New Welding Alloys: Computational Methods

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Metals are useful materials because of their sophistication and low cost. The many phase transformations and processing variables associated with them can be exploited to achieve a very large range of desirable properties. The very complexity that makes metals so useful also makes their design difficult. This is particularly so for welding alloys which have an additional level of complexity given that the ultimate properties have to be achieved in the *as–welded* condition.

The modelling of welds is a vast subject covering arc physics, heat and fluid flow, solidification, solid–state transformations and the development of mechanical properties for the fusion zone, the heat–affected zones and the joint as a whole (Table 1). The present paper focusses on just one of these aspects, the structure and properties of the fusion zone in steel welds.

Arc phenomena	Plasma processes
Vapourisation	Heat transfer
Fluid flow	Surface tension effects
Mass transfer	Gas absorbtion
Oxidation phenomena	Flux–metal interactions
Solid–state transformations	Tempering reactions
Mechanical property models	Joint integrity

Table 1:Variety of topics covered in the general subject of *weld modelling*.

The Variables

The majority of welding alloys are produced for the fabrication of structural steels. The engineering requirements are usually expressed in terms of a specified yield strength, ductility (elongation and reduction of area) and the toughness (Charpy tests or K_{IC} measurements). The toughness is a prime requirement in most cases but particularly for service at sub–zero temperatures.

The variables affecting these properties include the chemical composition which might include deliberate additions of C, Mn, Si, and Ni as elements which primarily influence the stability of the variety of phases. Trace additions such as titanium and boron are usually in concentrations so small that they do not affect phase stability *per se* but instead have profound kinetic effects, for example by segregation to interfaces. There are also the "impurity" elements, such as phosphorus, sulphur, nitrogen, oxygen and aluminium which have complex consequences on the microstructure and mechanical properties. The welding process determines the solidification microstructure and cooling conditions, and hence influences the final properties. In arc welding the parameters of importance include the welding current, voltage, speed and interpass or preheat temperature. The welded joint in structural steels is rarely heat treated after fabrication so that tempering reactions need not be taken into account except in the context of multirun welds where the sequential deposition of layers causes incipient heating of the underlying weld metal.

How does one begin to calculate the engineering parameters as a function of this myriad of variables? Surprisingly, the answer begins with a consideration of equilibrium!

Equilibrium

Equilibrium is a state in which there is no perceptible change no matter how long the system is observed. It takes time to approach equilibrium. The transfer of metal from an electrode, through an arc plasma, into the weld pool and finally its incorporation into the solid state occurs in a matter of seconds. This is not conducive to the achievement of equilibrium so it is reasonable to wonder why, in the context of welding, one should bother with thermodynamics at all.

The reason is simple: a system which is not at equilibrium may still have the characteristics of equilibrium on a local scale. Thus, a ball which is falling at a steady rate is not at equilibrium but an observer located on the ball will not see any change in the local environment as the ball falls. Similarly, phases such as ferrite frequently occur with *local equilibrium* at the moving transformation front.

Thermodynamic parameters are therefore essential inputs to kinetic theory, which describes the rate of approach to equilibrium. Thermodynamics also helps reduce the number of variables, for example by expressing the combined effect of carbon and manganese in terms of their effect on the relative stabilities (free energies) of the austenite and ferrite. The method thus "links together many variables so that they can be seen to be a consequence of a few".

Most people are familiar with phase diagrams, which give equilibrium phase fractions and the compositions of the phases as a function of solute content and temperature. Such diagrams become difficult to conceive in more than three dimensions. Thus, for steels with many alloying elements we have to be satisfied with just the numerical information on phase fractions and compositions. This is the friendly output of phase diagram calculations. There is other information which is of value in seeing what drives transformations.

Fig. 1 shows an example of phase diagram calculations which form an input to the kinetic theory which is essential in estimating the development of microstructure. Calculations like these can now be carried out routinely for alloys with many solutes, for example the duplex stainless steel, hardfacing alloys in addition to the vast range of low alloy steels.

