A MODEL FOR THE YIELD STRENGTH ANOMALY IN FeAl

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ABSTRACT

A phenomenological model is used to explain the yield strength anomaly in FeAl. The model incorporates hardening by thermal vacancies at intermediate temperatures, and dislocation creep at elevated temperatures. Since the vacancy concentration increases exponentially with increasing temperature, the model predicts an exponential increase in strength with increasing temperature. This increasing strength is terminated by the onset of dislocation creep. The model captures the experimentally-observed strain rate dependency of the yield stress at high temperatures, and yields an activation enthalpy for vacancy formation which is in excellent agreement with a previously measured value [1].

INTRODUCTION

Several studies on either large-grained or monocrystalline FeAl containing initially low vacancy concentrations have demonstrated anomalous strengthening at intermediate temperatures and a yield strength peak at ~0.40-0.45 Tm [2-13].

There have been a number of models developed to explain the yield strength anomaly in B2 compounds. In the cross-slip pinning model [14], <111> dislocations are assumed to cross-slip from {110} to {112} planes, where they become pinned. This process is thermally-activated, hence, the density of pinning points and, thus, the yield strength increase with increasing temperature. The driving force for this cross-slip is either a reduction in the anti-phase boundary (APB) energy or the torque term arising from the anisotropy in elastic constants [15]. For FeAl, the APB energy on the primary {110} slip plane is lower than that on the cross-slip {112} plane [16], and the torque term does not exist on the {110} slip plane [17]. Therefore, cross-slip pinning is unlikely to occur in FeAl.

Xiao and Baker [3] first noted that the yield strength peak occurred in FeAl at about the temperature of the well-known transition from glide by APB-coupled a/2<111> dislocations at low temperature to <100> slip at high temperature [13,18-19]. However, this slip transition alone cannot explain the yield strength peak since for a yield peak to occur there has to be a mechanism whereby <111> slip becomes more difficult with increasing temperature - a slip transition would presumably simply produce a change in the slope of the yield stress-temperature curve. Contemporaneously, Yoshimi and Hanada [5] suggested, based on the occasional observations in FeAl [4] of dislocations with non-<111> Burgers vectors below the yield peak, that the gliding <111> dislocations decompose (locally) into <001> and <110> segments which act as pinning points. If the density of these pinning points increases with temperature, an increase in strength with increasing temperature occurs. However, the applicability of this model is unclear since Munroe and Baker [20] could not find evidence of this decomposition in a boron-doped Fe-45Al alloy which exhibited the anomalous yield behavior even though they specifically looked for it.

Morris [21] suggested a model, based on a mechanism that was originally proposed to explain dislocation locking in β brass [22-27], which utilizes the local climb of APB-coupled dislocation partials. Vacancy diffusion was suggested to occur between the partials' cores such that locally one partial climbs up whilst the other climbs down. These segments act as pinning points. If the density of the climb-dissociated partials increases with increasing temperature, then the yield strength increases with temperature. This model is intriguing but it is unclear what terminates the rising yield stress with increasing temperature, and, hence, what is the cause of the peak. At present, there is a lack of experimental data to evaluate whether this mechanism operates in FeAl. However, the climb-lock model appears to imply a strain-rate dependency of the yield stress, i.e. increasing yield stress with decreasing strain rate, which is the opposite of that observed experimentally [28].

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THE VACANCY-HARDENING MODEL

This paper outlines a vacancy-hardening model for the yield peak in FeAl and discusses its implications. The model, which is described in detail elsewhere [29], is based on an idea proposed by Carleton, George and Zee [10]. In this model, the increasing yield stress with increasing temperature arises because of vacancy pinning/drag on gliding APB-coupled a/2<111> dislocations. How the vacancies pin or cause drag to the dislocations is unclear, but that they do is well-established [30,31]. One possible mechanism whereby vacancies could impede dislocation motion involves a pair of a/2<111> partial dislocations gliding along a (110) plane separated by an APB, in which the second partial restores the disorder (within the APB) generated by the first. If a vacancy is now placed at the core of either the leading or the trailing dislocation, the edge dislocation climbs up one plane at a single atom. Now the disorder generated by the leading dislocation is no longer restored by the trailing dislocation at the point on the dislocation where the vacancy has condensed. The resulting disordered "tube" exerts a drag on the dislocation. Such tubes have, indeed, been observed in FeAl behind gliding edge or near-edge APB-coupled a/2<111> dislocations after room temperature deformation [32-34]. This would result in an increased work-hardening rate in Region III, as has been observed [9]. Interestingly, condensation of a vacancy on the <001> dislocations which are observed at high temperature would not produce this effect since they are perfect dislocations. Thus, one might expect a lesser effect of vacancies on <001> dislocations.

