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Modelling of the influence of alloy composition on flow stress in high-strength nickel-based superalloys

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Abstract

A model is proposed for the variation of the yield strength of nickel-based superalloys as a function of chemical composition. Consistent with hardening theory, alloy strength is assumed to be proportional to the product of the anti-phase boundary (APB) energy and the square root of the fraction of the strengthening γ' phase. A relationship is established between the APB energy estimated using a CALPHAD database and predictions from density functional theory. Quantitative estimates of the role played by Ti, Ta, Nb, Cr, W and Mo suggest that these elements have a profound effect on APB energy. A procedure is proposed to enable the strength to be estimated from an initial input of the chemical composition alone. Predictions are made for new multicomponent alloys. Insight is provided into how composition may be isolated for optimal strengthening. However, the size and spacing of the γ' precipitates is not explicitly predicted or considered; future work must address this.

Keywords: Nickel superalloys; Modelling; Precipitation hardening; Alloy design

1. Introduction

Nickel-based superalloys display excellent high-temperature mechanical properties, particularly in creep and fatigue [1–3]. But why is this? The overarching reason is that deformation on the microscale is restricted by the precipitation hardening conferred by a significant fraction of the $Ni_3(Al, Ti, Ta)$ phase, which is commonly referred to as gamma prime (γ'). The origin of this effect cannot be explained by differences in the elastic moduli of matrix and precipitate, since these do not differ greatly from phase to phase. Instead, it is the fault energies associated with anti-phase boundaries (APBs) and stacking faults (SFs) which are responsible for it [4,5]. Their magnitudes severely limit the penetration of the γ' phase achieved by the dislocations introduced during deformation, and thus bulk plastic flow.

It follows that the fault energies are of great significance to the physical metallurgy of Ni-based superalloys. This is emphasized further by considering theoretical expressions which describe the how yield strength varies in the alloy with respect to precipitate size and distribution. Take the case of so-called weakly and strongly coupled dislocations; Eqs. (1a) and (1b) describe permeation of a superalloy containing a fraction f of precipitates. The shear yield stress τ_y varies according to [6]:

$$\tau_y = \frac{\Delta E_{\mathrm{APB}}}{2b}\left[\left(\frac{6\Delta E_{\mathrm{APB}} f r}{\pi T_L}\right)^{1/2} - f\right] \tag{1a}$$

$$\tau_y = \sqrt{\frac{3}{2}}\left(\frac{Gb}{r}\right) f^{1/2}\frac{w}{\pi^{3/2}}\left(\frac{2\pi\Delta E_{\mathrm{APB}} r}{wGb^2} - 1\right)^{1/2} \tag{1b}$$

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for the cases of weakly and strongly coupled dislocations, respectively. Here, ΔE_{APB} is the APB energy, b is the Burgers vector, r is the mean precipitate radius, T_L is the line tension, G is the shear modulus of the γ phase and w is a dimensionless constant to account for uncertainties, which is expected to be of the order of unity. One can see that the APB energy is expected to influence the flow properties substantially. Moreover, some of the dependence of mechanical strength on alloy chemistry is due to differences in the APB energy, which depends upon the chemistry of the γ' phase. Elements such as Ti and Ta which partition strongly to γ', which thus influence the APB energy, might therefore be expected to enhance the yield stress. The stoichiometry of $Ni_3(Al, Ti, Ta)$ is also likely to be important. However, calculations are needed to deduce the precise details of these quantitative relationships.

The work reported in this paper was motivated with the above in mind. We set out to identify quantitative alloy composition/mechanical property relationships in polycrystalline Ni-based superalloys. Emphasis is placed on the APB energy and its role in conferring static strength in these materials. The paper is structured in the following way. First, the experimental and theoretical evidence for the magnitude of the APB energy is considered. Next, the dependence of the APB energy on changes in chemistry of $Ni_3(Al, Ti, Ta)$ is quantified, using methods based upon computational thermodynamics and electron structure calculations. Finally, models for the yield stress which contain a composition-dependent APB energy are considered. These are used to rationalize the role played by the composition dependence of the APB energy in conferring strength.

