \cdot \delta x \tag{4b}$$

Equations 4 can be combined to give:

$$\tau = \frac{\tau(x_1) + \tau(x_2)}{2} \tag{5}$$

This result means that in the present approximation the shear stress τ required to move the superdislocation from any position is given by the arithmetic mean of the back stress values at the positions of the two partials. Some special cases, in which the leading dislocation is situated at the point of detachment, are illustrated in figure 3:

a) If the spacing of the partials exceeds the particle diameter d (figure 3, case a), then $\tau(x_2) = 0$ and the detachment stress for the leading dislocation is reduced to half its original value.

b) If the spacing is such that the trailing dislocation sits at the point of the climb barrier maximum (figure 3, case b), then the detachment stress for dislocation 1 is reduced only by a small amount. This is the optimum case, with the detachment stress being given by the average of eqs. 3a and 3c:

$$\left(\frac{\tau_d}{\tau_0}\right)_{max} = \frac{\sqrt{1 - k^2} + \left(k - \frac{h}{r}\right)^{3/2}}{2} \tag{6a}$$

c) If on the other band, dislocation 2 resides in the valley of the stress profile (figure 3, case c), then it aides dislocation 1 in the detachment process, to the extent that the detachment stress for that dislocation can become negative. This case provides a lower bound on the detachment stress:

$$\left(\frac{\tau_d}{\tau_0}\right)_{min} = \frac{\sqrt{1-k^2} - \left(k - \frac{h}{r}\right)^{3/2}}{2} \qquad (6b)$$

Figure 4 shows the resulting detachment stresses as a function of w/d. It is clear that the detachment stress is at a maximum when i) w/d = 0 (no dislocation splitting), and ii) w/d ≈ 0.55 (case b above). The position of the second maximum is relatively insensitive to the value of k. It dominantes over the first maximum when the attractive interaction is small (k ≈ 1).

The resulting detachment stresses can also be plotted as a function of k (figure 5). Note that in the range of k values usually encountered (0.8 < k < 1.0) the variation in detachment threshold can be enormous. Only for exceptionally attractive particles (k < 0.7) can a narrow range for the detachment stress be expected.

Discussion and Some Preliminary Conclusions

The model for the effect of an ordered matrix on the particle-dislocation interaction at high temperatures, as presented here, still contains many simplifying assumptions. Probably most seriously, we have neglected the change in APB area near the particle, and we have not considered the fault that may develop between the partials in the particle/matrix interface. In addition, we have only treated the effects on the athermal detachment stress. Further work to include thermally activated detachment and the statistics of the processes is currently in progress.

Nevertheless, even this simplified formulation leads to some possibly interesting conclusions for alloy design. It is striking that for a fixed partial spacing w, i.e. for a given APB energy, there appears to be an optimum particle size

$$d_{opt} \approx \frac{w}{0.55}$$

Because of the inverse dependence of w on the APB energy γ_0, d_{opt} is inversely proportional to γ_0.

In practice, this optimum may be difficult to achieve in a given material. The second best strategy would then be to choose a dispersoid size well in excess of w, in order to fulfill the requirement w/d ≈ 0, corresponding to negligible dislocation splitting.

A first estimate for the dispersoid sizes required in two different intermetallics leads to the following conclusions /16/: For NiAl, with $\gamma_0 \approx 800$ mJ/m^2 and w ≈ 0, a particle size of 10 nm should give good results. By contrast, in Fe-40at%Al, with $\gamma_0 \approx 150$ mJ/m^2 and w ≈ 7 nm, much larger particles (of order of 50 nm) would be required. We suggest that the relatively inconsistent creep strength data of dispersion strengthened Fe-40at%Al, as compared to the much more consistent NiAl /16/, may be accounted for by this effect.

Summary

We have presented a first model for the effect of superpartials on dispersoid-dislocation interactions relevant for creep strength of dispersion strengthened intermetallics. The analysis indicates that the particle size, relative to the spacing of the superpartials, can have a significant effect on the creep strength. This result suggests a connection between the APB energy and the optimum particle size in dispersion strengthened intermetallics.

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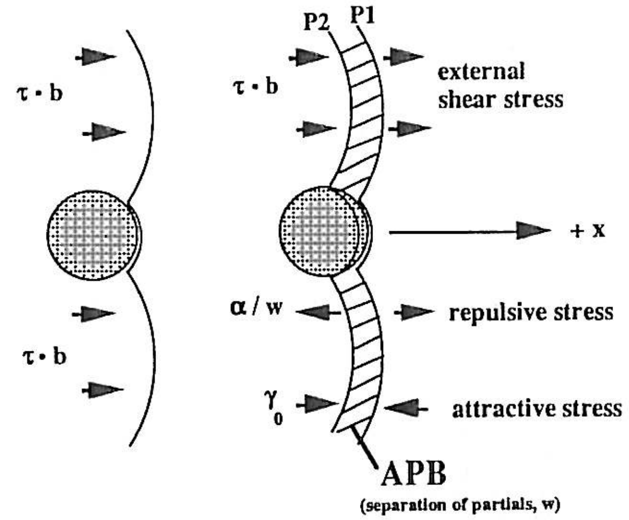

Fig. 1: The effect of an ordered matrix considered in this paper: dispersoid-dislocation interaction in a disordered matrix (left) is altered by the mutual forces on the superpartials (right).