Vacancy hardening can arise if the activation enthalpy for vacancy formation, E_f, is relatively low compared with the enthalpy for vacancy migration, E_m. In other words, at intermediate temperatures although vacancies are easily formed they move with difficulty. Since, the vacancy concentration increases exponentially with increasing temperature, the yield strength initially increases exponentially with increasing temperature. Eventually, at elevated temperature, the vacancies are able to migrate (E_m need not be high in absolute terms simply higher than E_f) and, hence, instead of impeding dislocation motion, the vacancies lead to dislocation creep. The onset of dislocation creep ends the rising part of the yield strength-temperature curve, and gives rise to the yield peak.

There are two clear implications of this model. First, if there are a large number of quenched-in vacancies. Then the low temperature strength will be raised and the yield peak will be obscured. This is one possible reason why the yield peak was not observed in many early studies [13,22,35-38]. Second, although the vacancy hardening regime would not, to a first approximation, be expected to be strain-rate dependent, the dislocation creep regime clearly is. The onset of dislocation creep will occur at high temperatures at higher strain rates and at lower temperatures at lower strain rates. These shifts in the onset of dislocation creep with strain rate will also produce changes in the magnitude of the peak: to higher values at higher strain rates and to lower values at lower strain rates. These suggestions are consistent with observations [28,39].

A less obvious implication is that if a specimen is tested, at a fixed strain rate, at the yield peak temperature after holding for different times at that temperature, then the yield strength will vary with hold time. This affect arises because the equilibrium vacancy concentration does not occur instantaneously but requires time, that is, after heating from room temperature, the vacancy concentration will increase with increasing hold time. Hence the yield strength increases with increasing hold time at the peak temperature. Conversely, if vacancies in excess of the equilibrium concentration are quenched (from elevated temperature) into a specimen at the yield peak temperature, then in short times the yield stress will be increased. Both of these features have been observed experimentally [28].

MATHEMATICAL FORMULATION

In order to test the validity of the vacancy-hardening model further, experimental data on large-grained, low-temperature annealed Fe-40Al have been fitted, as shown in Figure 1, using the phenomenologically-derived equations below (the derivation of these equations is described in greater detail elsewhere [29]). The experimental yield stress-temperature data are split into three regions corresponding to different physical mechanisms labeled II, III and IV. (Region I is data for below room temperature which is not relevant to the present discussion but is discussed elsewhere [29]).

