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Modelling of microstructure evolution in hot deformation

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This paper reviews various approaches to the modelling of microstructure evolution in hot deformation, for the purpose of predicting the flow stress during deformation or for predicting the subsequent annealing behaviour. Two contrasting approaches are discussed, and illustrated for the example of hot plane-strain compression testing of Al–Mg alloy. These approaches are (i) physically based state variable models, in which the microstructure and property evolution is modelled explicitly; and (ii) advanced statistical methods, for linking processing conditions empirically to properties, or to annealing rate and final microstructure.

The state variable models illustrate some general features of microstructure modelling and the level of experimental work that goes with it. Of particular importance are the accuracy of the data used to calibrate or validate a model, the implications that this makes on the volume of data needed, and the viable level of detail in the model that can realistically be verified. Various sensitivity analyses will be used to illustrate the need for a balanced view of model and experiment if a credible predictive capability is to emerge.

The statistical methods provide no physical insight, but, nonetheless, warrant further consideration for hot-deformation problems. They potentially provide a means to optimize time-consuming experimental work, and may provide useful predictive capabilities for industry rather sooner than can be expected from complex physically based modelling.

Keywords: modelling; microstructure; deformation; state variable methods; statistical methods; aluminium alloys

1. Introduction

Modelling of thermomechanical processing of metals is one of a number of industrial materials modelling activities reviewed recently in response to the Technology Foresight exercise (Shercliff 1997). This illustrated the breadth of industrial processes and alloys for which there are common underlying challenges in process modelling. Table 1 summarizes the dominant thermomechanical processes and alloys.

The level of model development varies greatly between processes and materials. This largely reflects the volume of production in each alloy system, but also the complexity of the deformation problem (e.g. flat rolling is more advanced than section rolling or forging). Thus, steels and aluminium alloys dominate, but much is to be gained by interaction across disciplines. Many industrial modelling challenges are generic to most of the combinations in table 1, as summarized in table 2.

For many deformation processes, there is a view that continuum mechanics finite-element (FE) methods are well established, both for simulating the manufacturing

Table 1. *Thermomechanical processes and alloy systems*

processes	materials
flat rolling	steels
section rolling	Al alloys
forging	Ni alloys
extrusion	Ti alloys
sheet forming	intermetallics
machining	metal matrix composites (MMCs)
friction welding	
'standard tests' (e.g. plane-strain compression (PSC))	

Table 2. *Major industrial modelling challenges in thermomechanical processing*

component design-for-manufacture
design of dies and tooling
shape and property control
reduction of defects, higher productivity
coupling in software of design, processing and product performance analysis
alloy development
scientific understanding

process itself and, also, the less obvious task of modelling the 'standard tests' used, for example, to determine constitutive behaviour (Shercliff 1997; Ricks, this issue; Melton, this issue; Beynon, this issue). The greatest limiting factors at the continuum level in all metal-forming analyses are poor characterization of interfacial friction conditions (and to a lesser degree heat transfer), and the need for improved models of material constitutive behaviour for complex deformation histories and for inhomogeneous materials.

FE methods now provide sufficient information for many 'mechanical' problems, such as load prediction, and for problems of flatness, residual stress, etc. By empirical means, a modest degree of prediction of microstructure can be achieved; for example, linking recrystallization after deformation to the average process conditions. Figure 1 illustrates the interactions in thermomechanical process modelling at this 'macro' level. Given the volume of detailed FE output about the distribution of deformation and temperature history, there is great potential to exploit this output for microstructure modelling (Shercliff 1997; Evans 1993). In most cases, microstructure modelling will be a 'post-processing' activity, but, in more complex situations, microstructure prediction may be in parallel, determining the constitutive response of the material in the next time-step. Figure 2 summarizes the additional connectivity in process modelling at this 'micro' level. It is clear that there is potentially great 'added value' that may be obtained by incorporating microstructure modelling, in particular offering (a) wider scope for predicting properties, damage and subsequent

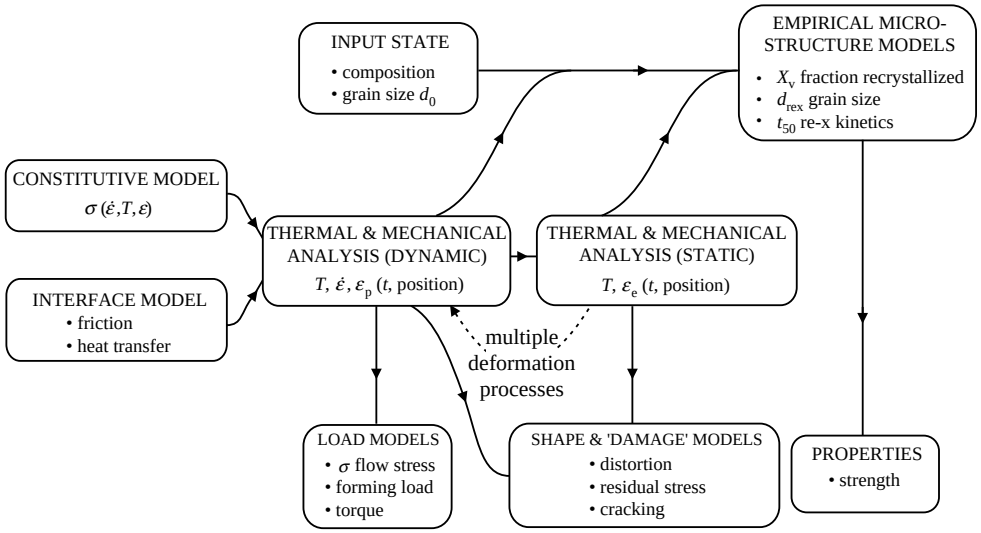

Figure 1. Thermomechanical process modelling: sub-models and connectivity at the 'macro' level.

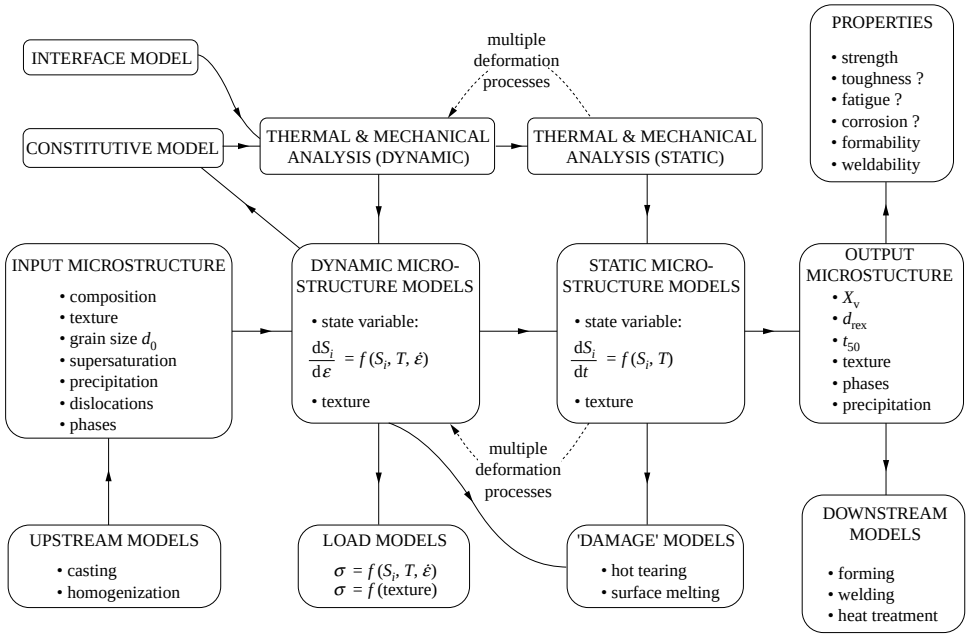

Figure 2. Thermomechanical process modelling: sub-models and connectivity at the 'micro' level.

material processability, and (b) linking upstream and downstream material behaviour through multi-stage process histories. It is the modelling interactions illustrated in figures 1 and 2 that currently provide the most fertile opportunities for collaborative research between academia and industry.

2. Approaches to microstructure modelling

Many diverse approaches to modelling microstructure evolution in hot deformation (and subsequent annealing) have been explored. Some are appropriate for coupling directly to real process histories (as in figures 1 and 2), while others seek to simulate the underlying physical behaviour under idealized conditions. The present discussion is limited to empirical, state variable and statistical approaches to modelling microstructure evolution, for prediction of flow stress and subsequent recrystallization. Other microstructure modelling activities in hot deformation include (a) texture prediction, which is a major field in its own right, (b) finite-element crystal plasticity (Dawson *et al*. 1994; Bate, this issue), and (c) annealing simulation by Monte Carlo methods (Rollett *et al*. 1989; Humphreys 1992), and cellular automata (Davies 1997).