2. Background

In Ni-based superalloys, precipitates of the ordered $L1_2$ phase (γ') reside within a coherent face-centred cubic (fcc) matrix, commonly referred to as the γ phase. The dislocations in γ have a Burgers vector of $a/2[1\bar{1}0]$ on the $\{111\}$ plane, but this is not a full dislocation in the γ' phase. Two dislocations with Burgers vector $a/2[1\bar{1}0]$, or superlattice partial dislocations, are required to generate a full dislocation within the precipitate. In practice, a superlattice partial dislocation can enter the γ' precipitates, forming a planar fault called an APB—see Fig. 1. Depending on the plane, the superlattice partial dislocation resides on either $\{111\}$ or $\{001\}$, with the order imposed by the $L1_2$ crystal structure being locally overcome by forcing undesirable first (in the case of $\{111\}$ planes) or second (in the case of $\{001\}$ planes) neighbour bonds. A trailing superlattice partial dislocation is then able to restore the ordered $L1_2$ structure.

Early approximations of the APB energy for the $L1_2$ phase appealed to an Ising model. In this approach the energy is determined by relating changes in internal energy—approximated from thermodynamic values—to the interaction of atom pairs at the planar defect. Flinn [7] proposed a model to calculate APB energy in superlattices based on atomic interactions. Applying this model to the $L1_2$ crystal structure yields the following equation:

$$\Delta E_{APB} = \frac{2\phi h}{a^2\sqrt{h^2+k^2+l^2}} \quad (2)$$

where h, k and l are the Miller indices of the plane on which the superlattice partial dislocation resides, and $\phi = \Omega_{AB} - 1/2(\Omega_{AA} + \Omega_{BB})$ is the ordering energy, with Ω_{AB}, Ω_{AA} and Ω_{BB} representing the interaction energies of the A–B, A–A and B–B bonds, respectively. A number of ordered structures, including Ni_3Al, exhibit a proportional relationship between the ordering energy and the disorder–order transition temperature, T_{ord}, consistent with:

$$\phi = kT_{ord}/w \quad (3)$$

where k is the Boltzmann constant and w is a constant determined by the crystallographic structure and model applied. For $L1_2$ alloys w can vary between 0.82 [8], 1.0 [9] and 1.5 [10]. Fig. 2, taken from Ref. [11], shows that Flinn's model gives a reasonable approximation of experimentally determined values for the APB on the $\{111\}$ plane for a number of $L1_2$ alloys; the plotted lines have been determined using Eqs. (2) and (3).

The APB energy can be determined experimentally by using transmission electron microscopy (TEM) to measure the distance between superlattice partial dislocation pairs in the γ' phase [12–27]. Repulsive forces exist between dislocations due to their associated strain fields, which decrease as separation between the dislocations increases. However, as the separation gets larger, the surface area of the APB and the energy associated with this fault acts to bring the partial dislocations together. Assuming elastic isotropy, the forces acting on the partial dislocations can be balanced to find their equilibrium separation. The APB energy and the separation distance of partial dislocations, d, are related using:

$$\Delta E_{APB} = \frac{\alpha\mu b^2}{2\pi d} \quad (4)$$

where α is dependent on the dislocation character, μ is the shear modulus and b is the Burgers vector [28]. In practice the measurements made using TEM methods may significantly deviate from actual APB energies. The most significant source of error arises from misrepresentation of separation distances in TEM images. Image-correction methods have been developed in order to determine true separation from TEM observations. Cockayne et al. [29] derived an isotropic correction for observations under weak beam conditions. Corrections have been further improved using image simulations—which provide an anisotropic Cockayne-like correction—to determine dislocation separation [15].

The APB energy in binary Ni_3Al has been studied extensively using TEM experiments [12–18]; this work has been predominantly focused on Ni- and Al-rich compositions. Douin and Veyssiere [16] showed that APB energy on $\{100\}$ is increased by excess Al and lowered by excess