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Selecting non-isothermal heat treatment schedules for precipitation hardening systems: An example of coupled process–property optimization

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Abstract

A physically based process model for the room temperature yield strength of an age-hardenable alloy subject to selected monotonic non-isothermal heat treatment schedules is developed and used to examine the possible efficiencies in processing and enhancements in strength that may be realistically achieved. 'Processing Maps' are generated which illustrate both the yield strengths achievable and the processing routes necessary to achieve them, as well as estimates of the energy consumed in the thermal treatment. A Fe–2Cu (wt.%) alloy is used as an example and the results of physical experiments are compared with the model predictions. For the conditions examined, enhancements in yield strength of ~8% above those achievable in comparable isothermal treatments are illustrated with 65% of the energy input. Alternatively, similar yield strengths to those from comparable isothermal treatment are shown to be achievable with ~35% of the energy input. The physical origins of the observed effects and the potential implications of coupled process–property optimization are considered.

Keywords: Precipitation; Ageing; Hardness; Modelling; Non-isothermal

1. Introduction

The in situ formation of a distribution of precipitates from a supersaturated metallic solid solution can have a very large effect on the properties of alloys. The effects on mechanical properties have been particularly well studied, especially their influence on the yield strength [1–3]. Much effort has been expended in attempts to manipulate the in situ precipitation behavior as a means of optimizing the property (or combinations of properties) of interest. A rational approach to this optimization requires an understanding of two aspects of the problem: (i) the effects of the available processing variables on the development and evolution of microstructure (processing–microstructure link); and (ii) the effect of the microstructure on the property of interest (microstructure–property link).

The processing variable which has received the most attention is temperature. The effect of temperature on the precipitation process from supersaturated solid solutions and the resulting hardening effects have been experimentally studied for nearly 100 years [4]. In the laboratory this is often achieved by monitoring the hardness as a function of isothermal annealing time and the precipitation products can be monitored using electron microscopy techniques or bulk techniques such as small angle X-ray scattering. More recently, theoretical treatments of the in situ formation and evolution of a distribution of precipitates from a solid solution have been developed (e.g. [5–7]), and these can now be readily implemented using modern computational thermodynamic and

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kinetic tools. Theoretical treatments relating the precipitation state to the yield stress are also now available and these are based on calculations of the shear stress required to propagate a dislocation through an array of obstacles [1–3]. In both cases, the theoretical treatments are reasonably mature for spherical particles.

The first researchers to couple theoretical descriptions of the effect of temperature on the evolution of microstructure in precipitation hardenable alloys and the corresponding microstructure effect on the hardening response into an overall process model were Shercliff and Ashby [8,9]. They applied this approach to the rationalization of isothermal age-hardening curves in a series of Al alloys. Since this first attempt, many treatments coupling the precipitation process with the mechanical response have appeared in the literature, with much success in rationalizing the observed mechanical response [6,10–19].

In those cases where process models have been validated for a range of processing conditions an opportunity arises to use the model to perform virtual experiments and generate 'processing maps' that can show both the ranges of properties that might realistically be achieved and the approximate processing routes to achieve them. In this work, we have performed 'virtual experiments' using a process model for the room temperature yield stress in a model Fe–2Cu (wt.%) alloy to identify potential non-isothermal heat treatment schedules that maximize the yield stress subjected to constraints on the maximum time and temperature of the process.

In the development of process models a number of approximations, simplifications and generalizations must be made. As a result, there is a limit to the numerical accuracy which can be expected. At the current level of development, it is important to emphasize that the role of such process models is not to completely replace experiments. Rather, as will be shown in the following work, they are complementary, and the purpose is to help identify, for example, the types of non-isothermal heat treatment schedules that are likely to be of most interest for experimental investigation.

The use of variations in temperature during processing as a means of enhancing the yield strength through modifications to the precipitation process date at least to the 1940s [20] and have been attempted many times since (e.g. [21–25]). In each case the optimal times and temperatures for treatments must be found experimentally and the number of possibilities for examination is necessarily restricted. It is therefore difficult to evaluate whether an optimal solution to the processing–microstructure–property question has been found. The nucleation, growth and coarsening processes governing precipitation are all strongly temperature dependent, as is the overlap and competition between each of the processes. It is because of this complexity in the coupled phenomena that it seems unlikely that optimal non-isothermal treatment schedules could be easily derived from any simple, general criteria.

2. Model description

A binary Fe–2Cu (wt.%) alloy was used for the study. This system has the advantage that the precipitation and hardening behavior has been studied previously [18,26,27] and our process model has been calibrated for the series of temperatures [18] of interest in this study. The model couples a description of the precipitation of Cu in α-Fe under non-isothermal heat treatment conditions with a summation of contributions to the room temperature yield strength.

2.1. Precipitation of Cu in α-Fe

Upon annealing a supersaturated Fe–Cu solid solution, the first phase to appear is a coherent metastable BCC Cu precipitate which transforms to the FCC structure upon reaching a size of ~9 nm [28]. In this study, we are concerned with conditions where the mean particle diameter rarely exceeds this value so precipitation is represented by a single process of spherical, BCC pure Cu precipitation.

The kinetics of Cu precipitation is described using a two-stage precipitation model [6,18] where the mean particle radius (R) and the particle number density (N) are monitored. The first stage consists of concurrent nucleation and growth and the second stage consists of coarsening. The experiments and calculations were conducted within a regime where no significant overlap between nucleation and coarsening is expected [29] and therefore this simple two-stage model is expected to satisfactorily describe the kinetics of precipitation.

2.1.1. Nucleation

The nucleation of Cu in α-Fe is described using classical nucleation theory [30]:

$$\left.\frac{\mathrm{d}N}{\mathrm{d}t}\right|_{\mathrm{Nucl}} = \beta^* Z N_0 \exp\left(\frac{-\Delta G^*}{kT}\right)\left(1-\exp\left(\frac{t}{\tau}\right)\right) \tag{1}$$

where N is the number of precipitates per unit volume, N_0 is the number of nuclei sites per unit volume, Z is the Zeldovitch factor, β^* is the absorption frequency of a Cu atom, ΔG^* is the activation energy for nucleation, τ is the incubation time, k is Boltzmann's constant, T is temperature and t is time. Classical derivations for a spherical nucleus assuming ideal solution thermodynamics are used for the evaluation of Z, β^*, τ and ΔG^* [30]. The diffusivity of Cu in α-Fe is described by an Arrhenius equation ($D^{\alpha}_{\mathrm{Cu}} = D_0 \exp(-Q/RT)$) with $D_0 = 4\times10^{-2}\ \mathrm{m^2/s}$ and $Q = 129{,}484$ J/mol [18] (Table 1). The equilibrium solubility of Cu in α-Fe as a function of temperature is described by the solubility product, $\log_{10}(\text{at.\% Cu}) = -1450.4/(T+1.05)$ [18].

2.1.2. Growth

Diffusion-controlled growth of the spherical Cu precipitates with local equilibrium interfacial conditions,