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Finite-element modelling of thermomechanical processing

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The finite-element method is the most widely used computer-based modelling technique for investigating the detail of metal-forming operations, particularly within the deformation zone. It is used for mechanical, thermal and microstructural events. The demands for greater detail keep pace with improvements in computer power, such that the technique remains an off-line tool, too slow for on-line use. Indeed, the complexity of the modelling requires significant simplifying assumptions to be made. Despite this, the finite-element method is often capable of answers that are potentially more accurate than can be achieved with the input data available. Considerable effort is now going on to provide better descriptions of constitutive behaviour, friction and heat transfer. This paper will consider these issues in assessing the current status of finite-element modelling as applied to the thermomechanical processing of metals.

Keywords: boundary conditions; oxide scale; coupling; constitutive behaviour; microstructure modelling; validation

1. Introduction

The complexity of hot working operations renders the finite-element method as the most comprehensive computer-based modelling tool for mechanical, thermal and microstructural events. The method is particularly well suited to modelling the deformation zone, despite the difficulties of dealing with large-strain plasticity. It dominates the field of modelling techniques for thermomechanical processing, sometimes acting as a host for other methods. Its all-embracing capacity stimulates the continuing development of the method, keeping pace with the growth in computer power. The demand for more and more detailed information shows no sign of abating. Despite many simplifying assumptions, the finite-element method still provides useful results now, and finds wide application in industry. In many cases, the method could be more accurate, but is restricted by the inadequacy of the input information available. This has led to a considerable research effort to improve the quality of such information. Thus, there are, broadly, two parallel developments in progress: improvement of the accuracy of prediction of the finite-element method; and exploitation of the method in its current state.

The remainder of this paper will consider these issues, in particular how they apply to boundary conditions and constitutive behaviour. This will form the basis for an assessment of the current status of the finite-element method for modelling the thermomechanical processing of metals, as well as indicating where research is needed.

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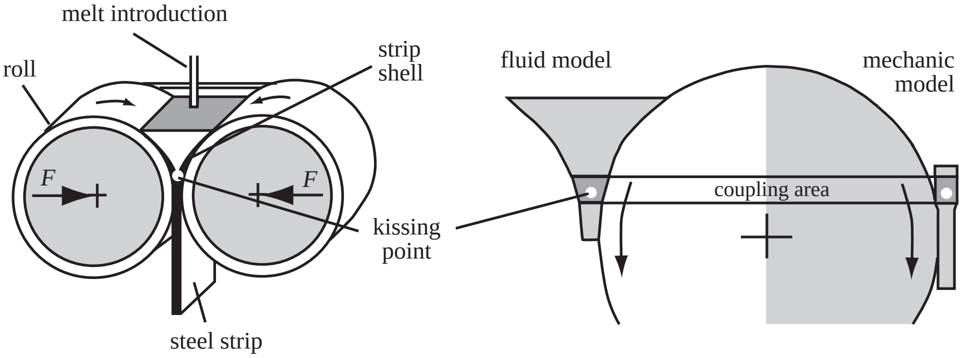

Figure 1. Twin-roll casting process and model layout (Adamidis *et al.* 1998).

2. Developments of the finite-element method

Although in-house finite-element code is still being used, more and more research groups are using commercially available software. Such code is often not ideally suited to thermomechanical processing with its large strain plasticity, having been developed for elastic structural analysis. It can, therefore, be much less efficient than software written expressly for a particular hot working operation. However, the documentation, support, compatibility, familiarity and alternative uses of commercial codes make them more attractive for many groups. This is particularly the case for metallurgists who do not wish to become experts in the finite-element method. There remain many pitfalls for the non-expert user of finite-element code, but they are steadily reducing in number. Many users rely on benchmarking to check their code and their use of it. 'NAFEMS' (1998) is an organization that was founded in 1983 to promote the safe and reliable use of finite-element and related technology, and it oversees a wide range of benchmark tests. This civilizing of the finite-element method has resulted in it being used as a tool by process engineers, that is by people whose first experience is with the process being modelled, rather than with the computational methods. This is a welcome development and brings with it much more appropriate application of computer-based modelling, germane to the current appreciation of the hot working operation.

The range of applications of the finite-element method is considerable and continues to expand. A recent development is the coupled modelling of the casting and solid deformation that takes place during the casting of thin strip between a pair of rollers. Adamidis *et al.* (1998) have used a multi-grid fluid solver for the liquid state, and a finite-element program for the solid strip. In the zone where these two states merge there is a 'coupling area' (figure 1), where the two programs share state variables. These variables have to be carefully mapped in space as well as synchronized in time. However, by careful interchange, Adamidis *et al.* (1998) have been able to couple what are essentially separate programs to provide a single model from liquid through to deformed solid. (It is interesting to observe that this hybrid modelling required a team of 12 people; see author list.) There remains scope for progress, perhaps through hybrid liquid–solid modelling within one program, which is being developed for other applications. One example is the modelling of the deformation of flexible heart valves pushed open by blood flow (Carmody *et al.* 1997).

