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Modeling of fundamental phenomena in welds*

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Abstract. Recent advances in the mathematical modeling of fundamental phenomena in welds are summarized. State of the art mathematical models, advances in computational techniques, emerging high-performance computers, and experimental validation techniques have provided significant insight into the fundamental factors that control the development of the weldment. The current status and scientific issues in the areas of heat and fluid flow in welds, heat source–metal interaction, solidification microstructure, and phase transformations are assessed. Future research areas of major importance for understanding the fundamental phenomena in weld behavior are identified.

1. Introduction

Welding has evolved in the last few decades from almost an empirical art to an activity embodying the most advanced tools of various basic and applied sciences [1, 2]. Significant progress has been made in understanding the welding process and welded materials. The improved knowledge base has been useful in automation and process control. In view of the large number of variables involved, creating an adequately large experimental database to understand and control the welding process is expensive and time consuming, if not impractical. A recourse is to simulate welding processes through a set of mathematical equations representing the essential physical processes of welding. The results obtained from the phenomenological models depend crucially on the quality of the physical relations contained in the models and the trustworthiness of the input data.

In order to assess the current status of knowledge and to explore new and emerging opportunities for basic research, a Research Assistance Task Force was organized to review the progress in the US as well as in Asian and European programs. The *Research Assistance Task Force on Modeling for Welding Science* was held in Cocoa Beach, Florida, 16–19 March, 1993, under the auspices of the Materials Science Division of the Office of Basic Energy Sciences, US Department of Energy, and the Electric Power Research Institute (EPRI). A panel of 26 scientists (four from industry, 14 from universities, six from national laboratories, and two from DOE and NIST), including the cochairpersons T Zacharia,

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Table 1. Workshop participants.

Dr Lee A Bertram	Sandia National Laboratories
Dr Harshad K Bhadeshia	University of Cambridge
Dr John A Brooks	Sandia National Laboratories
Dr Joseph B Darby Jr	Department of Energy
Dr Stan A David	Oak Ridge National Laboratory
Professor T DebRoy	Pennsylvania State University
Dr John A Goldak	Carleton University
Dr Linda L Horton	Oak Ridge National Laboratory
Dr Jerry Jones	Colorado School of Mines
Mr Larry Jones	Massachusetts Institute of Technology
Professor Hugh W Kerr	Waterloo University
Professor Jyoti Mazumder	University of Illinois
Dr Kenichi Ohsasa	Hokkaido University
Dr Anand J Paul	Concurrent Technologies Corporation
Dr Tim Quinn	NIST
Dr B Radhakrishnan	University of Alabama, Birmingham
Professor Michel Rappaz	Ecole Polytechnique Federale de Lausanne
Dr Alan Sprague	University of Alabama, Birmingham
Professor Julian Szekely	Massachusetts Institute of Technology
Professor R G Thompson	University of Alabama, Birmingham
Mr Michael L Tims	Concurrent Technologies Corporation
Dr Ravi Vishnu	University of Lulea
Dr R Viswanathan	Electric Power Research Institute
Dr John M Vitek	Oak Ridge National Laboratory
Dr Thomas Zacharia	Oak Ridge National Laboratory

J M Vitek, and R Viswanathan, were involved in the Task Force. The international weld modeling community was represented with participants from five countries. See table 1 for a list of participants.

Four major areas of modeling were addressed: (i) heat and fluid flow; (ii) heat source–metal interactions; (iii) weld solidification microstructures; and (iv) phase transformations. There were no parallel sessions, and the participants had diverse interests and backgrounds in welding research. As a result, the problems and issues discussed were interdisciplinary in nature. The present status and future recommendations for research in these four areas were discussed under the guidance of session chairpersons: J A Goldak, T A DebRoy, M Rappaz, and H K D H Bhadeshia, respectively. The original suggestion for this Research Assistance Task Force by J B Darby Jr made the workshop, and this subsequent report, possible.

