

Frontiers in the Modelling of Steel Weld Deposits*

鋼溶接金属予測モデルの最前線*

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鋼の溶接金属中で生じる凝固現象における変化は、その機械的特性に及ぼす影響が大きい。このレビューは、ミクロ組織と特性の観点から、これらの現象の数学的モデリングにおける最近30年にわたって得られた進歩に焦点を当てており、特に溶接金属の特性予測の能力に重点を置いている。それらのモデルはより経済的な溶接合金の開発につながるだけでなく、新しい発見を喚起させるものであり、それらの幾つかは既に商品化されている。

1. Introduction

It is often said that a welded joint covers the entire field of metallurgy and all states of matter. Here we focus on the *weld deposit*, which is the additional metal added to a welded joint in order to make it integral. There are few aspects of welding that can be treated in isolation, but the deposit is the part that is clearly separated from the rest of the assembly by the fusion surface. Consequently, its metallurgy can be treated somewhat independently, particularly with respect to the development of microstructure in the solid-state. We shall see nevertheless that this microstructure can have long-range consequences on the entire engineering assembly.

This paper is about the numerical modelling of weld deposits once solidification is complete. As in all technology, the problem is complicated and has to be faced at a level consistent with the technological goals. The ordinary method of science can fail in these circumstances whereas modelling is a pragmatic approach appropriate to the technology. The two procedures are contrasted in Fig. 1 and described in detail elsewhere¹ -the main point is that it is necessary to combine a large variety of techniques and methods of approximation, as will be evident in the discussion that follows.

A good deal of effort has, over the last 16 years, been spent on systematically archiving detailed reviews in the famous Graz symposia on the numerical modelling of weld

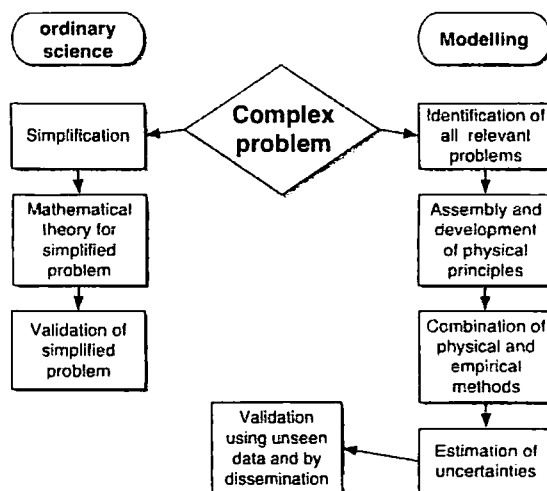


Fig. 1 The defining qualities of a model, compared with the conventional scientific method. Modelling has a greater focus on the original technological goal.

phenomena, resulting in eight published volumes containing both the detail and essence of the methods. For brevity, the present review makes liberal reference to these tomes. We begin by considering the most common welding alloys and then continue with the science which is not yet mature.

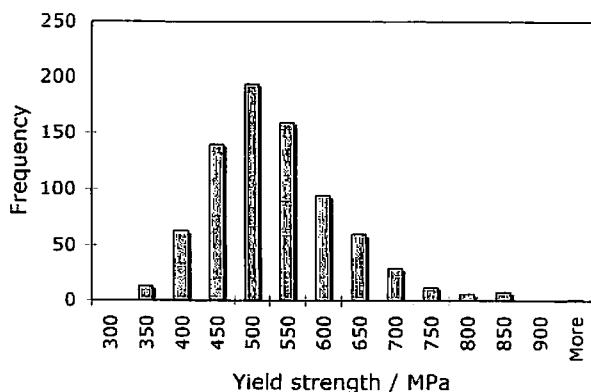
2. Common Welding Alloys

Solute additions to the vast majority of weld metals must be kept at a minimum to avoid the risk of brittle fracture.

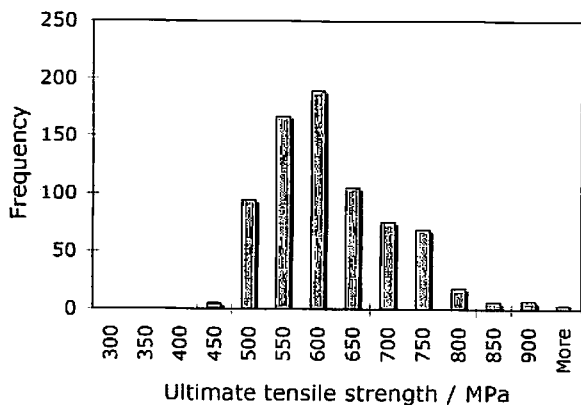
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Their yield strengths therefore usually lie in the range 350-550 MPa, with occasional higher values achieved at the expense of toughness, Fig. 2.