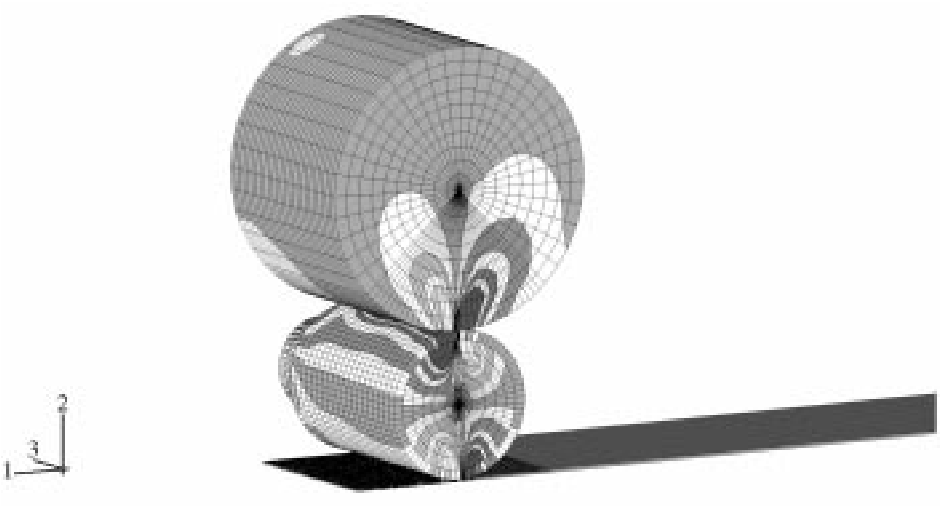

Figure 2. Stress in the plane of a roll section, showing high stresses at the contact regions and discontinuities between the skin and core of the work roll (after Wadsworth 1998).

Another type of coupling is to model the deformed body together with the deforming tool. Although computationally more expensive, there should be greater geometrical precision when both tool and stock are modelled fully. Wadsworth (1998) has produced a fully thermally coupled elasto-plastic three-dimensional model of a hot steel strip being rolled in a four-high stand (figure 2). Although such a large model is only required for specific cases in which dimensional accuracy is paramount, particularly for transient conditions, it does illustrate the capacity of modern commercial code in skilled hands.

Such large three-dimensional finite-element models are computationally very intensive. When dealing with multipass rolling or multistage forging, such models need to be run several times per schedule. With the computer power available to most industrial users, this leads to a time constraint on the modelling. Not enough modelling can be done in the time available. There are ways to short-cut the fully three-dimensional model with little loss in accuracy. Wen & Petty (1998) have predicted the shape of rolled cross-sections, a three-dimensional problem, using an approximation in combination with a two-dimensional model. The approximation is an analytical expression for the complexities of the shape change, which is claimed to be valid for a wide range of geometrically similar rolling operations. The quality of the approximation can be gleaned from figure 3, which compares the shape of the long product after seven rolling passes as predicted by two- and three-dimensional models.

An alternative approach to more economical modelling also exploits the similarity of many rolling operations. An artificial neural network has been trained with the output from a range of finite-element runs, and then used to predict deformation for rolling geometries not previously modelled (Trowsdale *et al*. 1998). Figure 4 shows two hot rolling sequences for steel: round-to-oval and oval-to-round. The grain size shown is based on strain calculated as a mean value, locally by the finite-element method, and locally from the artificial neural network. This illustrates the lack of detail that a single mean value provides, particularly when the grain size varies

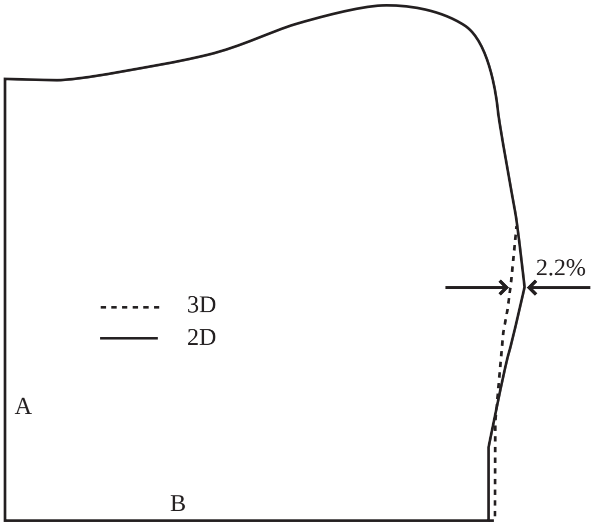

Figure 3. Predicted final cross-section shape for a 100 mm square billet, hot rolled through seven passes by full three-dimensional finite-element analysis and by a novel two-dimensional finite-element method. The maximum error is less than 2.2%; A and B are symmetry planes (Wen & Petty 1998).

significantly across the section (figure 4*d*–*f*). It also illustrates a reasonably close comparison between the finite-element and artificial neural-network predictions.

Although the development of the artificial neural-network model may take many iterations of the training set of data, once trained, it produces output almost instantaneously. Since the finite-element method, particularly when dealing with three-dimensional problems, can take several hours to compute each deformation, this is a remarkable time saving. It also offers the potential for on-line use of the finite-element method by proxy. The time constraints for on-line process calculations are very demanding. Consequently, most on-line models are very simple, only moderately accurate, and give mean rather than distributed values. Access to the sort of detail of which the finite-element method is capable, on-line, is an exciting prospect.