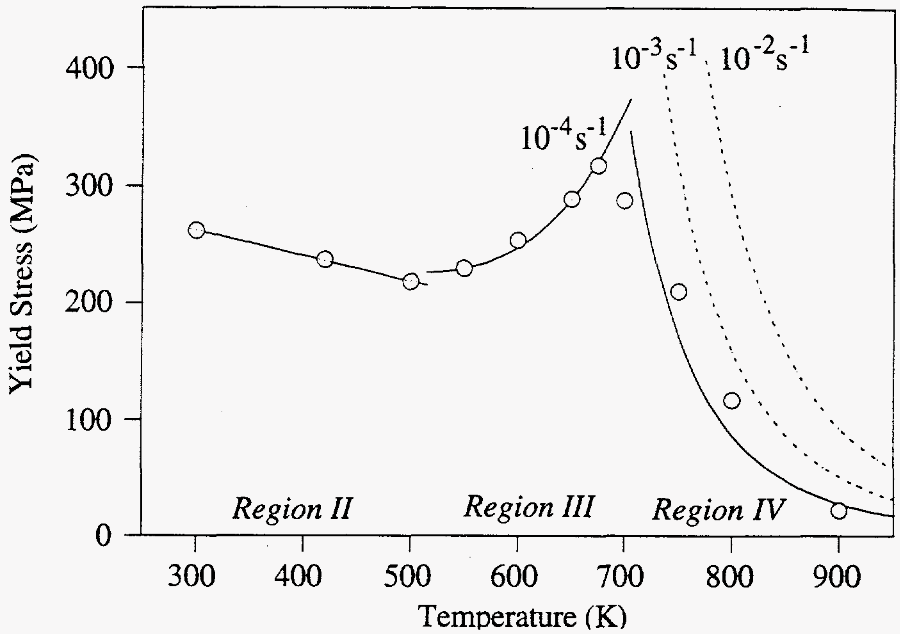

Figure 1. Graph of yield stress versus temperature for large-grained, low-temperature-annealed Fe-40Al strained under tension at 1 x 10^{-4} s^{-1}. See text for details. After reference 29.

In region II we assume that the yield stress scales with the shear modulus and therefore displays a weak linear temperature dependence:

$$\sigma_{II} = \sigma_o - \alpha T \qquad \textbf{Region II}$$

where σ_o is the yield stress extrapolated to absolute zero and α is a constant.

In region III, the increase in yield stress due to thermal vacancies, $\Delta\sigma$, is assumed to be a r[illegible] of a solid solution-type hardening. Utilizing the observed parabolic hardening due to v[illegible]cies in FeAl [30] and that the vacancy concentration increases exponentially with increasing temperature, one can write [29], $\Delta\sigma_{III}$ (= $\sigma_{III} - \sigma_{II}$, where σ_{III} is the yield stress in region III), as:

$$\Delta\sigma_{III} = \{C_o \exp(-E_f/kT)\}^{1/2} \qquad \textbf{Region III}$$

where C_o is a pre-exponential term, k is the Boltzmann constant and T the absolute temperature.

In region IV, vacancies are assumed to be present in a sufficient concentration and are sufficiently mobile so that deformation is by dislocation creep. At steady state, over a small temperature range, the yield stress can be written [29,40]:

$$\sigma_{IV} = \mu\{\dot{\gamma} \exp(E_d/kT) / D''_o\}^{1/m} \qquad \textbf{Region IV}$$

where μ is the shear modulus, $\dot{\gamma}$ is the shear strain rate, *m* is a material constant, E_d is the activation enthalpy for vacancy diffusion ($E_d = E_f + E_m$), and D''_o is a modified pre-exponential factor for diffusion, which is weakly temperature dependent.

At constant $\dot{\gamma}$, the temperature dependencies of the yield stress in the three regions can be fitted to the data for Fe-40Al [3] using $\sigma_{II} \propto T$; $\Delta\sigma_{III} \propto \exp(-1/T)$; and $\sigma_{IV} \propto \exp(1/T)$, respectively, see Figure 1. Since the equations in the model are empirical, and one can obtain arbitrarily good fits with the experimental data by choosing appropriate fitting parameters, the only way to judge whether the model is reasonable is by determining values for the various constants in the equations and examining whether they are physically reasonable. This has been done [29]. For Region II, values of σ_o and α of 330 MPa and 0.22 MPa·K^{-1}, are obtained. Unfortunately, there are no independent data with which to compare σ_o. However, if α is normalized with respect to the yield stress at absolute zero one obtains a rate of change of stress with temperature of $6.7 \times 10^{-4} T^{-1}$, which can be related to the rate of change of elastic modulus with temperature normalized with respect to the modulus at absolute zero, which is $3.5 \times 10^{-4} T^{-1}$ for Fe-40Al [41]. For region II, the physical constant, α, obtained from the model is in reasonable agreement with previously established data.