(*a*) *Empirical methods*

The established empirical approach (Sellars 1990; McLaren & Sellars 1992) to predicting flow stress during hot working and subsequent recrystallization is based on the Zener–Hollomon parameter, Z:

$$Z = \dot{\varepsilon} \exp(Q_{\mathrm{def}}/RT), \tag{2.1}$$

where $\dot{\varepsilon}$ and T are the average strain rate and temperature, respectively, and Q_{def} is an activation energy characteristic of the material. Flow stress is commonly described by an equation of the form

$$\sigma = \frac{1}{\alpha'} \operatorname{arsinh}\left(\frac{Z}{Z^*}\right)^{1/n}, \tag{2.2}$$

where α', Z^* and n are material constants. Recrystallized grain size, d_{rex}, and the time to 50% recrystallization, t_{50} (a common measure of recrystallization kinetics), are described by power laws:

$$d_{\mathrm{rex}} = \alpha d_0^a \varepsilon^{-b} Z^c, \tag{2.3}$$

$$t_{50} = \beta d_0^p \varepsilon^{-q} Z^{-r} \exp(Q_{\mathrm{def}}/RT), \tag{2.4}$$

where d_0 is the initial grain size, and ε is the von Mises equivalent strain. The other parameters are empirical constants.

This approach bypasses the evolving microstructure altogether, and relies on a test program covering the relevant ranges of strain, strain rate and temperature for each material to calibrate the many fitting parameters. It is used industrially for flat rolling of many steels, but is known to be unsatisfactory for rolling of aluminium alloys, and for any metal deformation involving more complex strain paths. There is, therefore, a well-established need for more sophisticated approaches to these problems.

(*b*) *'Surrogate' state variable methods*

A more complex approach to modelling flow stress in aluminium alloys was demonstrated by researchers at Alcoa (Sample *et al*. 1992), using internal state variables. Differential evolution laws with strain for one or more state variables S_i were proposed, and the flow stress σ was then a function of the instantaneous values of these variables. The state variables were 'surrogate' variables in the sense that they

were deemed to represent the underlying evolution of dislocation structure, rather than having a measurable physical meaning. The form of the evolution laws and the coupling to flow stress were mathematical functions adjusted to fit test data for individual alloys, but with no physical basis. The principal advantage over equation (2.2) was the ability to follow transients in strain rate and temperature with reasonable accuracy, but the approach offers no further physical insight, and is equally dependent on alloy-specific test data. No development for modelling recrystallization behaviour has been reported in the literature.

(*c*) *'Physically based' state variable methods*

Modelling of microstructure evolution explicitly in differential form has been the basis for most classical theories of work hardening and annealing. The internal state variables are now physically meaningful quantities that can, at least in principle, be measured by electron microscopy (dislocation densities and so on). Developments of this approach can now benefit from the recent advances in microscopy, such as semi-automated electron backscatter diffraction (EBSD), which enable substructures to be quantified with far greater speed and precision. Differential physically based state variable models have the potential to follow complex process histories and provide a means of carrying microstructure explicitly from one processing stage to the next. The use of physical state variables for modelling hot deformation and annealing of Al–Mg alloys is discussed below.

(*d*) *Advanced statistical methods*

A quite different recent development is the application of artificial intelligence methods to make predictions about materials processing. A variety of advanced statistical methods are now available, which essentially enable nonlinear regression analyses to be performed on complex data-sets. These methods, therefore, offer no physical insight, but are, nonetheless, of interest, due to their ability to seek trends in the data for multi-parameter problems, and to indicate the apparent importance of each input to the problem on the basis of the data provided. Such approaches are often regarded with deep suspicion or even hostility by physical metallurgists, while industrialists who are used to empirical methods readily make use of them. Recent work in hot working using artificial neural networks and 'Gaussian process models' is discussed further below. A preliminary analysis is conducted on the same data for hot working and annealing of Al–Mg alloys, to explore whether these approaches could be usefully developed in parallel.

3. Microstructural modelling in hot working and annealing of Al–Mg alloys

(*a*) *Status of physically based modelling*

Hot deformation and annealing of non-heat-treatable aluminium alloys has been extensively studied in recent years. The approach summarized here comes largely from the research groups in Trondheim, Sheffield and Cambridge. There are three separate modelling tasks: (a) describing evolution of deformation substructure, in

particular the subgrain size, dislocation density and subgrain boundary misorientation; (b) coupling substructure to flow stress; and (c) predicting recrystallization behaviour.

The Trondheim group (Nes *et al*. 1994; Nes 1995; Nes & Furu 1995) have used evolution laws for subgrain size and dislocation density to study steady-state flow stress in constant strain-rate hot deformation, when work hardening and dynamic softening processes are balanced. Complex developments of this approach have been proposed to provide a 'universal' model for work hardening (at constant strain rate) across all deformation temperatures for pure FCC metals and Al–Mg alloys, based on a statistical view of dislocation storage (Nes 1998; Marthinsen & Nes 1997). This model introduces many adjustable parameters, and cannot yet be straightforwardly applied in a practical context.

Recrystallization modelling by the same group has exploited the expanded data acquisition of EBSD methods, to link recrystallized grain size and kinetics to substructure; in terms of the average behaviour (Furu *et al*. 1990) and, more recently, allowing for different texture components explicitly (Nes *et al*. 1994; Vatne *et al*. 1996). This reflects the dominant interest in the development of cube texture in hot rolling of aluminium alloys for canstock.

The Sheffield group have approached hot working of aluminium alloys from a background of FE analysis of the transient nature of the deformation history in flat rolling; in terms of temperature, strain rate and strain path. The transient strain-rate work (in collaboration with researchers in Cambridge) is summarized and developed further in this paper; progress with strain-path effects is described elsewhere (Davenport *et al*., this issue).

(*b*) *Conceptual framework of state variable models*

A general form for a differential state variable model for hot deformation is

$$\left.\begin{aligned} \frac{\mathrm{d}S_1}{\mathrm{d}t} &= f_1(S_1, S_2, \ldots, T, \dot{\varepsilon}), \\ \frac{\mathrm{d}S_2}{\mathrm{d}t} &= f_2(S_1, S_2, \ldots, T, \dot{\varepsilon}), \\ &\vdots \end{aligned}\right\} \tag{3.1}$$

where S_i represents the chosen measurable state variables. The quantity of most interest during the deformation is the flow stress σ, which is described by a function of the instantaneous values of the state variables:

$$\sigma = g_1(S_1, S_2, \ldots). \tag{3.2}$$

Subsequent static microstructure evolution may be described in various ways depending on the problem. For static recovery, a further differential evolution model for the substructure could be used to explicitly link the dynamic to the static stage:

$$\left.\begin{aligned} \frac{\mathrm{d}S_1}{\mathrm{d}t} &= f_3(S_1, S_2, \ldots, T), \\ \frac{\mathrm{d}S_2}{\mathrm{d}t} &= f_4(S_1, S_2, \ldots, T), \\ &\vdots \end{aligned}\right\} \tag{3.3}$$

Static recrystallization is driven by the substructure at the end of deformation, S_i^f, which governs both the density of nuclei activated and the growth rate. This process may be described by a differential evolution of the fraction recrystallized X, which would be necessary if the temperature varied during annealing:

$$\frac{\mathrm{d}X}{\mathrm{d}t} = f_5(S_1^f, S_2^f, \ldots, X, T). \tag{3.4}$$

For isothermal annealing, it is sufficient to use an integrated form from which the recrystallized grain size, d_{rex}, and the time to 50% recrystallization, t_{50}, may be inferred:

$$\left.\begin{aligned} d_{\mathrm{rex}} &= g_2(S_1^f, S_2^f, \ldots, T), \\ t_{50} &= g_3(S_1^f, S_2^f, \ldots, T). \end{aligned}\right\} \tag{3.5}$$

As noted earlier, the first-order elements of the substructure in hot working of aluminium alloys are considered to be the subgrain size, δ, the dislocation density within the subgrains, ρ_i, and the subgrain boundary misorientation θ. δ and θ can be measured relatively easily using modern SEM techniques, including their statistical distributions, while ρ_i presents more difficulties and needs conventional TEM. Extensive microscopy on hot- and cold-worked aluminium has revealed considerable complexity in subgrain structure (Hansen & Juul Jensen, this issue; Duly *et al*. 1996), but it may prove sufficient to consider that the structure has two main subcomponents: geometrically necessary and statistically stored dislocations. This is of particular importance in characterizing and quantifying the development of misorientation with strain.