3. Boundary conditions

The previous section gave two examples of accelerated solution techniques based on the finite-element method. Both compared the fast with the standard approach to demonstrate their predictive accuracy. This does not, though, necessarily mean that either compares well with reality. Very often the use of the finite-element method to model thermomechanical processing operations is limited in its accuracy by uncertainty about the boundary conditions.

In the rolling of wide thin plate or strip, the deformation is highly constrained, other than at the very start and end of the metal stock. The only 'free' deformation is the shear deformation, which is dictated by the roll gap geometry and the friction conditions pertaining between the roll and stock (Ponter *et al.* 1993). Currently, the shear deformation cannot be determined *a priori* and must be determined experimentally. Since the intimacy of the contact between the cold tool and the hot

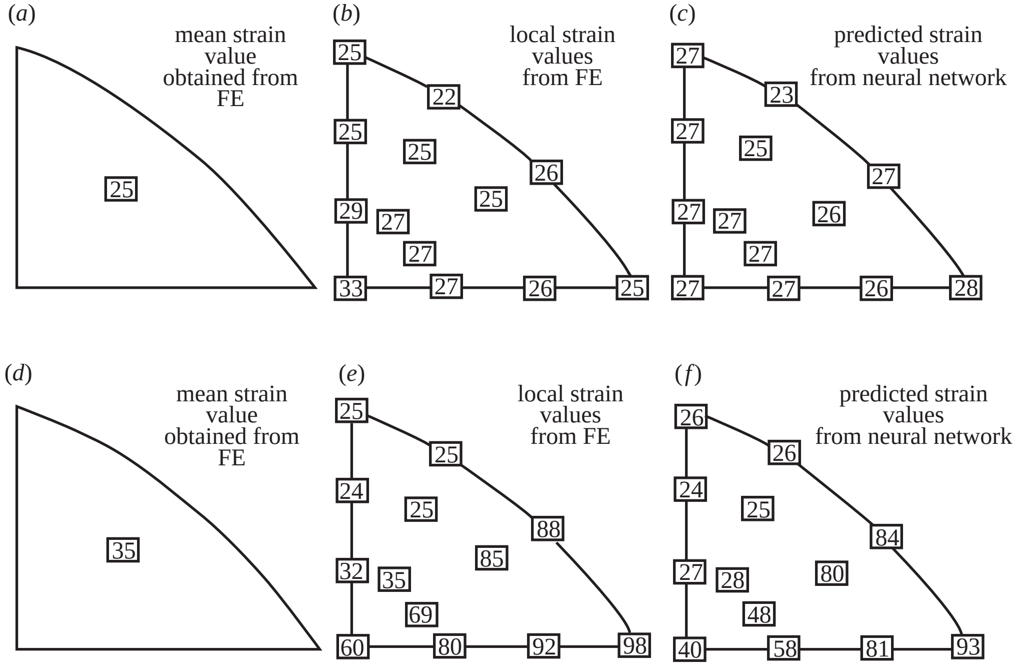

Figure 4. Comparison of grain size (μm) predicted using strain calculated as a mean value, locally by the finite-element method, and locally from an artificial neural network trained on other finite-element output. Two hot rolling sequences for steel are shown: round-to-oval (*a*)–(*c*) with a fairly uniform strain distribution; and oval-to-round (*d*)–(*f*) with more inhomogeneous strain (Trowsdale *et al.* 1998).

Table 1. *Measured heat-transfer coefficients between roll and stock for hot rolling of steel and aluminium*

steel		aluminium	
(kW m^{-2} K^{-1})	reference	(kW m^{-2} K^{-1})	reference
18–38	Stevens *et al.* (1971)	19–22	Pietrzyk & Lenard (1989*b*)
23–81	Murata *et al.* (1984)	10–50	B. K. Chen *et al.* (1992)
2–20	Malinowski *et al.* (1994)	15–20	Semiatin *et al.* (1987)
5–50	Pietrzyk & Lenard (1989*a*)	15	Timothy *et al.* (1991)
200	Sellars (1985)	100–350	Hlady *et al.* (1993)
10–260	W. C. Chen *et al.* (1992)	200–450	Hlady *et al.* (1995)

workpiece is critical to both the traction and the rate of heat transfer, the friction and thermal behaviours are interrelated and must be considered together (Beynon 1998).