2. Heat and fluid flow

During welding, the development of the weld pool is determined by the arc–metal interaction, heat flow and fluid flow, the thermophysical properties of the material, and the associated boundary conditions. Understanding the development of the weld pool during welding is of considerable practical significance. Because of the complexity of the process and the presence of the arc plasma, direct experimental investigations are extremely expensive and often impossible. There have been a number of theoretical studies of welding in order to understand the underlying mechanism that controls the development of the weld bead and its properties [3–21]. The influence of heat flow and fluid flow and its effect on the weld pool shape are well documented [10–21]. Besides the information on weld pool shape and size, computational modeling of welding can provide detailed information on such

parameters as weld cooling rate, temperature gradient in the weld pool, and macroscopic growth rate.

Modeling of melting and solidification during welding provides a good example where rational descriptions of turbulence, multiphase flow, electromagnetic and surface tension flow, transient heat transfer, and evaporation can be used to characterize complex physical phenomena. Figure 1 shows a schematic of the welding process, indicating the various regions of interest. Initial attempts at studying the effects of heat flow in welding concentrated on the development of analytical solutions [3] or semiempirical expressions [4] for heat flow in the weldments. Rosenthal developed an analytical solution for moving heat sources and applied these solutions to arc welding operations [3]. Since then, there have been a number of attempts to study the effect of plate thickness on cooling rates, the temperature distribution in a plate of finite thickness, and the effect of cooling rate on the weld cross-sectional area. Even though these studies provided significant insight and had the advantage of simplicity, the applications of these solutions were fairly restrictive and could not be used for a generalized study of the welding operation.

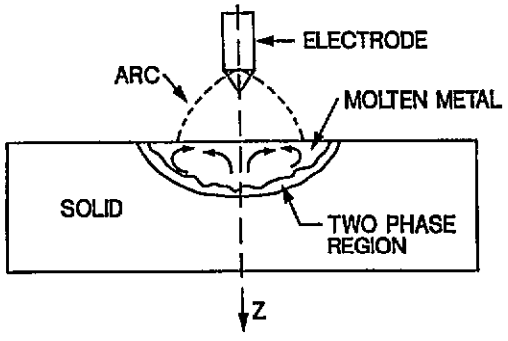

Figure 1. A schematic of the weld pool.

In the past decade, the capability of computing transient temperature, velocity, and pressure in weld pools has been developed [10–21]. This is done by solving the equations for the conservation of mass, momentum, and energy for appropriate boundary conditions. In the simplest case, if (i) the geometry of the weld pool is assumed, (ii) the velocity of the liquid on the liquid–solid boundary is assumed to be zero, (iii) the traction is assumed to be known on the liquid arc surface, (iv) the 'body' forces due to buoyancy and electromagnetic forces are assumed to be known, and (v) the viscosity is assumed to be known, then Navier–Stokes equations can be solved for sufficiently small Reynolds numbers. If (i) the thermal flux is known on the arc–liquid surface, (ii) the temperature is known on the liquid–solid boundary, and (iii) the thermal conductivity and specific heat are known for the liquid, then the energy equation can be solved to compute the temperature in the weld pool [3]. Figure 2 shows the convective flow in a stationary weld pool as a result of the complex interaction between the various driving forces. Depending on the welding conditions, the resulting convective flow can be a relatively simple recirculating flow, or a more complex flow with several convective cells operating in the weld pool.

As a result of these studies, important physical insight into the mechanism of weld pool development was achieved. These studies demonstrated that, in most cases, the fluid flow and heat transfer in the weld pool are controlled by the spatial variation of surface tension that exists on the weld pool surface. The spatial variation of surface tension causes the