Rate

The simplest assumption in kinetic theory is to take a "flux" to be proportional to a "force". The flux could represent an interface velocity, an electrical current or a heat flux, with the driving force, the electromotive force and temperature gradient representing the corresponding forces. The assumption of proportionality is probably reasonable for small departures from equilibrium. The proportionality can be generalised, so that a given flux can be expressed as a function of a combination of forces. In a ternary Fe–Mn–C alloy, the diffusion flux of carbon depends not only on the gradient of carbon, but also on that of manganese. Consequently, a uniform distribution of carbon will tend to become inhomogeneous in the presence of a manganese concentration gradient. Similarly, the flux of heat can be driven by an electromotive force (Peltier effect).

If the mechanism of a transformation is known, it is possible to apply kinetic theory to model the development of microstructure. An example for welding is illustrated in Fig. 2. The calculations have over many years proved to be sufficiently reliable for the models to be used routinely in industry, both for alloy design and to address customer queries with confidence. The experimental determination of the data illustrated in Fig. 2 would cost in excess of £100,000.

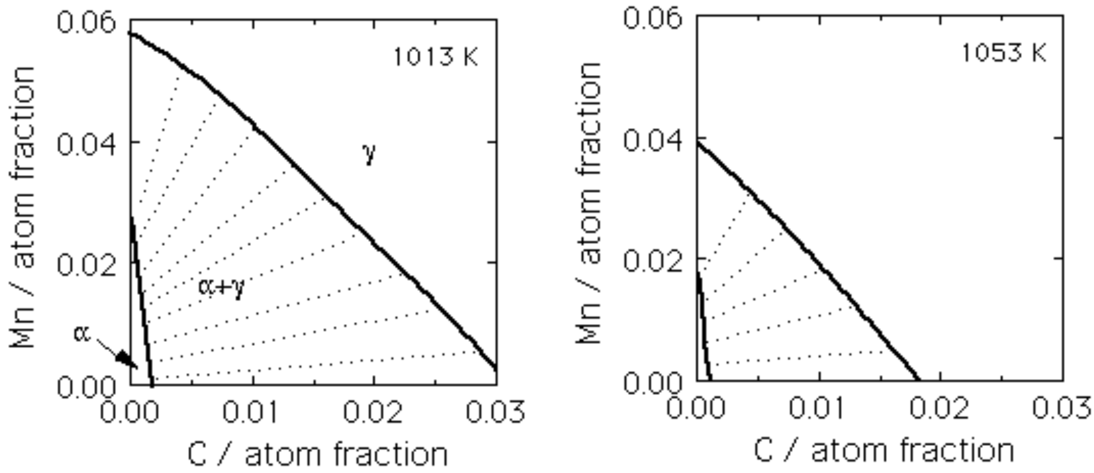

Fig. 1: Calculated isothermal section of the Fe–Mn–C phase diagram illustrating how the ferrite (α) and austenite (γ) phase field changes with solute concentration and temperature. The end points of the dotted lines represent the compositions of the austenite and ferrite which are in equilibrium. It has been possible to do such calculations for multicomponent steels for many decades.

EMPIRICAL MODELS

The physical models described above are capable of predicting entirely new phenomena. But there are difficult problems where the general concepts might be understood but which are not as yet amenable to mathematical treatment. We are at the same time told that good engineering has the responsibility to reach objectives in a cost and time–effective way. Any model which treats a small part of the required technology is therefore unlikely to be treated with respect. Empiricism can in these circumstances be extremely useful in filling in any gaps whilst striving for longer term solutions.

Most people are familiar with regression analysis where data are best–fitted to a specified relationship which is usually linear. The result is an equation in which each of the inputs x_j is multiplied by a weight w_j; the sum of all such products and a constant θ then gives an estimate of the output $y = \sum_j w_j x_j + \theta$. Relationships like these are used widely in the welding industry, for example, in the formulation of the famous *carbon equivalents*:

$$\mathrm{IIW} \qquad > 0.18\,\mathrm{wt.\%\ C}$$

$$\mathrm{CE} = \mathrm{C} + \frac{\mathrm{Mn}+\mathrm{Si}}{6} + \frac{\mathrm{Ni}+\mathrm{Cu}}{15} + \frac{\mathrm{Cr}+\mathrm{Mo}+\mathrm{V}}{5} \qquad \mathrm{wt.\%}$$