The hot metal invariably begins with an oxide on its surface. With aluminium alloys, the oxide forms a thin adherent film. With steel, the thickness and composition of the oxide scale depend on temperature, time at temperature, steel composition and availability of oxygen (Chang & Wei 1989). The plastic straining imposed during hot-

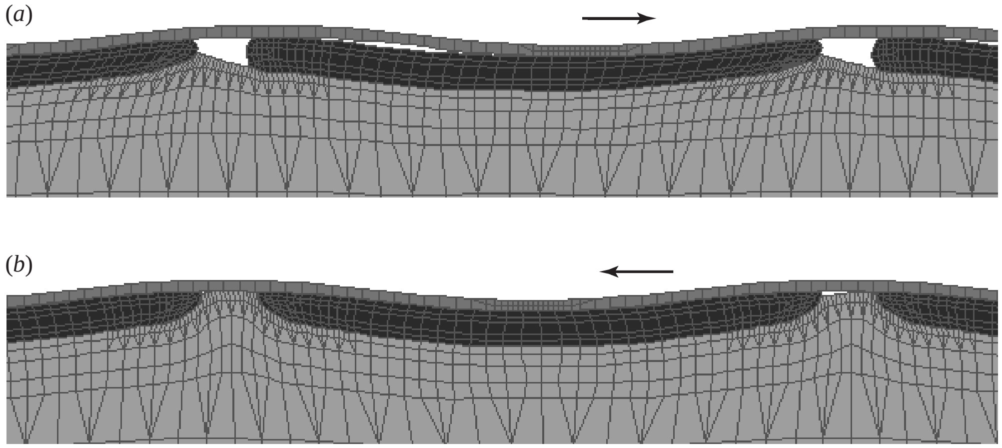

Figure 5. Predicted deformation in the vicinity of wide cracks in the oxide scale for two positions in the hot rolling of a plain carbon steel strip initially 1.8 mm thick, at 911 °C, and travelling at 13.2 m s^{-1}, reduced during the pass by 13% (Fletcher *et al*. 1998). The two figures are taken at 24% through the arc of contact, and at 92%. Metal can be seen to extrude up through the crack to make contact with the roll (represented by the single row of elements at the top). The arrows indicate the movement of the roll relative to the stock.

metal forming causes deformation and/or fracture of the oxide scale. If such fracture occurs when the hot metal is in contact with the cold tool, clean metal–metal contact can occur as the hot metal extrudes up through the crack. This will produce a sharp rise in friction, and a dramatic rise in heat transfer compared with contact through an oxide barrier. What is not known is under what conditions such fracture occurs, since making measurements of the interfacial events is fraught with difficulties, particularly under industrial hot working conditions. As a consequence, modellers have generally resorted to single coefficient values for friction (Montmitonnet & Buessler 1991). Similarly, measured values of heat-transfer coefficient vary enormously (see table 1). Even worse, the values in table 1 were obtained under laboratory conditions, which differ significantly from industrial circumstances, most notably in terms of speed, lubrication and the state of the surface oxide.

Current research is, therefore, focused on detailed modelling of the tool–stock interface itself, at a geometrical scale-level below that of the whole metal working operation. The finite-element method has been applied to this problem also, for the deformation of asperities in cold forming (Korzekwa *et al*. 1992), and the hot compression of a single asperity (Lin *et al*. 1993). More recently, multiple-asperity contact has been modelled using the finite-element method to determine friction and heat transfer during the relatively high-speed rolling of thin (*ca*. 1 mm) flat steel strip in the last stand of a seven-stand tandem mill, and for the hot rolling box passes of long steel products (Fletcher *et al*. 1998). Figure 5 illustrates such modelling for the strip rolling case, modelling that can include fluid pressurization, oxide scale deformation, fractured scale, all in a thermally coupled model. Yet again, finite-element modelling has been taken to a reasonably advanced level, only to be thwarted by a lack of information on how metal oxides behave under the extreme conditions of the tool–stock interface. This shortfall has triggered subsequent experimental investigations

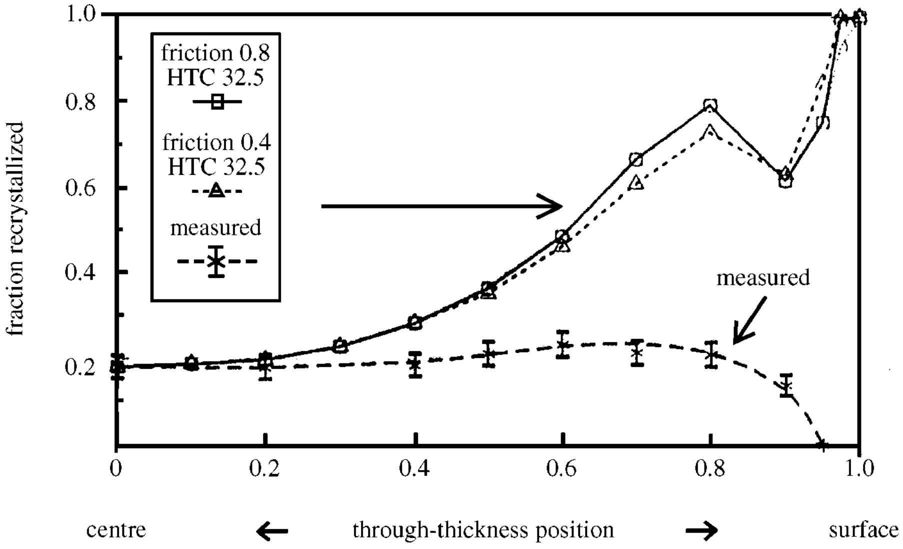

Figure 6. Predicted through-thickness gradient in microstructure for a type 316 stainless steel, following laboratory hot rolling, using two values of friction coefficient and two values of heat-transfer coefficient, comparing poorly with the experimental results (after McLaren *et al.* 1995).

into oxide behaviour under hot working conditions. Nevertheless, there remains an enormous amount of investigation, both experimental and computer based, before friction and heat transfer can be adequately described for a comprehensive range of thermomechanical processing of the main group of structural alloys.