(*c*) *Differential substructure evolution laws*

The approach adopted by the Trondheim group (Nes *et al*. 1994; Nes 1995; Nes & Furu 1995) for evolution of dislocation structures might be termed a 'profit and loss' approach. For dislocation density, the evolution law contains a positive storage term and a negative annihilation term, representing the independent processes of work hardening and dynamic recovery. Subgrain size is treated similarly with terms for subgrain refinement and for growth. In the simplest form, the evolution of each state variable only depends on its own value and the deformation conditions:

$$\frac{\mathrm{d}\rho_i}{\mathrm{d}\varepsilon} = \frac{1}{\dot\varepsilon}\left(\frac{\mathrm{d}\rho^+}{\mathrm{d}t} + \frac{\mathrm{d}\rho^-}{\mathrm{d}t}\right) = \frac{1}{\dot\varepsilon} f_1(\rho_i, \dot\varepsilon, T), \tag{3.6}$$

$$\frac{\mathrm{d}\delta}{\mathrm{d}\varepsilon} = \frac{1}{\dot\varepsilon}\left(\frac{\mathrm{d}\delta^+}{\mathrm{d}t} + \frac{\mathrm{d}\delta^-}{\mathrm{d}t}\right) = \frac{1}{\dot\varepsilon} f_2(\delta, \dot\varepsilon, T). \tag{3.7}$$

Misorientation is the least well-characterized of the three parameters, so it may initially be assumed that a similar form of evolution law may be found:

$$\frac{\mathrm{d}\theta}{\mathrm{d}\varepsilon} = \frac{1}{\dot\varepsilon}\left(\frac{\mathrm{d}\theta^+}{\mathrm{d}t} + \frac{\mathrm{d}\theta^-}{\mathrm{d}t}\right) = \frac{1}{\dot\varepsilon} f_3(\theta, \dot\varepsilon, T). \tag{3.8}$$

Given sufficient experimental data it may prove of interest to explore the separate evolution of geometrically necessary and statistically stored dislocations. In steady state, the storage and annihilation terms balance, so that steady-state values for δ and ρ_i may be derived in terms of the Zener–Hollomon parameter, and linked to the steady-state flow stress (Nes *et al*. 1994; Nes 1995; Nes & Furu 1995).

For transient deformation, the structure evolution is more complex, particularly if the strain rate is varying in the early hardening part of the deformation when the substructure and flow stress would in any case be evolving at constant strain rate. Recognizing this complexity, an alternative pragmatic approach has been investigated. Zhu & Sellars (1996) noted that at constant strain rate, the observed microstructure was well approximated by an exponential evolution with strain, and proposed a general equation of the form

$$S_i = S_0 + (S_{\rm ss} - S_0)[1 - \exp(-\varepsilon/\varepsilon_{S_i})], \tag{3.9}$$

where, in this instance, S_i represented $1/\delta$, $\rho_i^{1/2}$ or θ. S_0 and $S_{\rm ss}$ are the initial ($\varepsilon = 0$) and steady-state values of S_i, respectively, and ε_{S_i} is a characteristic strain that controls the strain over which steady-state is reached. In view of the similarity to the corresponding expression for flow stress, equation (3.9) might be termed a 'microstructural Voce equation'.

Differentiating equation (3.9) gives a possible empirical form of evolution law. A characteristic of the resulting evolution law is that the rate of change of microstructure scales with the difference between the current and the steady-state values (giving an exponential approach to steady state at constant strain rate). While it is perhaps physically unrealistic that the initial rate of accumulation of dislocations could be governed by the eventual steady-state density, it does lead to a convenient general form for substructure evolution laws:

$$\frac{{\rm d}S_i}{{\rm d}\varepsilon} = \frac{1}{\dot\varepsilon}\left(\frac{{\rm d}S_i^+}{{\rm d}t} + \frac{{\rm d}S_i^-}{{\rm d}t}\right) = f(\dot\varepsilon, T)\left(\left[\frac{S_i}{S_{i,\rm ss}}\right]^a - \left[\frac{S_i}{S_{i,\rm ss}}\right]^b\right), \tag{3.10}$$

where now $S_i = \delta$, ρ_i or θ (as before), and $S_{i,\rm ss}$ is the steady-state value of S_i. This form of equation is convenient as the substructure values are normalized, being equal to unity in steady-state. By appropriate choice of the constants a and b, both increasing (ρ_i) and decreasing (δ) behaviour can be described. The form of $f(\dot\varepsilon, T)$ will depend on the relationship between steady-state structure and the Zener–Hollomon parameter, commonly given by expressions such as

$$1/\delta_{\rm ss} = A \ln Z + B \tag{3.11}$$

$$\delta_{\rm ss}\sqrt{\rho_{i,\rm ss}} = \text{const.} \quad \text{(the principle of similitude)}. \tag{3.12}$$

The steady-state average misorientation may be assumed to be constant, for lack of evidence to the contrary. Comparison with physically derived evolution laws for δ and ρ_i (Nes *et al.* 1994; Nes 1995; Nes & Furu 1995) shows that equation (3.10) approximates these if the following expressions are used.

$$\text{For } \delta\text{:} \quad f(\dot\varepsilon, T) \propto Z^{1/2}, \quad a = -1, \quad b = 2,$$

$$\text{For } \rho_i\text{:} \quad f(\dot\varepsilon, T) \propto Z^{-1/2}, \quad a = \tfrac{1}{2}, \quad b = \tfrac{3}{2}.$$

Equation (3.10) can be used to describe transient strain rate and temperature conditions, including strain-rate jumps (since the 'instantaneous' steady-state values can be updated at every time-step). So even though the physical basis is limited, this semi-empirical evolution law has the attraction of responding stably to varying deformation conditions: the microstructure is always seeking to change to the current 'equilibrium', i.e. the steady-state microstructure that would evolve if the strain rate stopped changing and was continued at a constant level.

A preliminary application of this approach has been made for hot plane-strain compression of Al–1%Mg alloy (Zhu *et al*. 1997). Equation (3.10) was calibrated to constant strain-rate data for the evolution of δ, ρ_i and θ with strain, and then applied to the substructure evolution in decreasing and increasing strain-rate tests. The method captured the right trends, but the small amount of substructure data and considerable uncertainty in the values did not provide a very rigorous test.

In view of the difficulty in validating evolution laws for substructure during transient deformation, continuous predictions of flow stress and recrystallization behaviour with strain could not be made with confidence. However, models for these aspects were investigated by using the measured substructure data directly as input to models for σ, d_{rex} and t_{50} (Furu *et al*. 1996, 1999). The recrystallization predictions are summarized here, and used as an illustration of the need, in modelling, for proper sensitivity analysis before reaching any conclusions about the level of agreement between models and data.

(*d*) *Recrystallization model*

The recrystallization model adopted is the simplest form of that proposed by Furu *et al*. (1990) and Vatne *et al*. (1996) for the prediction of d_{rex} and t_{50}. This is summarized in Appendix A. The experimental work is described in detail elsewhere (Baxter *et al*. 1996, 1999). Figure 3 summarizes the critical transient experiments that the model aimed to predict. Three strain-rate histories were applied at a temperature of 385 °C to the same final strain rate of 2.5 s^{-1} at a strain of 1.0, which was followed by further deformation at that strain rate (figure 3*a*). It was found that following a decreasing strain rate, a short transient in d_{rex} occurred (figure 3*b*), which followed the observed transient in subgrain size. A longer transient in t_{50} was observed (figure 3*c*), which was consistent with a more prolonged transient in both ρ_i and θ. In the significantly slower-increasing strain-rate tests, no transient in substructure or subsequent recrystallization was observed.

The model summarized in Appendix A was calibrated to constant strain-rate data, and then applied to the varying strain-rate data by substituting in the measured values of δ, ρ_i and θ on a test-by-test basis. The predicted and measured values of d_{rex} and t_{50} (from Furu *et al*. 1999) are compared in figure 4. Figure 4 shows that, overall, the model captured the transients in recrystallized grain size, but the kinetics was largely underestimated after decreasing strain-rate tests (predicted t_{50} being up to a factor of 2 too high). Some of this disagreement was possibly due to systematic error in measuring dislocation density. However, it was only considered meaningful to evaluate this disagreement in the light of a proper sensitivity analysis, i.e. considering the uncertainties in the model predictions, due to uncertainties in the measured substructure data used as input to the model. This uncertainty could then be considered alongside that in the experimental recrystallization data, to see if the disagreement between model and data was really significant. This aspect of microstructural modelling is so rarely addressed in the literature that it is developed further here to highlight its significance.

(*e*) *Sensitivity analysis*

Furu *et al*. (1999) conducted a sensitivity analysis by exploring the uncertainty in the recrystallization model due to uncertainty in each of the substructure parameters.