$$\mathrm{Ito} - \mathrm{Besseyo} \qquad < 0.18\,\mathrm{wt.\%\ C}$$

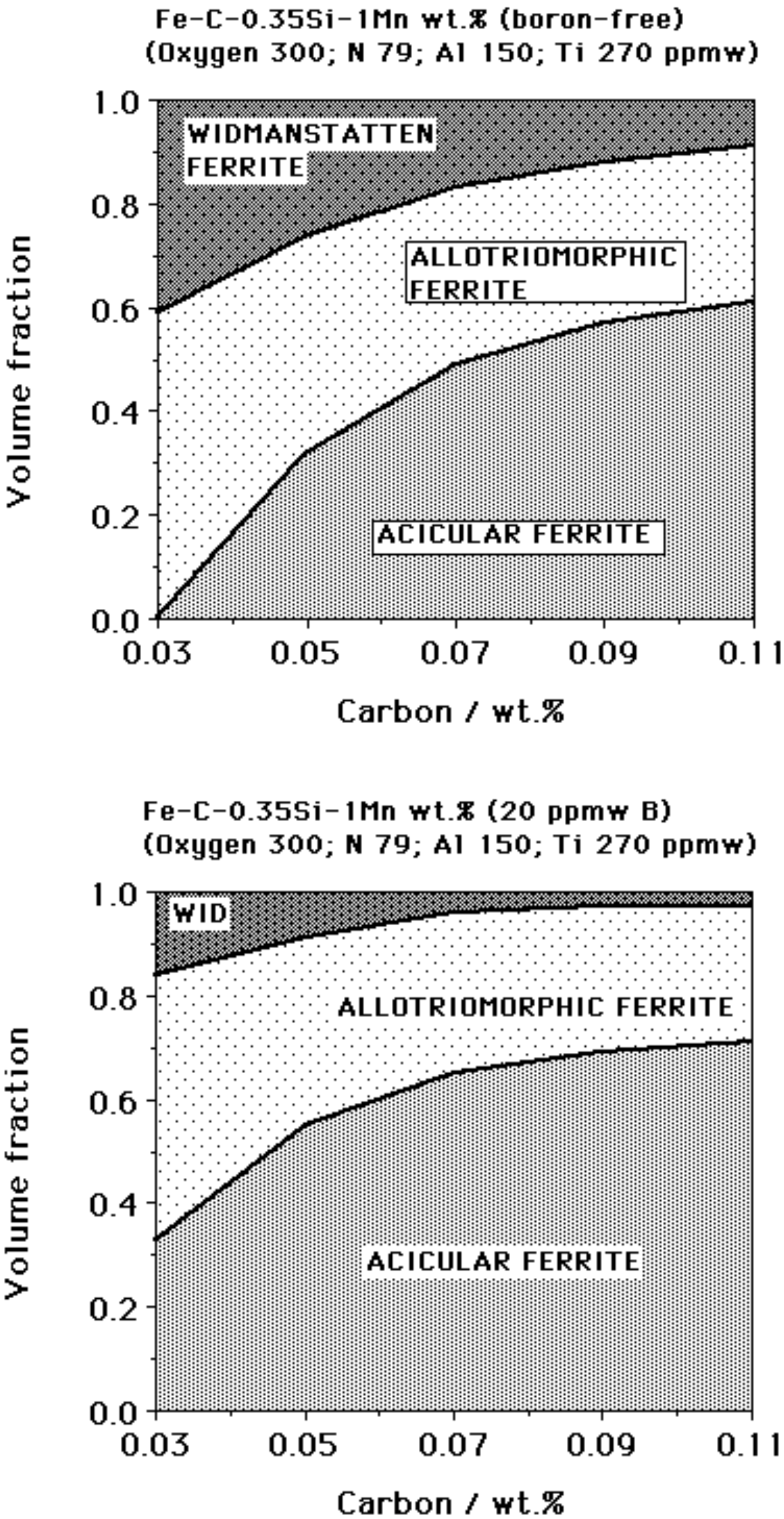

Fig. 2: Calculated microstructures of manual metal arc weld deposits as a function of chemical composition. The boron concentration makes a remarkable difference to the microstructure.