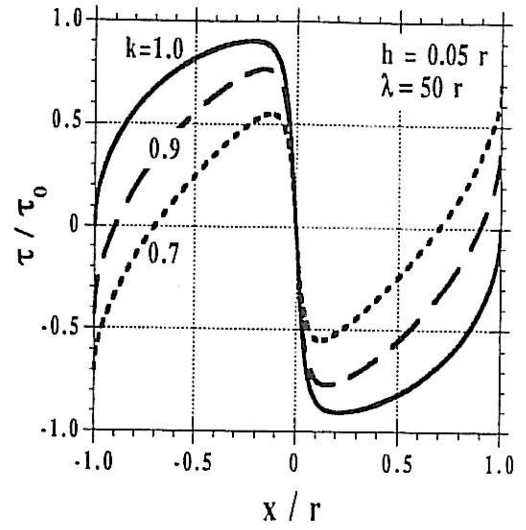

Fig. 2: Shear stress σ on the dislocation (normalized by the Orowan stress τ_0) vs. position x along the particle of radius r. Glide plane is assumed to intersect the particle near its equator.

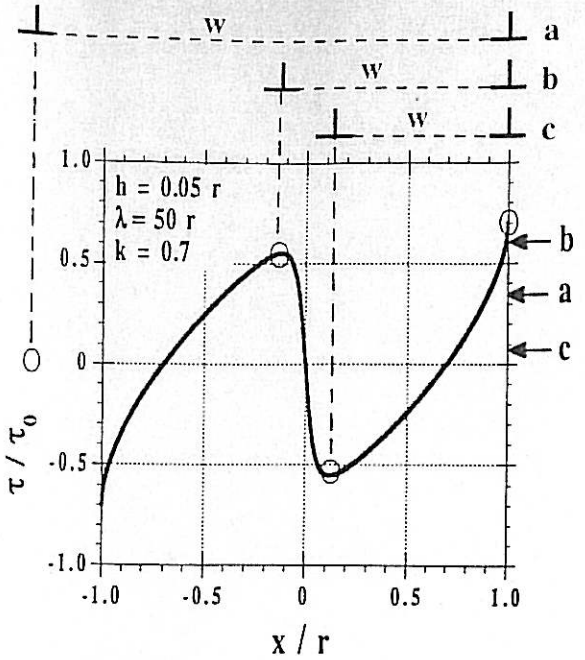

Fig. 3: The effect of the spacing w between superpartials on the detachment stress of the leading partial:
a) w > d
b) w ≈ 0,55 d
c) w ≈ 0,45 d, where d = 2 r is the dispersoid diameter. The arrows indicate the resulting stress level for detachment in the three cases.

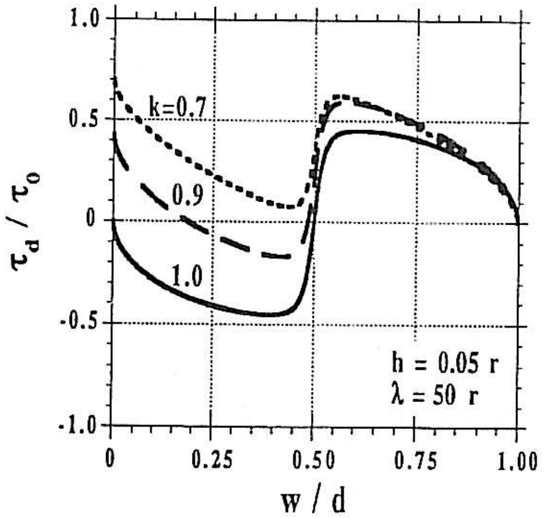

Fig. 4: The detachment stress for the leading partial with the aid of the trailing partial, as a function of partial spacing / dispersoid diameter, d = 2 r.

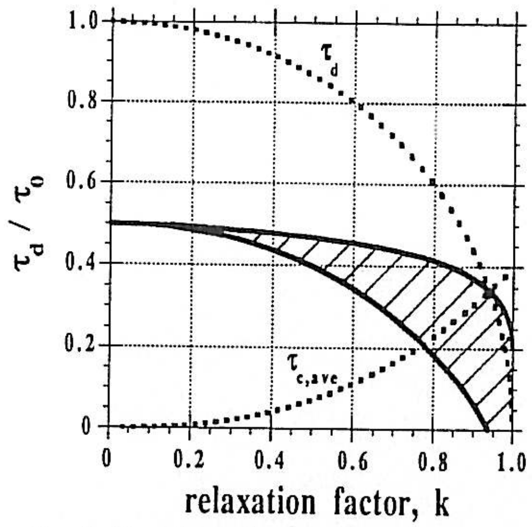

Fig. 5: Bounds on the detachment stress for the leading partial as a function of the relaxation factor k (eqs. 6a and 6b). Also shown are the detachment stress (eq. 3c) and the average climb stress (eq. 3b) for the disordered case (broken lines)