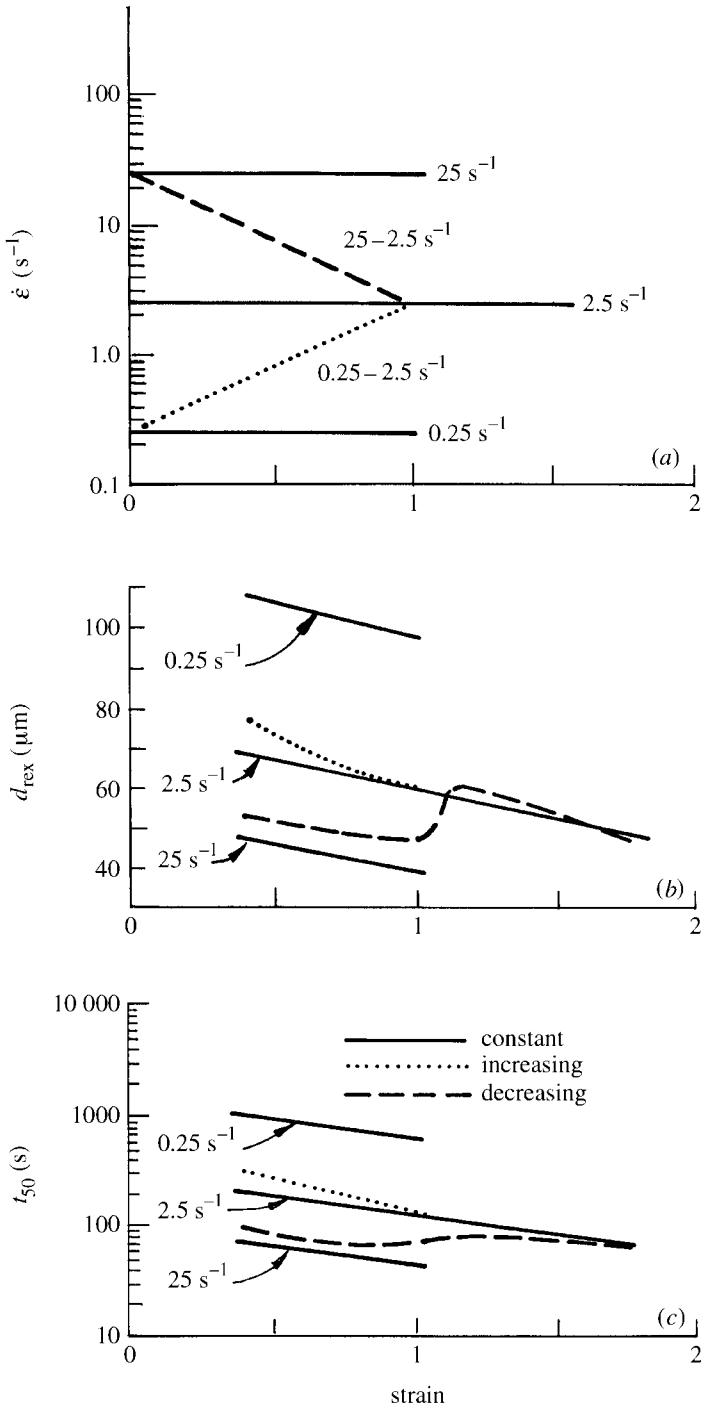

Figure 3. Schematic summary of recrystallization behaviour after transient strain-rate testing of Al–1%Mg: (*a*) strain-rate histories; (*b*) recrystallized grain size; (*c*) time to 50% recrystallization (after Furu *et al*. 1999).

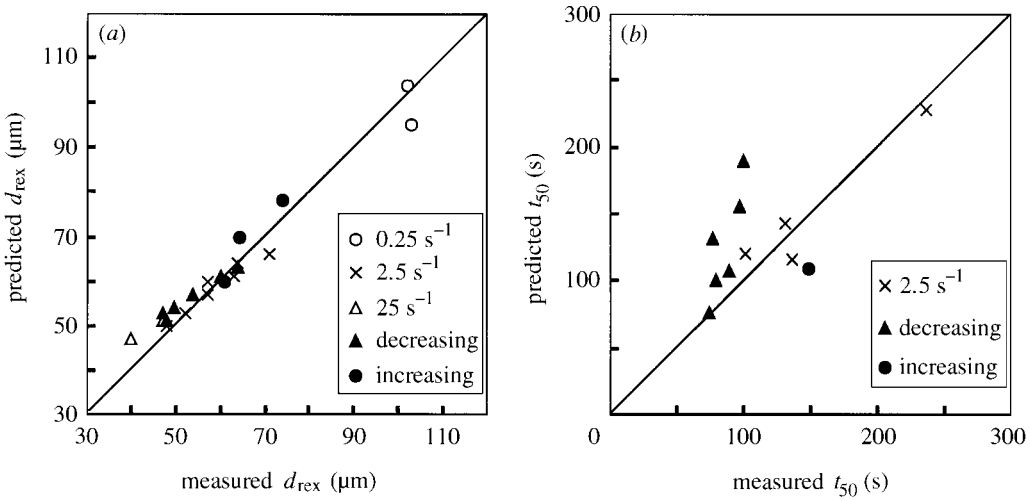

Figure 4. Predicted versus measured recrystallization behaviour for constant and varying strain-rate testing of Al–1%Mg: (*a*) recrystallized grain size; (*b*) time to 50% recrystallization (after Furu *et al*. 1999).

Values were substituted in at the 95% confidence limits for each of δ, ρ_i and θ in turn to calculate d_{rex} and t_{50}. This gave valuable insight into the relative significance of each of δ, ρ_i and θ, particularly since their measurement is laborious, so future experimental work needs to be well focused. An estimate was also made of the overall 95% confidence limits for d_{rex} and t_{50} due to uncertainty in all of the parameters combined. The analysis indicated that the low density of data and the size of the uncertainty in the model for t_{50} made it difficult to reach any firm conclusions about the validity of the kinetic model.

This sensitivity analysis is now taken further. Simple error bars at 95% confidence limits tend to disguise the fact that values within the error bar are not equally probable: they represent the limits of significance of a distribution (assumed to be Gaussian). The models for d_{rex} and t_{50} combine many nonlinear functions of the input parameters, so it is of interest to calculate the actual *distribution* of the model predictions, rather than just finding a 95% confidence limit by propagation of errors.

The general problem of predicting the distribution of a model prediction given the 95% confidence limits on the inputs (which are assumed to be Gaussian) has been addressed by a Monte Carlo technique, as follows. Each of the uncertain inputs was assigned a mean value and a standard deviation. A numerical procedure was then used to sample a value at random from each of the input distributions, which are assumed to be independent. These are then used as a set of inputs to the model, yielding a single predicted value. This procedure is repeated many times, generating a probability distribution for the output. Eventually, the input parameter distributions have been thoroughly sampled and a smooth output distribution is found. This may take up to 100 000 or more iterations, depending on the number and uncertainties of the inputs, and the nonlinearities of the model. This approach was adapted from a technique for modelling the uncertainty in manufacturing cost using 'activity-based cost' models (Emblemsvåg & Bras 1994), and has recently been used to illustrate