For region III, a value of C_0 of 2.5×10^{11} MPa^2 is obtained. Again, there are no data with which to compare. However, the value obtained for E_f of 92 kJ/mol is in remarkable agreement with that determined experimentally (95 kJ/mol) by Würschum, Grupp and Schaefer [1], a result which strongly supports the vacancy-hardening model. In region IV, a value of E_d/mk of $8.2 \times 10^3$is obtained. Using the E_d of 259 kJ/mole measured by Würschum et al. [1] yields a value for *m* of 3.8, which is reasonable for dislocation creep where values typically lie between 3 and 7 [40].

DISCUSSION

The modeling results make it evident why FeAl shows a yield stress peak. The activation enthalpy for vacancy formation (~95 kJ/mole) in FeAl is relatively low compared with the activation enthalpy for vacancy migration (~164 kJ/mole) [1]. In other words, as noted earlier, it is easy to form vacancies but difficult for them to migrate. This feature is evident from the observation that large vacancy concentrations are retained in FeAl after annealing at elevated temperatures and cooling even quite slowly [31].

Given that the model reasonably fits the experimental data and can make predictions which seem to be borne out (see The Vacancy-Hardening Model section), it is reasonable to consider, using the model, how variations in Fe:Al ratio would affect the temperature dependence of the yield stress. Consider first the iron-rich alloys containing from 40 to 45 at. % Al. At lower temperatures, there are few vacancies in these materials and anti-site atom strengthening appears to be very weak. Thus, in Region II, the yield stresses are very similar, see Figure 2. The onset of Region III occurs at about the same temperature (and the same homologous temperature since the melting points of these three compositions are also very similar) in all three alloys as does the onset of Region IV. Thus, the yield stress peak occurs at about the same temperature in all the alloys. The only distinction appears to be that the difference between the peak yield stress and the valley stress (i.e. the lowest yield stress, which corresponds to the onset of Region III) decreases h increasing aluminum concentration. This difference may be related to changes in the alpies of vacancy formation and migration.

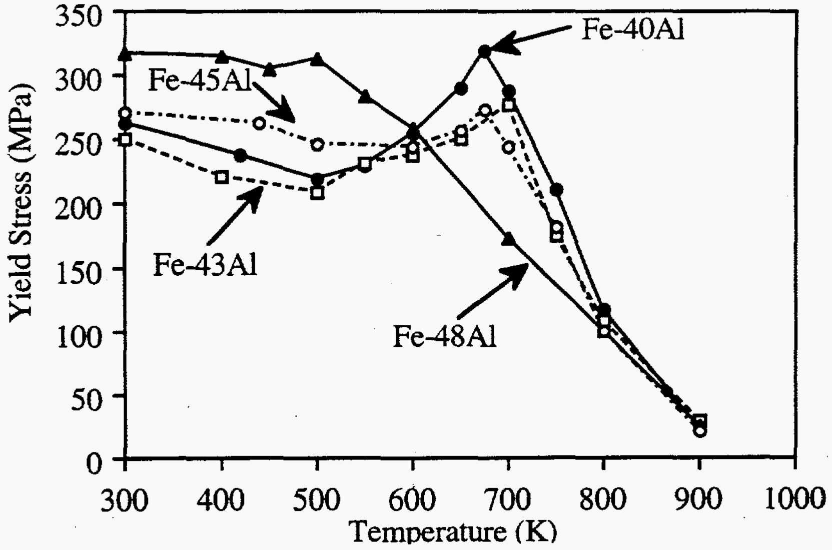

Figure 2. Yield stress versus temperature for large-grained binary FeAl. After reference 9.