4. Constitutive behaviour

It is not only at the tool–stock interface that the deficit in information is handicapping application of the finite-element method. Strain-path effects are well known in (cold) sheet metal forming and in fatigue, but have only recently revealed their considerable impact in thermomechanical processing. Even in flat rolling there is a strain-path effect, arising from the shear reversal as the stock passes the neutral point, accelerating past the roll speed as its thickness is reduced. Figure 6 shows the results of an attempt to reconcile finite-element predictions with experimental measurements (McLaren *et al.* 1995). Despite great care with both methods, the difference remained. This has resulted in a growing experimental programme to determine strain-path effects under hot working conditions, which is discussed elsewhere (Davenport *et al.*, this issue). This work is an excellent example of computer-based modelling acting as a stimulus for scientific research.

An important application of the finite-element method is its modelling of experimental tests, which is being used to determine the constitutive behaviour of a material. Particularly for thermomechanical processing, deformation and thermal gradients can be considerable within the specimen gauge zone. Subsequent interpretation of the microstructure requires detailed knowledge of the prevailing hot working conditions, which is provided by the finite-element modelling. Inverse analysis, or parameter optimization, techniques are being increasingly applied so as to extract reliable

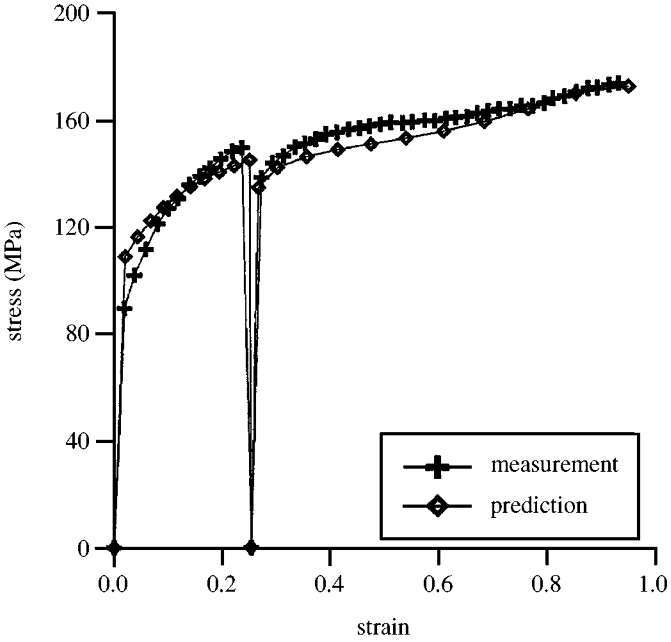

Figure 7. Measured and calculated stress–strain relationships for a two-stage uniaxial compression of an 0.49wt% carbon steel at 996 °C, inter-pass time 1.4 s, following an interruption after a strain of 0.25. The calculation is based on parameter optimization (Kusiak *et al*. 1996).

and accurate constitutive behaviour (Kusiak *et al*. 1996). Figure 7 reveals reasonable comparison between measured flow stress data and predicted values based on parameter optimization. Both work hardening and inter-pass static recrystallization are included in the model.

5. Integration of microstructure models

At its simplest, microstructure evolution is implicitly modelled in the form of the equation for flow stress. The early finite-element models assumed ideal plasticity, which is a fair approximation of, for instance, some aluminium alloys deformed under hot working conditions (see figure 8 and Shi *et al*. (1997)). Most aluminium alloys exhibit dynamic recovery under these conditions, whereas steels can dynamically recrystallize. The key feature of such a stress–strain curve is the peak followed by a small reduction to a steady-state flow stress (see figure 9 and Sakai & Jonas (1984)). To a first approximation, and to a sufficiently large strain, this can also be described by ideal plasticity.

Such simplifications have become less common since incorporating the full shape of the stress–strain curve is no longer problematic. As the metal is deformed, perhaps by passing through a roll gap, the local strain rate and temperature change. Most material models ignore the effect of accumulating strain under varying conditions of strain rate and temperature, and simply use the appropriate stress–strain curve for the prevailing conditions at the accumulated strain value. By following the locus of the various stress–strain curves, it has been shown (Beynon *et al*. 1993) that the