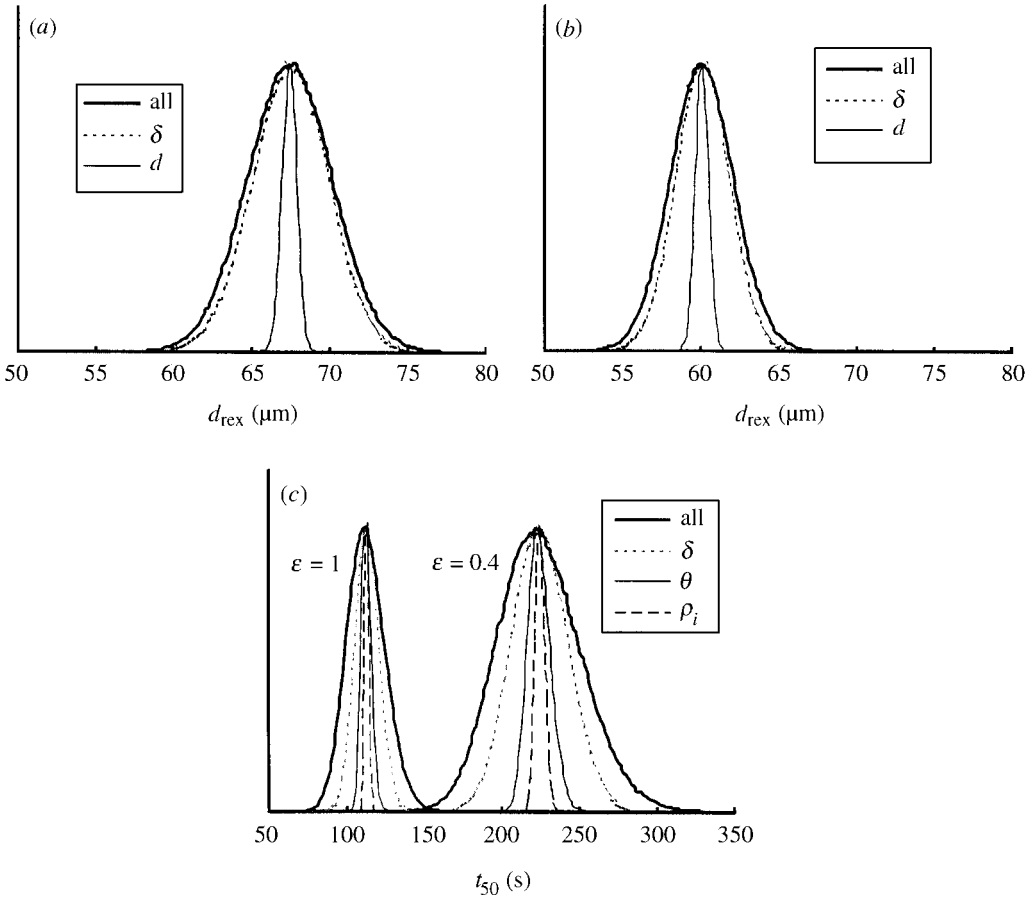

Figure 5. Statistical distributions of predicted recrystallization behaviour at constant strain rate, using a Monte Carlo approach to allow for uncertainty in the input parameters (d = initial grain size; δ = subgrain size; θ = misorientation; ρ_i = dislocation density): (*a*) recrystallized grain size, $\varepsilon = 0.4$; (*b*) recrystallized grain size, $\varepsilon = 1.0$; (*c*) time to 50% recrystallization, $\varepsilon = 0.4$ and 1.0.

the uncertainty in a model to predict the hardness of the heat-affected zone in steel welds (Lovatt 1998).

Figure 5 shows the distributions of predicted recrystallized grain size and kinetics, using the same test conditions as Furu *et al.* (1999), but now aggregating all of the uncertainties via the Monte Carlo technique above. Uncertainties were included in the three substructure parameters, and in the calibration constants in the model (which were themselves based on observed microstructure). The figures show the overall distribution in each case, superposed with the distribution generated when individual input parameters are uncertain but the rest are assumed to have fixed values. This indicates the relative significance of each parameter, and, hence, the importance of its uncertainty, in determining the predicted result.

This analysis provides a new perspective on the quality of the model, compared with assigning simple error bars. The cases shown in figure 5 are mostly near-Gaussian, but the predictions for t_{50} are somewhat skewed, with a longer tail towards

Table 3. *Inputs and outputs in hot deformation and annealing*

inputs	outputs
composition	flow stress
initial structure	recrystallized grain size
deformation temperature	recrystallization kinetics
deformation strain rate	deformation and recrystallization texture
total strain (or strain path)	
annealing temperature	
annealing time	

high predicted values. This is a result of assuming a ±95% confidence limit on the misorientation, which then enters a log term in the stored energy (see Appendix A).

In summary, therefore, sensitivity analysis should be an essential part of microstructure modelling, and should be conducted with care, since nonlinearities in the model can amplify the uncertainties assumed in the inputs. The analysis acts as an important guide as to where further effort should be targeted, for example:

(i) Is the model or the data more uncertain, and which uncertainty could be reduced most easily by further experiment?

(ii) Which of the substructure parameters are most significant to the problem?

(iii) What is the target accuracy in the substructure measurement to provide a statistically significant test of the model?

Finally, this analysis serves as a reminder that further development of a differential substructure model should not stop at an evaluation of the fit between model and substructure, but should consider the consequences for the macroscopic properties of interest, such as flow stress and recrystallization, which may not be particularly sensitive to uncertainty in the substructure model.

4. Advanced statistical methods

A completely different approach to providing predictions of material behaviour is to take the available data for process conditions and the required output behaviour and to interrogate this database by statistical means. Empirical nonlinear regression methods have grown in sophistication, and merit exploration as tools for 'data mining' in the field of thermomechanical processing, which is not short of data. The essential task is to link multiple inputs directly to one of a number of outputs, where the underlying physical behaviour is inherently complex. For the current problem of hot deformation and annealing, the target inputs and outputs are summarized in table 3.

The potential of artificial intelligence techniques has recently been explored for hot deformation of selected alloys (Sabin *et al*. 1997, 1998; Bailer-Jones *et al*. 1997, 1998). The same methods are also being used for studying phase transformations in steels, and toughness of steel welds, problems in which composition information has been central to the analysis (Bhadeshia *et al*. 1995; Ichikawa *et al*. 1996; Gavard

et al. 1996; Bailer-Jones *et al*. 1999). Two approaches based on Bayesian methods have been illustrated: neural networks and Gaussian process models (the latter being something of a misnomer in this field, since 'process' refers to the statistical process, while some regard 'models' as an inappropriate term for an empirical technique). Bayesian methods automatically embody a number of useful working principles for materials processing problems: (a) the analysis seeks the minimum complexity consistent with the data provided; (b) predicted outputs come with error bars indicating the reliability of the prediction; and (c) an indication is given of the apparent importance of each input.

(*a*) *'Static' neural networks*

Neural network architectures link a set of inputs to an output via a number of 'hidden units': parameters with no physical meaning, which are evaluated from the inputs by means of weighted nonlinear transfer functions (usually hyperbolic tan functions), and then linked to the output via a set of weighted linear functions. The number of hidden units (and the number of layers of units) is open but can be optimized to give the fairest representation of the data on various criteria while avoiding over-fitting the data. Training a given network minimizes the squared errors on the basis of the data provided and returns the transfer functions and weights. Once trained, the network predicts the expected output (and its uncertainty) for any other sets of input data using the trained functions and weights, without reference to the original data. The term 'static' implies that single values of the process conditions are used as inputs (for instance, final, average or maximum values), so that the network has no knowledge of the path of the deformation; a limitation currently being addressed by development of 'dynamic' neural networks (see below).

(*b*) *Gaussian process models*

Gaussian process (GP) models are a probabilistic variant of static neural network methods. For a set of N observations, the model assumes the joint probability of these observations is given by an N-dimensional Gaussian. Training the model consists of finding a set of hyperparameters within the assumed statistical function. This is done by maximizing the probability of the hyperparameters given the training data. The apparent level of noise in the data may be inferred by the training exercise, or known information on uncertainty can be fed into the analysis. Once trained, the model returns a Gaussian probability distribution for the output, on the basis of the data provided. GP models thus predict the most probable value of an interpolated output, i.e. the centre of the predicted Gaussian distribution, with the standard deviation being a measure of the uncertainty of the prediction. They do not fit a set of functions and weights to represent the behaviour of the training data, like a neural network, but use the original data (or a subset of it) to make each individual prediction.

(*c*) *'Dynamic' neural networks*

As noted earlier, the methods outlined above are considered to be 'static', since the input and output values embody no information about the evolution of material behaviour through the deformation and/or annealing processes. Static approaches

may be sufficient for relatively 'monotonic' deformation, such as plane-strain compression, or the centreline of flat-rolled products. However, given the strong path-dependencies in processes such as forging, section rolling, or flat rolling (in the near-surface regions), consideration has recently been given to developing a 'dynamic' neural network architecture with an added time dimension (Bailer-Jones *et al*. 1998; Withers *et al*. 1998).

The objective in training a dynamic network is to capture the history dependence of the problem, rather than using only final or average values of the process conditions. This is achieved by introducing 'state variables', which evolve in parallel with the known time-dependence of the process conditions (predicted by FE analysis). The state variables may be a combination of readily measurable quantities (such as grain boundary area per unit volume), and 'surrogate' variables, which are deemed to capture the effect of underlying unmeasurable (or simply unmeasured) features. A static neural network architecture is used to find the nonlinear functional dependence between the current values of the state variables and the process conditions (as inputs), and the time-derivative of the state variables (as outputs). Training the network is then a recurrent process, optimizing the weights at each time-step and calculating the next set of input values for the state variables from the predicted derivatives. It is sufficient to provide an initial value and one other value during the process for each measurable state variable in order for the network to 'learn' the evolution law.

This approach has recently been tested for predicting the evolution of damage in a forged MMC brake disc (Withers *et al*. 1998), using FE analysis to provide the process history at a number of points in the component. This was a suitable first problem since there was one measurable state variable, the damage (in terms of a fraction of broken particles), and the required output was the state variable itself. Since damage could both increase (due to tensile stress) and decrease (due to healing of damage under compressive stress), the couplings between process conditions and the state variable were non-trivial and provided a good test of the approach.