More intriguing is that both polycrystalline Fe-48Al and Fe-50Al strained at 1×10^{-4} s^{-1} do not show the yield stress peak at all but simply a change from Region II straight to Region IV, see

Figure 2. The reason for this change in behavior is probably related to the fact that for both of these compositions the room temperature yield stress is strongly controlled by vacancies which appear to be present in substantial numbers [30,42]. The effect of such vacancies is to raise the yield stress in Region II substantially. The lack of a yield stress peak in stoichiometric or near-stoichiometric alloys is somewhat analogous to iron-rich alloys which have not been equilibrated at low temperature and, hence, contain high vacancy concentrations. Here, again, the yield stress in Region II is raised and Region III is not observed [8,10]. The shift in Region IV to lower temperature in stoichiometric or near-stoichiometric alloys is presumably affected by the strain rate. Straining at a higher rate would shift Region IV to a higher temperature and, possibly allow the occurrence of Region III and, hence, result in a yield stress peak. Data again seem to confirm this trend. In Fe-48Al no yield stress peak has been observed after straining at 1×10^{-4} s^{-1} [9] but a peak has been observed after straining at 1×10^{-3} [8]. This observation suggests that perhaps even the stoichiometric alloy may show a yield stress peak if strained at a high enough strain rate.

We can also consider the effects of solutes. Boron doping would be expected to raise the yield stress in Region II by a simple solute strengthening mechanism. Since the yield stress in Region III is controlled by vacancies we might expect little effect of the interstitial boron at lower dopant levels, particularly at higher temperatures in this region, since the strengthening from the vacancies will far outweigh the strengthening from boron. (Data show that at room temperature, boron strengthening and vacancy strengthening produce yield stresses less than those expected by simple addition, implying an association of the interstitial boron atoms with the vacancies [43].) Boron, as with most solutes, would be expected to decrease dislocation creep and hence offset the onset of dislocation creep to higher temperatures. Thus, the onset of Region IV would move to higher temperatures. This would result in a shift of the peak yield stress to higher temperatures and higher stresses. Examination of the available data, see Figure 3, tend to confirm these trends.

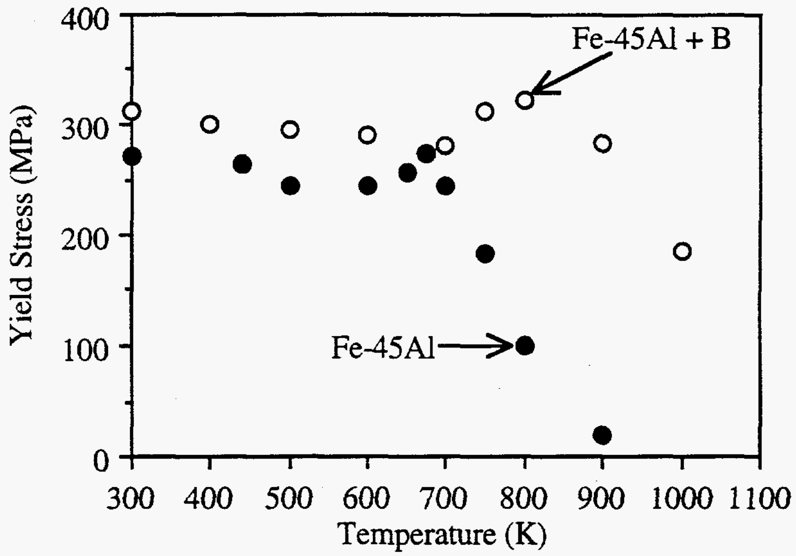

Figure 3. Graph of yield strength versus temperature for large-grained, low-temperature-annealed Fe-45Al and Fe-45Al + B. After reference 7.

Interestingly, the model does not rely on a slip system change to explain the yield anomaly. The change in slip system presumably occurs because the vacancies impede <111> dislocation glide to such an extent that <001> slip becomes easier. However, the slip system change is not necessary to cause the peak since above the peak there is a mechanism change to dislocation creep. That the slip vector change is not the root cause of the yield stress peak, but a by-product of vacancy-hardening, suggests that this mechanism may explain the yield stress anomaly in some other B2 alloy systems where no slip vector change is observed [44-46].

CONCLUSION

A model has been presented which can explain the yield strength anomaly in FeAl. The increasing yield strength with increasing temperature is ascribed to vacancy pinning/drag on gliding APB-coupled a/2<111> dislocations. The decreasing strength with increasing temperature at elevated temperature is ascribed to creep of <100> dislocations. Some physical parameters derived from the model compare well with experimentally-determined values derived by others, and some predictions of the model appear to be borne out.

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