The microstructure of such weld metals consists of mixtures of allotriomorphic ferrite (α), Widmanstätten ferrite (α_w), acicular ferrite (α_a) and the so-called microphases (small quantities of retained austenite and martensite)². Allotriomorphic ferrite is weak, and Widmanstätten ferrite suffers from poor toughness. This leaves acicular ferrite as a good strengthener which also has the ability to frequently deflect cracks; its fraction in the microstructure should therefore be as large as possible. The techniques for calculating the microstructure are now well-established and comprehensively reviewed¹⁻⁷. The basic method is based on thermodynamics, nucleation and growth kinetics and overall transformation kinetics (Fig. 3a), with some accounting for the formation of inclusions^{8, 9}. The heat-flow models for representing the actual process vary from empirical¹⁰ to a full treatment of heat and fluid flow¹¹. The underlying theory is based on the atomic mechanisms of phase transformations as reviewed in^{12, 13}. There are of course, other interpretations of the mechanisms of transformations in welds

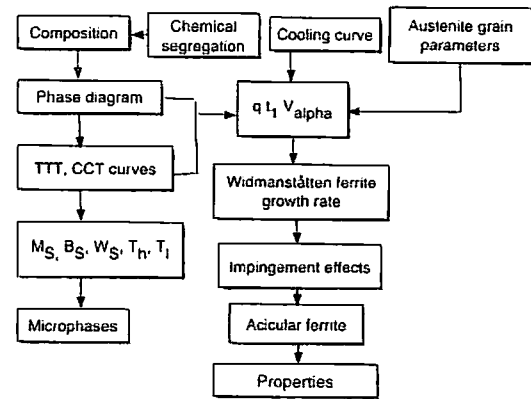


(a)

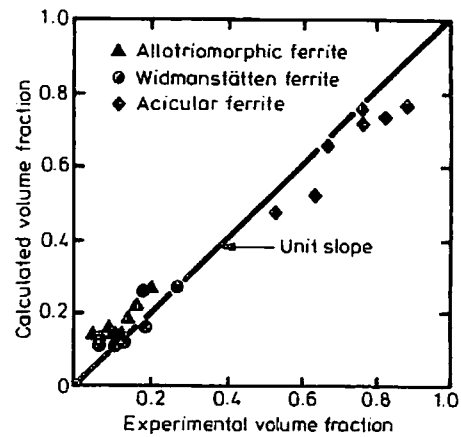


(b)

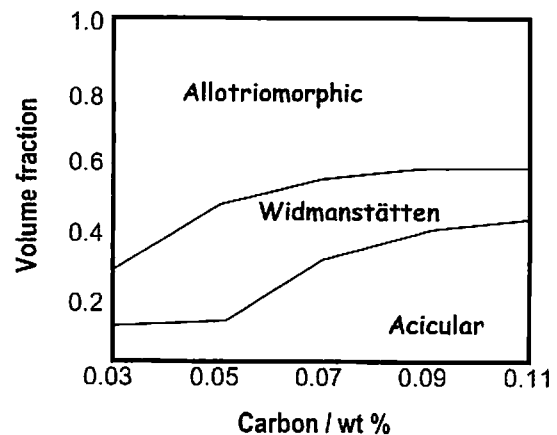
Fig. 2 Distribution of strength in ferritic steel weld metals. (a) Yield strength, 779 welds. (b) Ultimate tensile strength, 734 welds. Data from²⁵.



(a)



(b)



(c)

Fig. 3 (a) Flow chart illustrating the steps in the calculation of weld microstructure². TTT and CCT stand for time-temperature-transformation and continuous cooling transformation diagrams. q is related to the thickness of α layers. M_s , B_s and W_s to martensite, bainite and Widmanstätten ferrite-start temperatures. T_h and T_l are the start and finish temperatures for allotriomorphic ferrite. (b) An illustration of the agreement between the calculated and measured microstructures of arc-welds. (c) An example calculation taking account of C, Mn, Si, Ni, Mo, Cr, V, N, O, B, Al, Ti, current, voltage, speed, preheat and austenite grain size.

particularly regarding the nature of acicular ferrite^{14, 15}, but these are qualitative and cannot be used in predictive models, nor have they been established from a fundamental point of view.