The progress reported so far with the dynamic neural network shows real promise, but requires considerable development for characterizing hot-working problems generally. The method should be able to characterize the evolution of flow stress and recrystallization behaviour during transient deformation by treating the flow stress, or recrystallized grain size d_{rex}, as a state variable. The flow stress is clearly the actual flow stress at the time, but, in the latter case, the state variable 'd_{rex}' implies the recrystallized grain size at a point in the component if the deformation was instantaneously stopped and the component was subsequently annealed. This needs careful distinction from the actual current grain size, which would of course also be evolving during deformation. Alternatively, real or surrogate state variables could be used, and a functional dependence of the flow stress or d_{rex} on these state variables incorporated.

Perhaps the better way forward is the hybrid approach, where the state variables (and thus outputs of the dynamic network) are deemed to be actual or surrogate features of the microstructure. These are then linked to the true desired output (flow stress, recrystallization behaviour, etc.) by a separate function. Hence, the outputs of the dynamic neural network become the inputs to a subsequent static calculation. This mapping could be done by a physically based model, or could itself be an empirical fit, such as a static neural network or GP model. The benefit of this hybrid

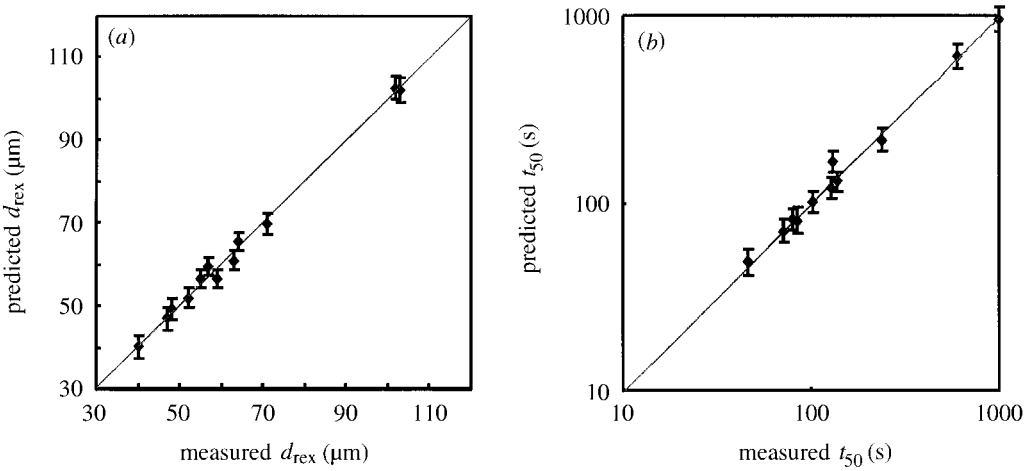

Figure 6. Predicted versus measured recrystallization behaviour at constant strain rate, using a Gaussian process model: (*a*) recrystallized grain size; (*b*) time to 50% recrystallization.

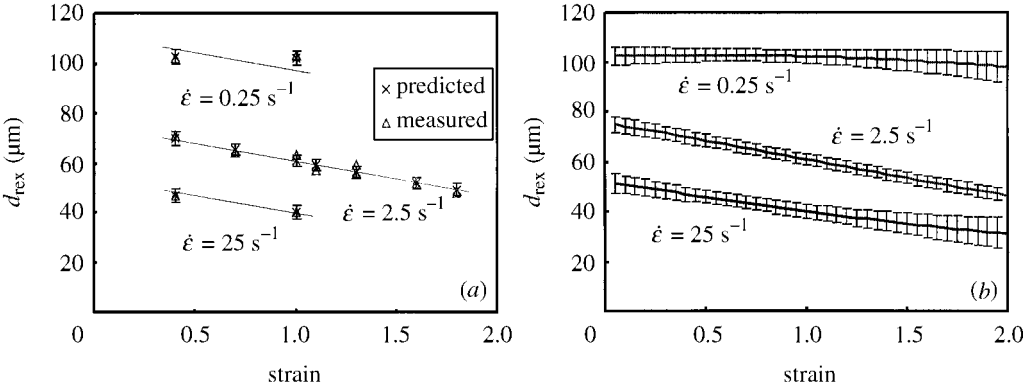

Figure 7. Predicted recrystallized grain size against strain at constant strain rate, using a Gaussian process model: (*a*) predicted and measured data; (*b*) predicted trend with strain at each of the three strain rates.

approach is that physical knowledge and data may be embedded in the problem wherever it is readily available, and, hence, the maximum predictive capability from these statistical methods is likely to be obtained.

(*d*) *Preliminary application of Gaussian process software to Al–1%Mg data*

Since a physically based model has been explored for the problem of hot plane-strain compression of Al–1%Mg alloy, it is of interest to try one of the static statistical methods on the same data-set. A preliminary analysis was, therefore, conducted using the static Gaussian process software and the available data for σ, d_{rex} and t_{50} at constant strain rate. A single alloy and a single deformation and annealing temperature were used, so the only inputs are the strain rate and the strain (though the analysis could extend to all of these variables given enough data).

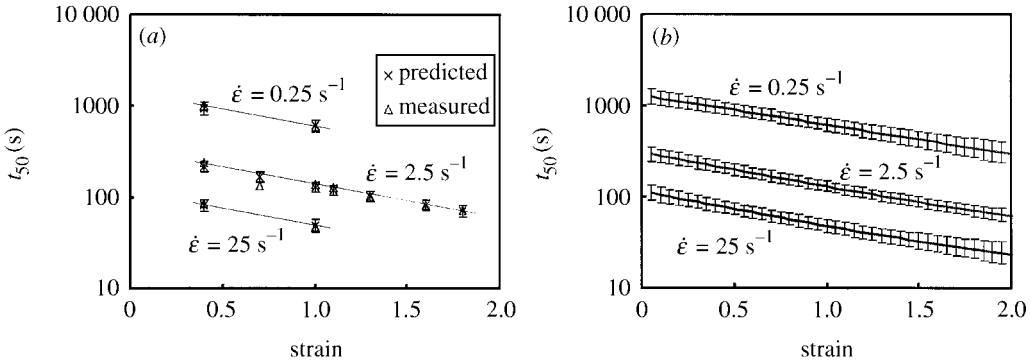

Figure 8. Predicted time to 50% recrystallization against strain at constant strain rate, using a Gaussian process model: (*a*) predicted and measured data; (*b*) predicted trend with strain at each of the three strain rates.

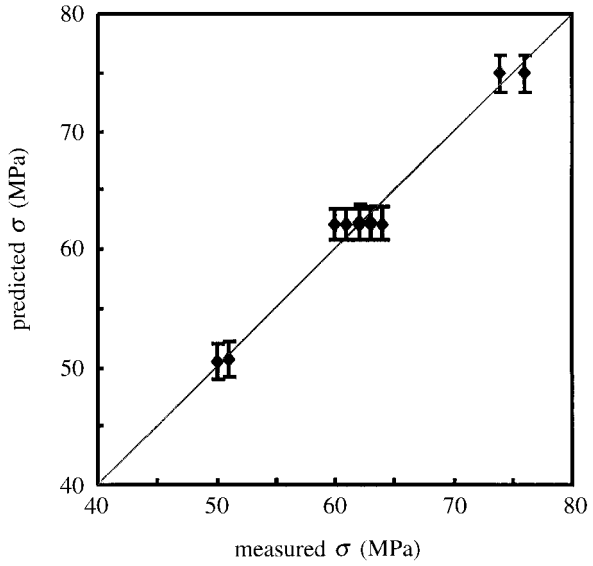

Figure 9. Predicted versus measured flow stress at constant strain rate, using a Gaussian process model.

The Gaussian process software (Gibbs & Mackay 1998) was used to make two types of prediction, given the data-set of measured outputs for all constant strain-rate tests (at 0.25, 2.5 and 25 s^{-1}): (a) the expected output for each of the input combinations in the training set; (b) the expected evolution of each output with strain, at each value of constant strain rate. Figures 6–9 show the results. In all cases, the predictions were made using all of the available data as the evidence, since the data-set is small.

Figure 6 shows the predicted versus measured values for d_{rex} and t_{50}. The error bars indicate the uncertainty inferred in the prediction (one standard deviation), and do not reflect uncertainty provided on the input or output data. These may be compared directly with the constant strain-rate data and physical model predictions from Furu

et al. (1999), plotted in figure 4. This indicates that the statistical method captures this relatively simple behaviour with equal certainty. Figures 7*a* and 8*a* show the predicted and measured data plotted against strain (as in Furu *et al*. 1999), which illustrate the limited scope and simple form of the original data-set.