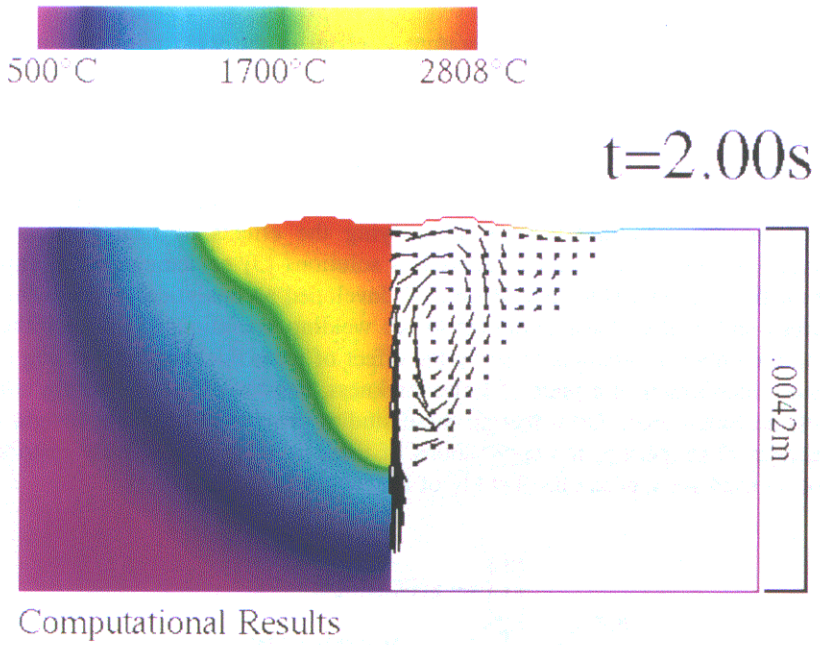

Figure 2. The calculated convective flow in the weld pool.

molten metal to be drawn along the surface from a region of lower surface tension to one of higher surface tension, resulting in large surface flows. For pure metals and alloys, the temperature dependence of surface tension ($d\gamma/dT$) is negative, causing outward flow at the surface. On the other hand, surface active elements such as sulfur can produce a positive $d\gamma/dT$, resulting in an inward flow.

The change in $d\gamma/dT$, from a positive value at low temperature to a negative value at high temperature, has important consequences on the weld pool fluid flow and heat transfer, and the ultimate development of the weld. Directly below the welding heat source, a hot zone exists where the temperature experienced by the molten weld metal is likely to be above the critical temperature, such that a negative $d\gamma/dT$ prevails in this region. This would cause two opposing surface tension gradients to exist on the weld pool surface: a positive surface tension gradient at the periphery of the weld pool, and a negative surface tension gradient at the center of the weld pool. Depending on the relative magnitude of these two driving forces, either a radially outward flow or a radially inward flow, or even a combination of both resulting in two opposing vortices, may develop.

Several studies have examined the detailed heat flow and fluid flow resulting from the surface tension gradient that exists on the weld pool surface [14–21]. These studies provide an improved understanding of the free surface effects and the surface tension gradient driven flow. The weld pool surface was treated as a free deformable surface. An improved understanding of the surface tension gradient effect was achieved by calculating $d\gamma/dT$ as a function of temperature and concentration of surface active elements. It was shown that, depending on the material composition and welding conditions, surface tension γ may go through an inflection point, initially increasing before decreasing with temperature.

Even though most of the numerical studies of welding concentrated on stationary spot

gas tungsten arc (GTA) welding, there have been some notable works on moving arc welds. The work of Kou and Wang [14], Friedman [5], Kraus [16], and Zacharia *et al* [17] are some examples of previous work on non-stationary heat sources. All of these studies have overlooked some factors that are important for accurate modeling of weld development.

2.1. Outstanding problems

It has been argued that the flow in a weld pool is turbulent. If the flow is turbulent, then turbulence models will have to be developed for weld pools. Since this will be a critical issue, it will be important to demonstrate whether or not the flow is turbulent. If it exists, then the turbulence must be characterized in order to develop models for the effective viscosity and thermal conductivity.

The traction due to the gradient in the surface tension, the Marangoni effect, drives the flow in the weld pool. There is a need to determine whether the gradient in the velocity field normal to the surface is adequately resolved by current models. For example, does a fine-scale vortex structure exist near the surface layer and is it turbulent?

Progress is being made on the more difficult problem of predicting the weld shape. The free surface between the weld pool and the arc strongly couples these two domains. In many industrial welds, the deformation of the surface is large, and current models do not adequately deal with the coupling between the arc and the weld pool. The fluid flow near the junction between the liquid pool, the solid, and the vapor should be looked at more carefully.

The convection of nuclei and equiaxed grains within the weld pool is not adequately analyzed with current models. Since an equiaxed grain structure in the fusion zone can improve the mechanical properties of welds, the mechanism of microstructural evolution is an important issue. Useful progress could be achieved in this area in the near future.