The method³ has been used particularly in the design of arc-welding consumables in industry, laser welds using fillers¹⁶ and has even been reproduced at TWI¹⁷. It is illustrated in Fig. 3b, c.

It is possible to deduce some elementary mechanical properties directly from a description of the microstructure¹⁸. The total strength of a single-pass weld consists of contributions from the intrinsic strength of pure iron, solid solution strengthening and microstructural contributions (grain dimensions, defects) from the variety of phases. The method makes use of standard deformation theory but

frankly, in terms of the required accuracy, is only capable of giving a good estimate of the yield strength. Plasticity, elongation, the ultimate tensile strength, fatigue, creep or any complex property cannot be calculated in this way. There is no theory which has the rigour or sophistication to handle the large number of variables which are known to control such properties.

The conventional way to deal with this difficulty is regression analysis in which experimental data are best-fitted to some function which is usually linear. Very many such relations can be found in the literature, for example¹⁹⁻²³. A better approach is a neural network¹⁸:

- * there is no need to specify a function to which the data are to be fitted. The function is an outcome of the process of creating a network;
- * the network is able to capture of almost arbitrarily non-linear relationships (Fig. 4);
- * with Bayesian methods, it is possible to estimate the uncertainty of extrapolation.

Robust neural network models of the mechanical properties of weld metals^{24, 25} have been incredibly successful in avoiding experiments in the design of new materials, well outside of the range of data included in the creation of the models. One example is a weld metal for fire-resistant steels, invented without any prior experiments²⁶. Another is the tough high-nickel alloys^{24, 31}. Many of the models are freely available on MAP³².

3. Strength: Unconventional Microstructures

As described previously, there are many components to strength. The microstructural component is only 27 MPa when the fraction of allotriomorphic ferrite is $V_{\alpha} = 1$, 486 MPa when $V_{\alpha w} = 1$ and 406 MPa when $V_{\alpha s} = 1$. Since the intrinsic strength of pure iron is about 220 MPa at ambient temperature, and since the ability to solid solution strengthen is limited by hardenability considerations, it is not surprising that the vast majority of welds based on these microstructures have strength in the range quoted above. Fig. 2 shows that there are few alloys which exceed a yield strength of 800 MPa. The term "high-strength" is therefore reserved for welds whose yield strength exceeds 800 MPa.

To achieve even greater strength, it is necessary to suppress transformations to lower temperatures. This induces greater nucleation rates and leads to a refinement of microstructure. It also becomes possible to obtain phases such as lower bainite and martensite. Martensite is traditionally avoided because of its association with poor toughness in welds, but it should be recognised that not all martensite is brittle even in the untempered form. Instead,

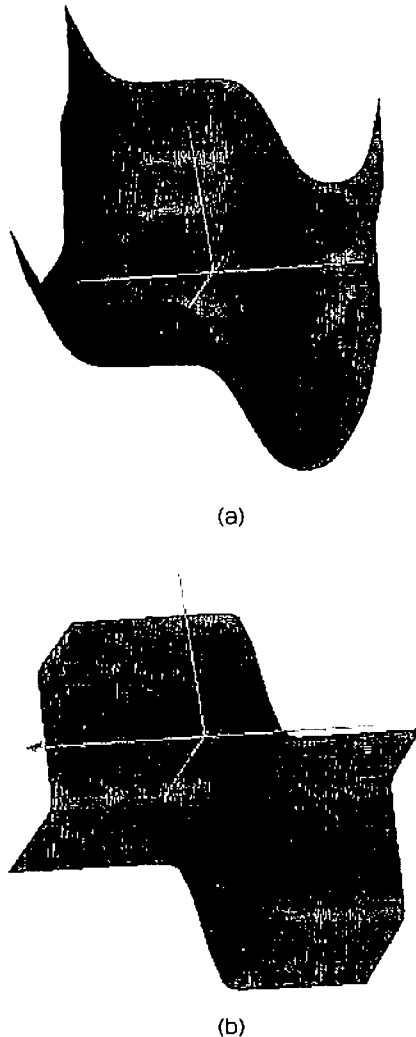


Fig. 4 An illustration of the complexity of the function (of two inputs) that can be created using a simple neural network with just four hidden units. The two figures are generated from the same mathematical function but different weights (w): $y = \tanh |wx_1 - 2| + \tanh |x_1^2 - 2| + \tanh |wx_2 + 2| + \tanh |z_2^2 - w| + 1$