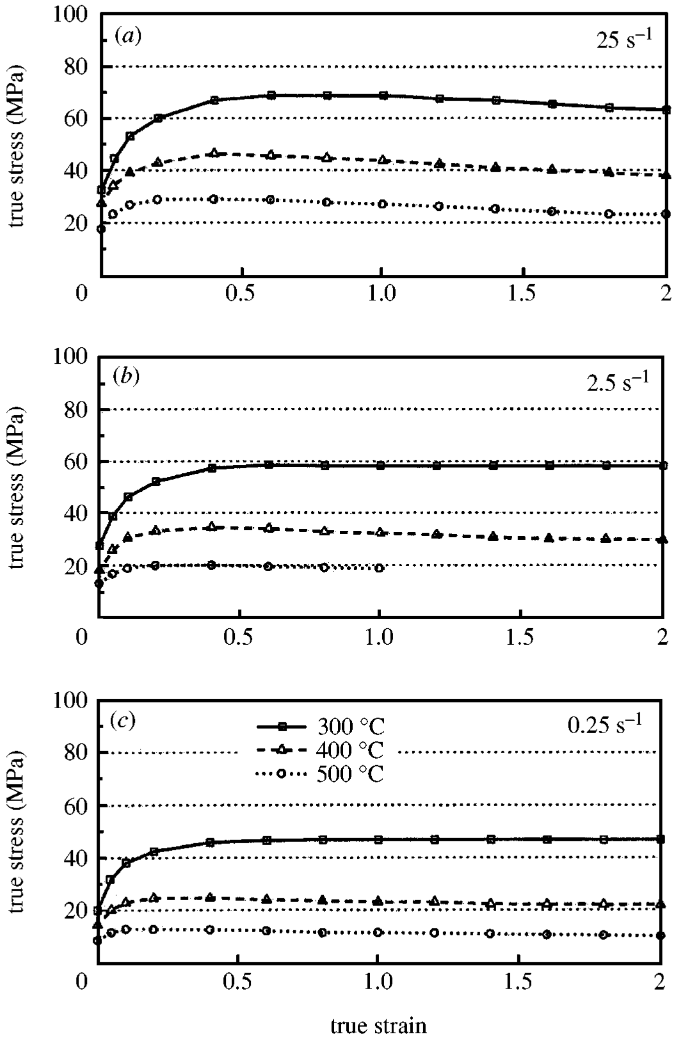

Figure 8. Measured stress–strain curves for commercial purity aluminium using hot plane-strain compression testing (Shi *et al*. 1997). The shape of the curves is typical of a wide range of aluminium alloys.

actual flow stress values used, for the bulk of the deformation, adhere closely to a single curve (figure 10).

For some applications, detailed microstructural predictions can be made without recourse to integration that is more than simply post-processing. This means running the finite-element model for a deformation with a description of material flow behaviour, which takes no account of the microstructural event of interest. The output from the model is then used to calculate the evolution of microstructure through the deformation. A good example of this is crystallographic deformation texture, which has been predicted with reasonable precision for a commercial aluminium can body alloy, where the industrial hot rolling was interrupted to crop ends off the stock to measure the texture. Figure 11 shows a comparison of measured and predicted

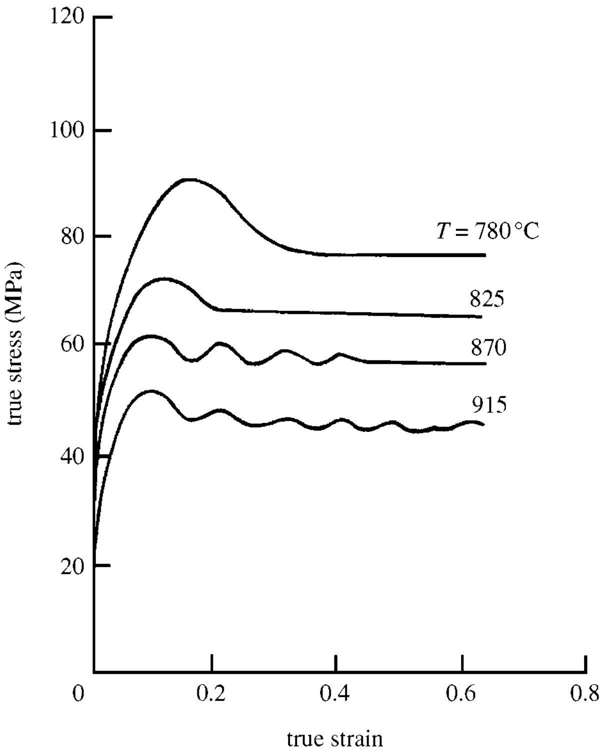

Figure 9. Measured stress–strain curves for an 0.68wt% carbon steel at a strain rate of $1.3 \times 10^{-3}\ \mathrm{s}^{-1}$ for a range of temperatures using uniaxial compression (Sakai & Jonas 1984). The curves illustrate different forms that can arise from dynamic recrystallization of the steel.

crystallographic texture for a roughing pass in an industrial flat mill (Oscarsson *et al*. 1994). It is for the user to decide whether the prediction is accurate enough. However, with the hard constraints of flat rolling, it is unlikely that the anisotropy of flow stress arising from such crystallographic textures would be enough to significantly alter the pattern of deformation.

For through-process models that attempt to follow microstructure evolution over multiple deformations, incremental formulations are required to allow integration into the finite-difference or finite-element model. Such a formulation for both dynamic and static events has been developed for hot worked austenite (Yanagimoto 1996).