$$\mathrm{CE} = \mathrm{C} + \frac{\mathrm{Si}}{30} + \frac{\mathrm{Mn} + \mathrm{Cu} + \mathrm{Cr}}{20} + \frac{\mathrm{Ni}}{60} + \frac{\mathrm{Mo}}{15} + \frac{\mathrm{V}}{10} + 5\mathrm{B} \qquad \mathrm{wt.\%}$$

or in the expression of mechanical properties as a function of the chemical composition (Evans *et al.*):

$$\text{yield strength / MPa} = 484 + 57 \times w_{Cu}$$

where w_{Cu} is the weight percent of copper in as–welded "carbon–manganese" manual metal arc welds. It is well understood that there are dangers in using such relationships beyond the range of fitted data. This is highlighted, for example, by the need to use a variety of carbon equivalent equations for different steels.

A more general method of regression is neural network analysis. As before, the input data x_j are multiplied by weights, but the sum of all these products forms the argument of a hyperbolic tangent. The output y is therefore a non–linear function of x_j, the function usually chosen being the hyperbolic tangent because of its flexibility. The exact shape of the hyperbolic tangent can be varied by altering the weights (Fig. 3a). Further degrees of non–linearity can be introduced by combining several of these hyperbolic tangents (Fig. 3b), so that the neural network method is able to capture almost arbitrarily non–linear relationships. For example, it is well known that the effect of chromium on the microstructure of steels is quite different at large concentrations than in dilute alloys. Ordinary regression analysis cannot cope with such changes in the form of relationships.

In the absence of a physical understanding, many models can in general be created to represent the same data. During the fitting of each model to the data, statistical methods such as that of Bayes can be used to infer the most probable parameter values and the error bars on those parameters. The sensible use of error bars reduces the danger of extrapolation or interpolation. Such error estimates are illustrated in the example given below. MacKay has shown that the Bayesian framework also permits different models to be distinguished on the bases of their complexity, with an automatic penalty to over complex methods. This follows the principle of the famous Occam's razor, that there should be a preference for simple theories. We should adopt the most simple explanation because such an explanation has beauty and because simple theories seem to be successful.

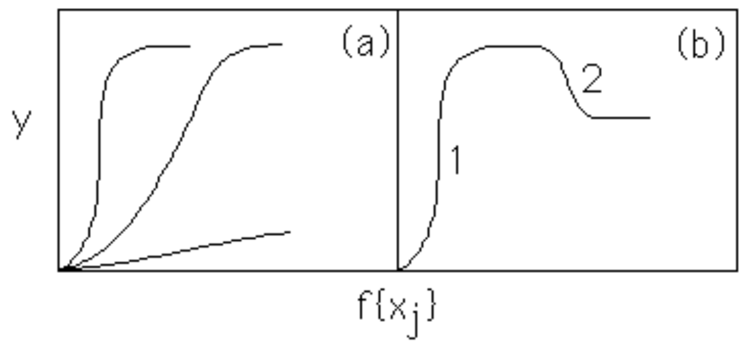

Fig. 3: (a) Three different hyperbolic tangent functions; the "strength" of each depends on the weights. (b) A combination of two hyperbolic tangents to produce a more complex model.

A potential difficulty with the use of powerful regression methods is the possibility of overfitting data (Fig. 4). For example, it is possible to produce a neural network model for a completely random set of data. To avoid this difficulty, the experimental data can be divided into two sets, a *training* dataset and a *test* dataset. The model is produced using only the training data. The test data are then used to check that the model behaves itself when presented with previously unseen data.