we shall see that embrittlement is more to do with poor alloy design so martensite need not be avoided in an effort to make stronger weld metals. Consider the classic case of welding alloys used in the manufacture of submarines which have high-strength tempered martensitic hulls. These typically have the composition Fe-0.05C-2Mn-0.3Si-0.45Cr-3Ni-0.6Mo wt% with a microstructure that is a mixture of bainite and martensite^{2, 39}. The carbon concentration is kept low, at a value not much greater than the maximum solubility in ferrite. Although the concentration exceeds the solubility, it is well known that excess carbon is trapped at defects in the bainite and martensite, to such an extent that the effective solubility is almost the same as the total concentration³⁹. It is possible in these circum-

stances, to completely avoid cementite precipitation²⁵. To summarise, low-carbon martensite need not be brittle—indeed, commercial welding alloys of the type described above are strong (yield 800-1000 MPa) and tough (60-70 J at -60°C).

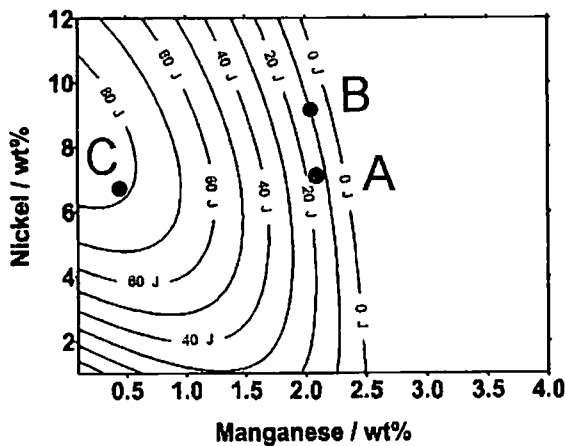
Unsuccessful attempts have been made^{36, 37} to go beyond these properties, by increasing the nickel concentration, based partly on the prevailing opinion that the addition of nickel to ferrite leads to an improvement in the toughness.

The problem was resolved when it was realised through mathematical models^{31, 38} that nickel is only effective in increasing toughness when the manganese concentration is small. This is illustrated in Fig. 5, where the contour plot shows the impact energy at -60°C for welds A (7Ni-2Mn), B (9Ni-2Mn) and C (7Ni-0.5Mn); the details are described elsewhere^{31, 38, 39}. Experiments validated the predictions so detailed studies were commenced to understand the mechanism of the Ni-Mn phenomenon.

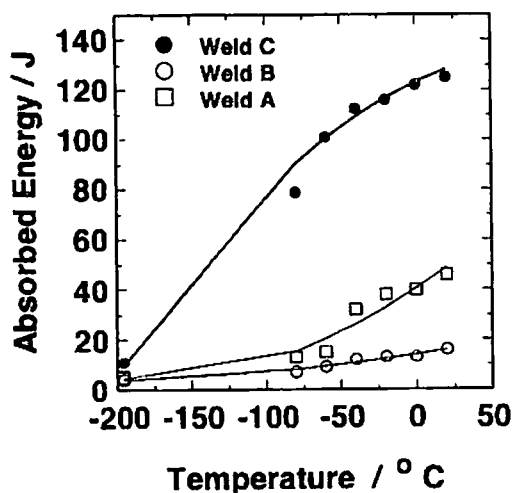
4. Coalesced Bainite

The mechanism by which a combination of high manganese and nickel concentrations leads to a deterioration in strength has been studied in detail by Keehan and co-workers^{40, 42}. It appears that when the transformation temperatures are sufficiently suppressed, leaving a narrow gap between the bainite and martensite-start temperatures, a coarse phase labelled *coalesced bainite* forms.

Coalesced bainite occurs when adjacent small platelets of bainite ("sub-units") merge to form a single, larger platelet⁴³. This striking change in form occurs at large undercoolings. Since adjacent sub-units of bainite have an identical crystallographic orientation, they may merge given sufficient driving force to sustain the greater strain energy associated with the coarser plate, and if there is nothing to stifle the lengthening of the sub-units⁴³. The first condition is satisfied by the large undercooling. The second implies that coalescence is only possible at the early stages in the transformation of austenite, when growth cannot be hindered by hard impingement with other regions of bainite.