Incremental formulations are a useful way to re-cast current equations. Other techniques are available that can contain advanced descriptions of materials' behaviour and allow the material to self-evolve the consequences. One promising prospect in this field is cellular automata, which have been used to model crystallographic texture (Marx *et al*. 1996). This modelling tool is particularly attractive for its visual presentation (figure 12), making the results relatively easy to interpret without sacrificing detail or precision. It is expected that cellular automata models will soon be embedded into finite-element models, the latter supplying details of the prevailing strain rate and temperature. Thus, the finite-element model can embrace each development in the modelling of texture. The definitive model for recrystallization texture under hot working conditions is still awaited.

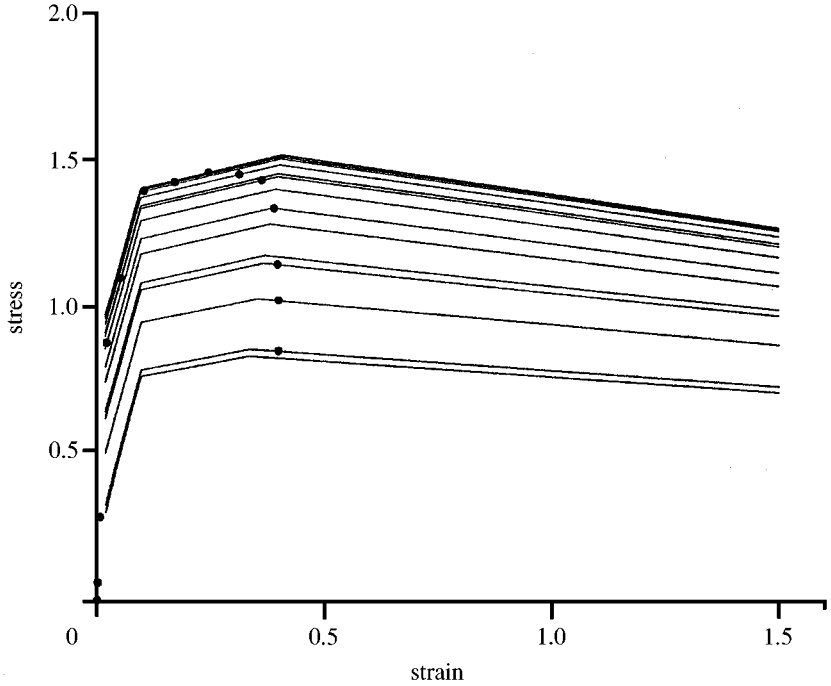

Figure 10. Stress (MPa/143)–strain curves for elements along the centreline of the stock in the roll gap for the laboratory hot rolling of type 316L stainless steel (Beynon *et al*. 1993). The closed circles show the locus of stress–strain for a particle moving along the flow line down the centre of the stock. The stress–strain curves have been simplified to linear fits between characterizing points.

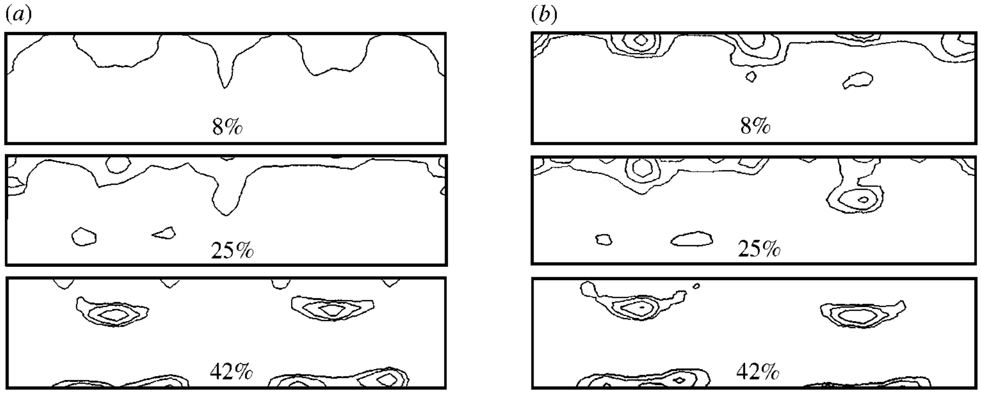

Figure 11. Comparison of measured and calculated (based on finite-element output) deformation textures for 80 mm AA3004 aluminium alloy plate that was industrially hot rolled (after Oscarsson *et al*. 1994). The orientation distribution functions ($\phi_2 = 45°$) are illustrated for three depths through the thickness (as a percentage of the thickness from the upper surface). The contour levels are 2, 4, 8 and 16.