When predictions are then made for the full strain range at all strain rates (figures 7*b* and 8*b*), it inspires some confidence to see that the uncertainty in the prediction varies in a way that reflects the density of the underlying data. The model is more confident of its predictions at the middle strain rate, where there are many more data points. Furthermore, as the prediction is extrapolated outside the range of the training data, the error bars grow; this is particularly marked at the higher strains at the high and low strain rate. This inbuilt warning that predictions are being made towards and beyond the fringes of the available data space is a great advantage of the Bayesian approach. In a simple problem, such as the one illustrated here, it is self-evident where the reasonable limits of the data lie, but in a multiple-input problem this is not the case. It would certainly be beneficial if physically based modelling was conducted with the same openness regarding the volume of data used to calibrate the model, and to the confidence associated with the predictions of the model.

Figure 9 shows the predicted versus the measured flow stress using the Gaussian software. It is now expected that there is only a dependence on strain rate and not on strain, since all of the data come from the steady-state region of the deformation. Figure 9 shows that the statistical method infers this from the data: it returns a virtually constant predicted value at each strain rate, having inferred (correctly) that the variations with strain (which are not systematic with increasing strain) are simply noise.

The transient strain-rate data could also be explored using the static analysis, by taking as input strain rate the strain-averaged or time-averaged strain rate, or just the final value. Of more general relevance, though, would be to use the dynamic neural network approach to characterize this and more complex deformation histories, and to link these to subsequent annealing behaviour. This is a matter of current research.

(*e*) *Summary*

This preliminary application of the Gaussian process model indicates that the statistical method captured the constant strain-rate trends as well as the physical model, and implied a ‘reasonable’ noise level in the data, and, thus, uncertainty in its predictions. While the method gives no physical insight at all, models of this type could serve various purposes:

(a) they may be sufficient in themselves for industrial data handling (an improvement on the traditional ‘power law’ empirical fit, as allowable nonlinearities are more complex);

(b) they give an alternative view of uncertainty in the data, and, thus, inform a comparison of physically based models and experiment;

(c) they may allow the number of experiments to be reduced by picking out trends in complex data-sets;

(d) they provide a 'significance test' on parameters of the problem, i.e. a measure of the apparent importance of different input parameters (similar to sensitivity analysis).

5. Conclusions

Microstructural modelling offers many opportunities to add value to the advanced FE analysis, which is becoming routine for hot working. Particular benefits include a wider predictive capability for product properties and subsequent processability, and the ability to link the steps in multi-stage processing. The long-term goal is to replace current empirical prediction of flow stress and recrystallization behaviour with physically based state variable models, which capture the essential material behaviour explicitly, but in a simple form suitable for coupling to FE analysis.

Some progress has been made to develop a state variable model for hot working in Al–Mg alloys. Fundamental differential microstructural evolution laws tend to be too complex for industrial use, or are not properly validated. A pragmatic semi-empirical approach may be sufficient to capture the first-order effects, but further progress at any level requires access to semi-automated microscopy to provide extensive substructure data, particularly for subgrain size and the distribution of subgrain boundary misorientation.

Transient strain-rate testing in Al–1%Mg has demonstrated that substructure evolution is more complex than in constant strain-rate testing, and, thereby, provides a more rigorous modelling test as the microstructural state variables are decoupled. Current recrystallization models capture some of the main effects in transient strain-rate deformation of Al–Mg. Physically based microstructural models establish the level of microstructural complexity that is needed for a given problem. For the problem of transient hot working of Al–1%Mg, recrystallized grain size is well characterized by a knowledge of the subgrain size (and perhaps its statistical distribution), whereas recrystallization kinetics requires a more complete picture of subgrain size, misorientation distribution, and, to a lesser extent, dislocation density. Other materials and processes might require different levels of detail; the guiding principle should be to make the model as simple as possible for the given target predictive capability.

Sensitivity analysis is an essential modelling activity. A Monte Carlo procedure was developed to illustrate the distribution of predicted output from the recrystallization model for hot worked Al–1%Mg. This indicated where subsequent experimental effort should be focused, and also demonstrated the dangers in placing too much confidence in the minimum amount of data needed to calibrate the model. A much greater level of data redundancy is needed (and, hence, semi-automated data gathering) before firm conclusions could be drawn as to the adequacy or otherwise of the models.

Advanced statistical methods provide a contrasting view of the problem. Static and dynamic neural networks, or Gaussian process models, are all being considered as tools for providing predictive capability for industrial hot working on a shorter timescale than is likely to be achieved from a fundamental physically based approach. A preliminary application of a Gaussian process model to the same data for hot worked Al–1%Mg indicated that the trends in the data were quickly established, with the added benefit of an automatic indication of the uncertainty of the prediction, and the sensitivity of the prediction to the different inputs. The best way forward with these advanced empirical tools may be via a hybrid approach, incorporating data for real

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measurable internal state variables and physical knowledge of material behaviour wherever possible.

H.R.S. acknowledges the contribution of the research groups in Cambridge and Sheffield, and the funding of the UK EPSRC, for the collaborative project on transient deformation of Al–Mg alloys. The stimulus for this work stems from many discussions, but in particular those with Dr Trond Furu, Dr Qiang Zhu, Professor Mike Sellars, Professor Philip Withers and Dr Owen Richmond. The authors also thank Dr Mark Gibbs and Dr David Mackay for making their Gaussian process software available on the Web. The financial support of the Körber Foundation and the Isaac Newton Trust for A.M.L. is also gratefully acknowledged.

Appendix A. Recrystallization model applied to hot PSC of Al–1%Mg

The recrystallization model used for predicting recrystallization behaviour in transient strain-rate compression of Al–1%Mg (Furu *et al.* 1999) is summarized below. The nucleation site density, N_v, is governed by the grain boundary area per unit volume S_v (assuming grain boundary nucleation):

$$S_v(\varepsilon) = (2/d_0)(\exp(\varepsilon) + \exp(-\varepsilon) + 1), \tag{A 1}$$

where d_0 is the initial grain size and ε is the strain. The probability of finding a critically sized subgrain on the grain boundary depends on the average subgrain size. An inverse square dependence was shown to be consistent with the data for constant strain-rate deformation of Al–1%Mg, giving

$$N_v = (C_d/\delta^2)S_v(\varepsilon), \tag{A 2}$$

where C_d is a calibration constant. The recrystallized grain size d_{rex} is then

$$d_{\mathrm{rex}} = (1/N_v)^{1/3}. \tag{A 3}$$

The driving force for recrystallization is assumed to come from the stored energy of the dislocations in the subgrain boundaries and the subgrain interiors. The stored energy P_{D} may be approximated by

$$P_{\mathrm{D}} = \alpha\gamma_{\mathrm{SB}}/\delta + \rho_i\Gamma, \tag{A 4}$$

where α is a constant (= 2). The sub-boundary energy γ_{SB} depends on the misorientation θ, and is given by

$$\gamma_{\mathrm{SB}} = \frac{Gb}{4\pi(1-v)}\theta(1 + \ln(\theta_{\mathrm{c}}/\theta)), \tag{A 5}$$

where G is the shear modulus, b is the Burgers vector, v is Poisson's ratio and θ_{c} is a characteristic misorientation for high-angle boundaries (15°).

The dislocation energy per unit length Γ is taken to be

$$\Gamma = \tfrac{1}{2}Gb^2. \tag{A 6}$$

The time to 50% recrystallization, t_{50}, is then

$$t_{50} = \frac{C_t}{M_{GB}P_{\mathrm{D}}}\left(\frac{1}{N_v}\right)^{1/3}, \tag{A 7}$$

where C_t/M_{GB} is a calibration constant.

References

Bailer-Jones, C. A. L., Sabin, T. J., Roberts, S. M., Mackay, D. J. C. & Withers, P. J. 1997 Prediction of deformed and annealed microstructures using Bayesian neural networks and Gaussian processes. In *Proc. Australasia Pacific Forum on Intelligent Processing and Manufacturing of Materials (IPMM '97), Gold Coast, Australia* (ed. T. Chandra *et al.*), pp. 2913–2919. Brisbane, Australia: Watson Ferguson.

Bailer-Jones, C. A. L., Mackay, D. J. C., Sabin, T. J. & Withers, P. J. 1998 Static and dynamic modelling of materials forging. *Aust. J. Intelligent Information Processing Systems* **5**, 10–17.

Bailer-Jones, C. A. L., Bhadeshia, H. K. D. H. & Mackay, D. J. C. 1999 Gaussian process modelling of austenite formation in steel. *Mater. Sci. Technol.* (Submitted.)