(a)



(b)

Fig. 5 (a) Calculated contours showing the combined effect of manganese and nickel on the calculated toughness for -60°C, of weld metal produced using arc welding with a heat input of 1 kJmm⁻¹, with a base composition (wt%) 0.034 C, 0.25 Si, 0.008 S, 0.01 P, 0.5 Cr, 0.62 Mo, 0.011 V, 0.04 Cu, 0.038 O, 0.008 Ti, 0.025 N, and an interpass temperature of 250°C.

(b) The results of subsequent experiments for welds A, B, and C.

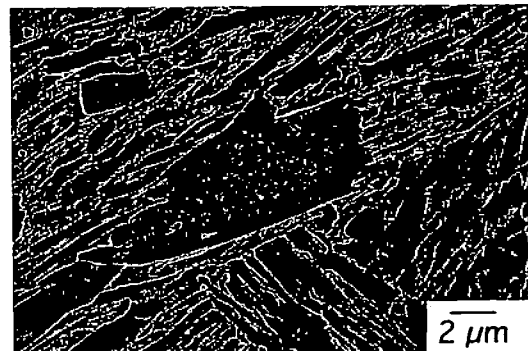


Fig. 6 Coalesced bainite in a 7Ni-2Mn wt% weld metal⁴⁰⁻⁴².

Experiments have now confirmed that the coarse, coalesced bainite appears in weld metals containing large concentrations of both manganese and nickel, such that the bainite forms at temperatures very close to the martensite-start temperature^{49, 49}. It leads to a deterioration in toughness and can be avoided by careful modifications of composition, for example, by reducing the manganese concentration when the nickel concentration is high.

5. Welding Alloys for Fatigue Resistance

Fatigue depends on many factors, one of the more important being the presence of residual stresses in the context of welded structures. Early work by Jones and Alberry⁴⁹ indicated that such stresses can be mitigated by compensating thermal contraction strains using transformation plasticity⁴⁹. Ohta *et al.*^{46, 50} designed a welding alloy with an exceptionally low transformation temperature (M_s), in which martensitic transformation in an unconstrained specimen starts at about 180°C and is just completed at ambient temperature (Table 1). By contrast, normal welding alloys have $M_s \approx 500 - 400^\circ\text{C}$. As illustrated in Fig. 7a, the net strain (ϵ) on cooling between M_s and ambient temperature is a contraction in the case of the high- M_s "conventional" alloy, whereas there is a net expansion for the new welding alloy. This results in a large residual tensile stress for the high- M_s sample and a compressive one for the low- M_s alloy (Fig. 7b).

When tests were done on welded sections, the structures joined using the low- M_s weld metal gave a much higher fatigue strength (Fig. 8). This improvement is attributed to the compressive residual stress which reduces the effective stress-range that the structure experiences during fatigue testing. The results are spectacular for engineering; benefits of the order illustrated in Fig. 8 will lead to radical changes in design and lifing philosophies for structural components. The achievement is based entirely on the fact that the reduction of the transformation temperature allows the shape deformation to compensate for the accumulated thermal contraction strains. The work done in Japan has recently been confirmed by Eckerlid *et al.*⁵¹ and Lixing *et al.*⁵².

Welding alloys used in civil constructions have to meet a range of requirements other than fatigue. Work is now

Table 1 The chemical compositions (wt.%), and measured M_s temperature of conventional and novel welding alloys. After Ohta *et al.*

Alloy	C/wt.%	Si	Mn	Ni	Mo	Cr	$M_s / ^\circ\text{C}$
Conventional	0.10	0.39	0.90	-	-	-	590
10Cr10Ni	0.025	0.32	0.70	0.10	0.13	10.0	180

needed to develop a system which gives a good portfolio of properties, such as strength, fatigue strength and toughness. Apart from this, the theoretical treatment usually adopted for transformation plasticity is rather weak, relying