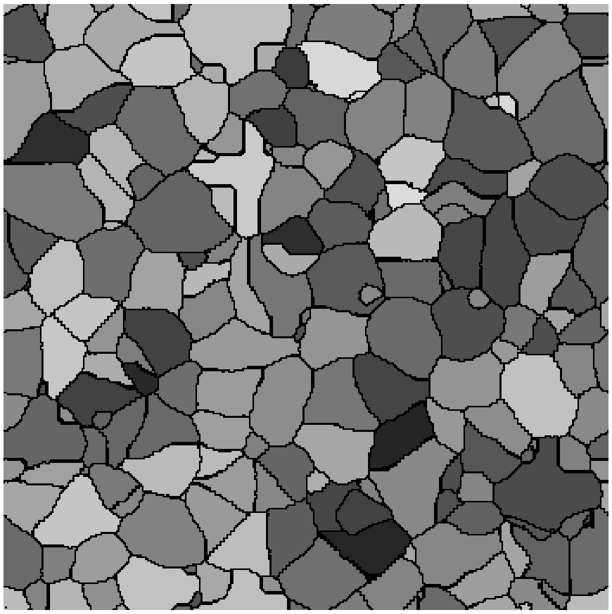

Figure 12. Typical image from a three-dimensional cellular automata calculation for static recrystallization, assuming site-saturated nucleation with homogeneous and isotropic boundary mobility. This output can be viewed live at the Web site of the Institut für Metallkunde und Metallphysik, RWTH-Aachen (http://www.imm.rwth-aachen.de/∼sim_dem/rx/welcome.htm).

6. Validation

The physical metallurgy of hot working has always provided limited opportunity for direct observation of events. Much has been determined from piecing together partial information, for instance from as-quenched specimens. In this sense, validating finite-element models for thermomechanical processing is no different.

The finite-element model can be checked against analytical solutions for simple cases, and against measurements for laboratory conditions. Unfortunately, industrial conditions for thermomechanical processing are often impractical to reproduce in a laboratory. Furthermore, making measurements on an industrial plant is very difficult. A good example is trying to measure temperature on a hot rolling mill. Embedding thermocouples is not practical for multipass rolling, so radiation pyrometers are used. With water, steam and oxide obscuring the metal surface, pyrometer measurements are prone to error. Indeed, Hodgson *et al*. (1993) have demonstrated that temperature can be more accurately determined from the measured roll force with the use of accurate roll force and hot strength models (figure 13).

For validating predictions of microstructure evolution, the best measurement would be of the microstructure itself during thermomechanical processing, rather than in a cooled sample. One example of such a development is *in situ* laser-based ultrasonic methods for monitoring microstructures and transformation kinetics (Scruby *et al*. 1995). With increasing use of warm rolling of steels around the austenite–ferrite phase transformation, on-line detection of the phase transformation would be a very valuable tool.

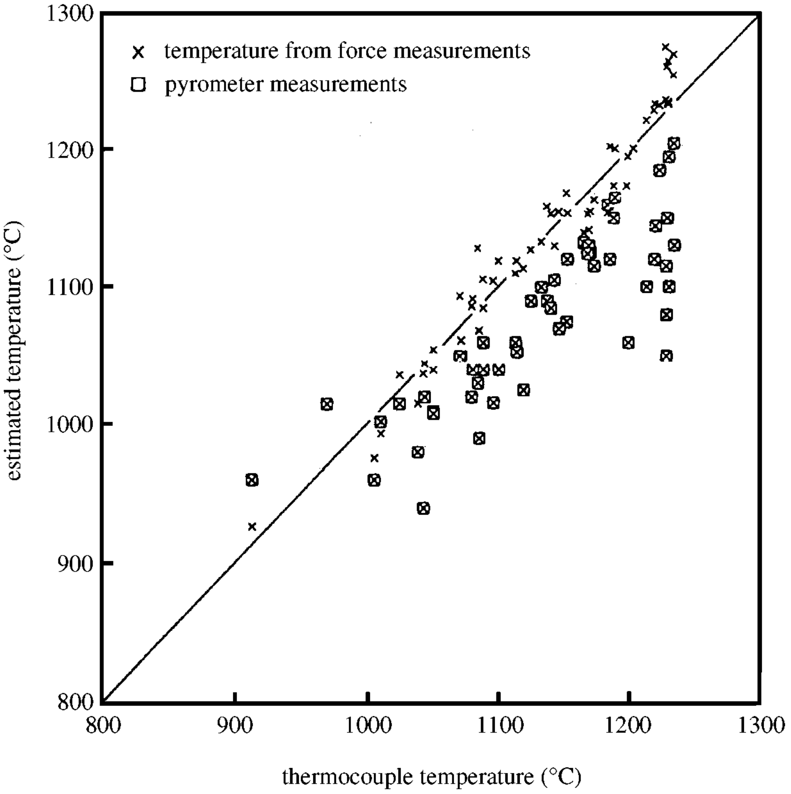

Figure 13. Comparison of temperature measured by thermocouples and pyrometers and estimated from force measurements during experimental rolling (Hodgson *et al.* 1993). This estimation requires very good roll force and hot strength models, but can provide a better measure of temperature (as determined by the thermocouples) than by using a pyrometer.

7. Conclusions

The finite-element method is in a mature state, capable of providing valuable insight into the deformation conditions prevailing in industrial hot working operations. It will find increasing application as a vehicle for models, which feed off its output of strain rate and temperature, to predict details of the evolution of microstructure during thermomechanical processing. The priority now is to improve the quality and precision of the boundary conditions and the microstructural models.

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