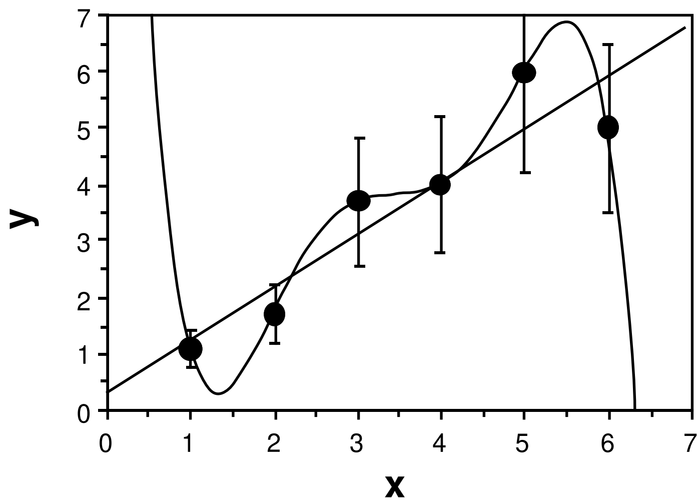

Fig. 4: A complicated model may overfit the data. In this case, a linear relationship is all that is justified by the noise in the data.

Neural network models in many ways mimic human experience and are capable of learning or being trained to recognize the correct science rather than nonsensical trends. Unlike human experience, these models can be transferred readily between generations and steadily developed to make design tools of lasting value. These models also impose a discipline on the digital storage of valuable experimental data, which may otherwise be lost with the passage of time.

An example of the use of a neural network model in predicting the strength of steel weld deposits, as a function of a very large number of variables, is illustrated in Fig. 5. The inputs included the detailed chemical composition (almost twenty elements), heat treatment and welding parameters. Models like these have been trained for many complex phenomena for which physical models do not exist; the fatigue strength of nickel–base superalloys, the formation of austenite during the heating of steels, the toughness of arc welds *etc.* They are particularly powerful in serving as a bridge between microstructure and mechanical properties.

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PROGRESS

"Modelling" has now become a very prominent subject not only in welding but in materials science as a whole. There are many university departments which specialise in the subject and there are numerous examples of similar work in industry. It is a very attractive area for

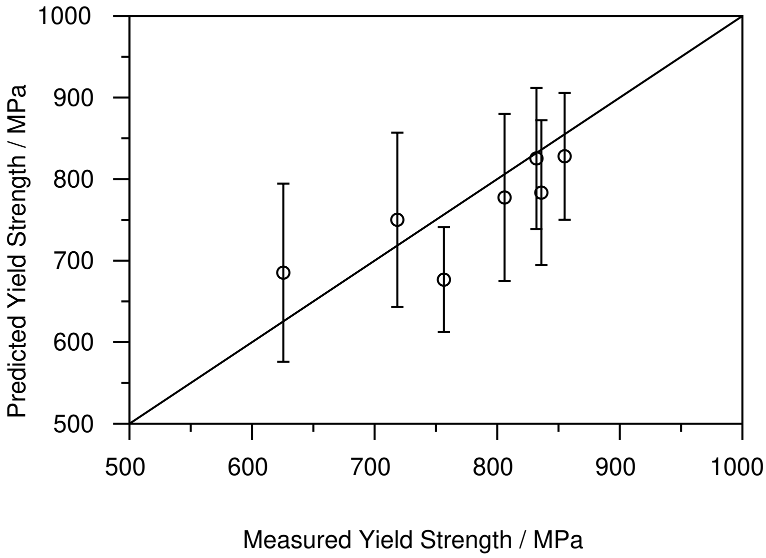

Fig. 5: The neural network predicted versus measured yield strength for a variety of welds previously unseen by the model.

collaboration between universities and industry because it combines the excitement of science with the focus on complex technological issues.

To help in making the subject accessible to a wider audience, there now exists a perpetual electronic library accessible via the world wide web:

http://www.msm.cam.ac.uk/map/mapmain.html

It contains elementary subroutines that can enable a user to develop new concepts using existing methods as a foundation. It is intended to make established work much more accessible and usable in both research and development projects. It embodies the essential features of publications, that the code included is validated, documented and open to scrutiny by the scientific and industrial communities.

The growth of the subject will only be sustained in the long term if it is seen to produce results which are useful to the entire community, not just one partner in the industry/university alliance.