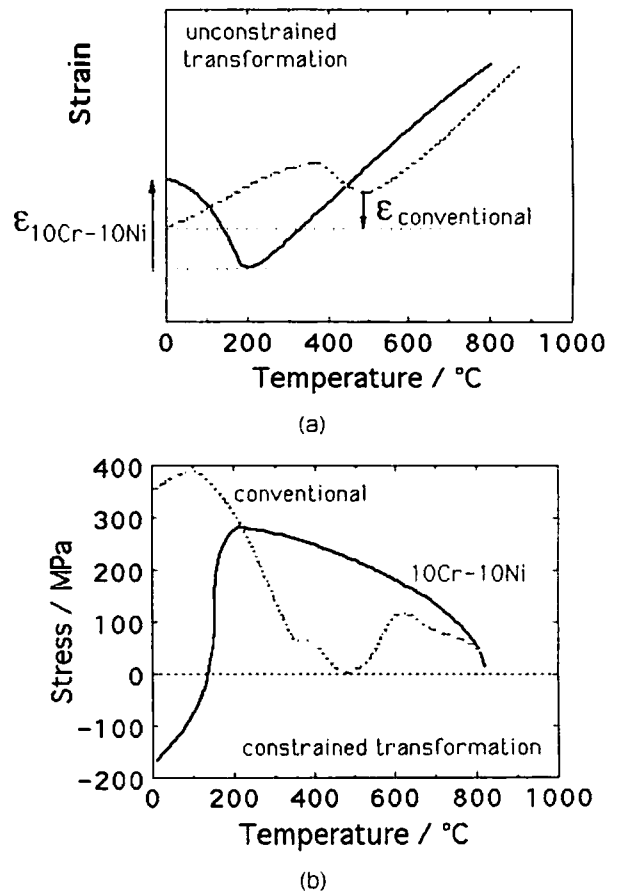


Fig. 7 (a) Transformation of weld metal during unconstrained cooling; (b) development of stress during constrained cooling. The chemical compositions of the alloys are given in Table 1. The low- M_s alloy is designated 10Cr10Ni in Table 1. After Ohta and co-workers.

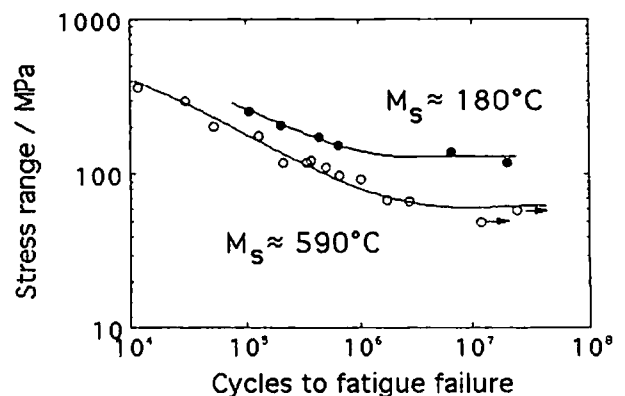


Fig. 8 Improvement in the fatigue performance of welded structure using a low transformation temperature welding alloy. After Ohta *et al.*

on the assumption that the transformation strain is an isotropic volume change. This is not appropriate for displacive transformations of the type that occur in high-strength weld deposits^{45, 53, 54}, where the shape strain due to the formation of bainite or martensite is very large, a shear of about 0.26 on the habit plane and a dilatational strain directed normal to the habit plane of about 0.03. It is necessary to use the proper transformation strain and the crystallographic theory to calculate the extent by which transformation plasticity is able to accommodate the stresses that develop due to constraint in welded joints. Such a theory should not only be able to predict the anisotropic transformation strains but also the crystallographic texture resulting from the development of a biased microstructure when those crystallographic variants which comply with the external stress are favoured. An advance has recently been made in this respect⁵⁵ which with further work, promises to be a useful approach for weld deposits designed to mitigate residual stresses.

The need for good theory is emphasised by the fact that the current low-transformation-temperature weld metals provide rather small transformation strains (0.01), largely because the degree of stress-induced bias in the microstructure is rather small. It has been demonstrated that the potential of transformation plasticity is much greater than this⁵⁶. The science needs to be developed to allow greater variant selection in the welding alloys.

6. Summary

Modern research has tended to emphasise fashions, for example the current trend for everything prefixed with the adjective *nano*. History tells us that many of these fashions are short-lived and fail to achieve the exaggerated claims made at their birth. I hope that in this review I have demonstrated that the mathematical modelling of steel weld deposits has lived up to expectations over some 30 years of continuous research. Furthermore, the methods are now routinely used in industry and academia alike, with novel products emerging as a result of predictions rather than accidents of research.

In this review, I have covered conventional weld metal microstructures consisting of allotriomorphic ferrite, Widmanstätten ferrite and acicular ferrite, together with associated properties. This is now a mature field with models which are sufficiently sophisticated and accurate to be applied across a broad range of requirements.

I have also covered two fields which are emerging, that of exceptionally strong weld metals dependent on bainitic and martensitic microstructures, and welding alloys designed to mitigate residual stresses. It would be appropriate to review these in another ten years time, perhaps in another special issue of the Proceedings of the Japan Welding Society.

7. Acknowledgments

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