Baxter, G. J., Furu, T., Sellars, C. M. & Whiteman, J. A. 1996 The influence of transient deformation conditions on strength, microstructure and recrystallisation during thermomechanical processing of aluminium alloy Al–1%Mg. *Mat. Sci. Forum* **217**–**222**, 459–464.

Baxter, G. J., Furu, T., Zhu, Q., Whiteman, J. A. & Sellars, C. M. 1999 The influence of transient deformation conditions on the deformed microstructure of aluminium alloy Al–1%Mg. *Acta Mater.* (In the press.)

Bhadeshia, H. K. D. H., Mackay, D. J. C. & Svensson, L.-E. 1995 Impact toughness of C–Mn steel arc welds—Bayesian neural network analysis. *Mater. Sci. Technol.* **11**, 1046–1050.

Davies, C. H. J. 1997 Growth of nuclei in a cellular-automata simulation of recrystallisation. *Scr. Mater.* **36**, 35–40.

Dawson, P. R., Beaudoin, A. J. & Mathur, K. K. 1994 Finite element modelling of polycrystalline solids. In *Proc. 15th Risø Int. Symp. on Materials Science, Roskilde, Denmark, September 1994*, pp. 33–44. Roskilde: Risø National Laboratory.

Duly, D., Baxter, G. J., Shercliff, H. R., Whiteman, J. A., Sellars, C. M. & Ashby, M. F. 1996 Microstructure and local crystallographic evolution in an Al–1%Mg alloy deformed at intermediate strain-rate and high temperature. *Acta Metall. Mater.* **44**, 2947–2962.

Emblemsvåg, J. & Bras, B. 1994 Activity-based costing in designing for product retirement. In *Proc. 1994 ASME Design Technical Conf.* (ed. B. Gilmore *et al.*), DE vol. 69–2, pp. 351–362. ASME.

Evans, R. W. 1993 Modelling of the hot-working of high performance alloys. *Key Engng Mater.* **77**–**78**, 227–240.

Furu, T., Marthinsen, K. & Nes, E. 1990 Modelling recrystallisation. *Mater. Sci. Technol.* **6**, 1093–1102.

Furu, T., Shercliff, H. R., Sellars, C. M. & Ashby, M. F. 1996 Physically-based modelling of strength, microstructure and recrystallisation during thermomechanical processing of Al–Mg alloys. *Mater. Sci. Forum* **217**–**222**, 453–458.

Furu, T., Shercliff, H. R., Baxter, G. J. & Sellars, C. M. 1999 The influence of transient deformation conditions on recrystallisation of aluminium alloy Al–1%Mg. *Acta Mater.* (In the press.)

Gavard, L., Bhadeshia, H. K. D. H., Mackay, D. J. C. & Suzuki, S. 1996 Bayesian neural network model for austenite formation in steels. *Mater. Sci. Technol.* **12**, 453–463.

Gibbs, M. N. & Mackay, D. J. C. 1998 Gaussian process software Web site. `http://wol.ra.phy.cam.ac.uk/mng10/GP/`.

Humphreys, F. J. 1992 Modelling mechanisms and microstructures of recrystallisation. *Mater. Sci. Technol.* **8**, 135–143.

Ichikawa, K., Bhadeshia, H. K. D. H. & Mackay, D. J. C. 1996 Model for solidification cracking in low alloy steel weld metals. *Sci. Technol. Welding Joining* **1**, 43–50.

Lovatt, A. M. 1998 Process selection in engineering design. PhD thesis, Department of Engineering, University of Cambridge.

McLaren, A. J. & Sellars, C. M. 1992 Modelling distribution of microstructure during hot rolling of stainless steel. *Mater. Sci. Technol.* **8**, 1090–1094.

Marthinsen, K. & Nes, E. 1997 A general model for metal plasticity. *Mater. Sci. Engng* A **234**–**236**, 1095–1098.

Nes, E. 1995 Constitutive laws for steady-state deformation of metals: a microstructural model. *Scr. Mater.* **33**, 225–231.

Nes, E. 1998 Modelling work hardening and stress saturation in FCC metals. *Progr. Mater. Sci.* **41**, 129–193.

Nes, E. & Furu, T. 1995 Application of microstructurally based constitutive laws to hot deformation of aluminium alloys. *Scr. Mater.* **33**, 87–92.

Nes, E., Vatne, H. E., Daaland, O., Furu, T., Ørsund, R. & Marthinsen, K. 1994 Physical modelling of microstructural evolution during thermomechanical processing of aluminium alloys. In *Proc. 4th Int. Conf. on Aluminium Alloys, Atlanta, USA* (ed. T. H. Sanders & E. A. Starke), pp. 18–49. Atlanta, GA: Georgia Institute of Technology.

Rollett, A. D., Srolowitz, D. J., Doherty, R. & Anderson, M. 1989 Computer simulation of recrystallisation in non-uniformly deformed metals. *Acta Metall.* **37**, 627–639.

Sabin, T. J., Bailer-Jones, C. A. L., Roberts, S. M., Mackay, D. J. C. & Withers, P. J. 1997 Modelling the evolution of microstructures in cold-worked and annealed aluminium alloys. *Proc. Int. Conf. on Thermomechanical Processing (Thermec '97), Wollongong, Australia* (ed. R. Chandra & T. Sakai), pp. 1043–1049. Warrendale, PA: The Minerals, Metals and Materials Society.

Sabin, T. J., Bailer-Jones, C. A. L., Roberts, S. M. & Withers, P. J. 1998 Gaussian process modelling of the evolution of microstructure in cold-worked aluminium–magnesium alloys. In *Proc. Int. Conf. on Forging and Related Technology (ICFT '98), April 1998, Birmingham, UK*. London: Institute of Mechanical Engineers.

Sample, V. M., Lalli, L. A. & Richmond, O. 1992 Experimental aspects and phenomenology of internal state variable constitutive models. In *Proc. 3rd Int. Conf. on Al Alloys, Trondheim, Norway* (ed. L. Arnberg, O. Lohne, E. Nes & N. Ryum), pp. 385–431. Trondheim: Norwegian Institute of Technology.

Sellars, C. M. 1990 Modelling microstructural development during hot rolling. *Mater. Sci. Technol.* **6**, 1072–1081.

Shercliff, H. R. 1997 Modelling of materials and processes. Department of Engineering, University of Cambridge, Technical Report CUED/C-MATS/TR243.

Vatne, H. E., Furu, T., Ørsund, R. & Nes, E. 1996 Modelling recrystallisation after hot deformation of aluminium. *Acta Mater.* **44**, 4463–4473.

Withers, P. J., Reed, R. C., Roberts, S. M., Mackay, D. J. C. & Bailer-Jones, C. A. L. 1998 Neural network process modelling for the microstructural management of forged components. Final report to EPSRC, grant number GR/L10239.

Zhu, Q. & Sellars, C. M. 1996 Microstructural modelling of hot deformation behaviour of single phase alloys in continuous and reversing deformation. In *Proc. 2nd Int. Conf. on Modelling of Metal Rolling Processes*, pp. 158–167. London: Institute of Materials.

Zhu, Q., Shercliff, H. R. & Sellars, C. M. 1997 Modelling hot deformation behaviour based on evolution of dislocation substructures. In *Proc. Int. Conf. on Thermomechanical Processing (Thermec '97), Wollongong, Australia* (ed. R. Chandra & T. Sakai), pp. 2038–2046. Warrendale, PA: The Minerals, Metals and Materials Society.

Discussion

D. Juul Jensen (*Materials Research Department, Risø National Laboratory, Roskilde, Denmark*). Concerning Dr Ricks's Monte Carlo sensitivity test, I wondered what kind of effects an incorrect equation relating $t_{0.5}$ or d_{rex} to the input parameters

(δ, d, θ) will have on the resulting distributions—and thus can the distributions be trusted?

H. R. Shercliff. The importance of the predicted distributions of t_{50} or d_{rex} is that it is only possible to judge the validity of the models if the uncertainty in both model and experiment is properly considered. It is true that a second level of sensitivity analysis could be conducted, where the form of the equations is modified to investigate other models. This should then include the altered sensitivity to the input parameters.

J. H. Beynon (*Department of Mechanical Engineering, University of Sheffield, UK*). Dr Shercliff gave an example of a 'Gaussian process model' based on 12 measured data. The predictions included error bars which to me look overly optimistic. Is this because Gaussian distributions are being used inappropriately, or because far too few input data have been used?

H. R. Shercliff. The error bars are somewhat optimistic—with a small data-set the analysis may tend to 'over-fit' the data. It is important not to read too much into the predicted uncertainty in absolute terms. The analysis does show, however, that the method can quickly explore combinations of parameters which have not been tested, and gives a good indication of increasing relative uncertainty as predictions are made further away from the training data.

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