Most current weld pool heat and fluid flow models ignore the geometric structure of the liquid–solid boundary caused by solidification, i.e., the formation of columnar grains or dendrites. Clearly, the casting community is studying this problem in detail, and the welding community should build on the knowledge that they develop. In the mushy zone, the volume change on solidification can cause a flow. This is expected to be most important at the root of dendrites. It could influence microsegregation. There is a need to develop numerical methods for those cases where the coupling of flow in the mushy region and the weld pool is significant.

The energy equation can be solved to compute the transient temperature in the solid region with useful accuracy if (i) the liquid–solid interface position and the temperature at the interface are known, (ii) a convection–radiation coefficient is known for the rest of the boundary, (iii) the thermal conductivity and specific heat are known (possibly as a function of temperature), and (iv) the initial temperature is known. Since the thermal conductivity varies with microstructure, there is a need to develop models of thermal conductivity as a function of microstructure. Although the latent heat of most solid state transformations is not large, to include latent heat in the thermal analysis would provide a small increase in accuracy. This could be done easily if the microstructure model can compute the rate of phase transformations.

In the past decade, considerable progress has been made on the computation of stress distribution in the solid region. The models usually assume an elastoplastic, stress–strain relationship that can be a function of temperature and strain hardening. They usually ignore the high-temperature strain rate dependence and creep. There is a need to develop models of the stress–strain relationship that are functions of the microstructure. Developments in microstructure modeling make this a feasible research goal. This is particularly important

since the material properties can vary rapidly in the HAZ. Without accurate stress–strain relationships, accurate stress analysis will not be possible.

The continuum mechanics analyses assume that sufficiently smooth density functions such as temperature, stress, strain, displacement, and density exist. As the spatial scale is reduced towards the scale of the microstructure, the validity of this assumption must be considered more carefully. For example, in transformation plasticity, current models assume the grains are randomly oriented. They consider only the volume component of the phase transformation and they assume the length scale is sufficiently large that the effects of shear in the phase transformation can be ignored. Continuum mechanics models also ignore effects of texture. The fusion zone of welds can be strongly textured [22], which could have a strong effect on both the plastic and elastic behavior of welds and must be considered in the modeling of stresses in welds.

Many of the numerical simulations described above are computationally intensive despite the simplicity of the models considered. Even on current supercomputers, some relatively small problems can be intractable. For example, to accurately simulate the heat transfer in a 1 m^3 block using a simple computational method requires 10^{12} arithmetic operations per second of simulated time. For a computer to do the simulation in real time would require a sustained computation rate 1000 times faster than that achievable by current supercomputers. Massively parallel computer systems, which combine several thousand processors able to operate concurrently on a problem, are expected to provide orders of magnitude increases in performance. Calculations of heat and fluid flow, stress analysis, and microstructural evolution [23] have been performed on massively parallel computers with very encouraging results. Massively parallel computers provide exciting new opportunities for weld process modeling in areas such as the interaction between arc plasma and molten metal, resolution of fluid flow along the interface layers, fully coupled macro–microscopic modeling, modeling of residual stresses, and damage prediction/modeling.

3. Heat source–metal interaction

Heat source–metal interaction affects heat and mass transfer, fluid flow, and, consequently, the structure and properties of the weld pool. Several interesting physical phenomena take place at and above the weld pool surface. These include transmission of power through the medium containing gas plasma, metal vapors, and solid and liquid particles. Often, intense vaporization of the alloying elements takes place at the surface. Inside the weld pool, the weld metal undergoes vigorous circulation, driven by Marangoni, electromagnetic, and buoyancy forces. Hydrogen, nitrogen, and oxygen are partitioned between the weld metal and its surroundings. The deformation of the 'free' weld pool surface, the presence of charged particles close to the surface, and the presence of a strong temperature gradient make the nature of the liquid metal surface significantly different from the metal surfaces commonly encountered in conventional high-temperature metals processing.

Crucial problems and issues related to heat source–metal interactions were addressed in the second session of the workshop. The discussion focused on the progress made, important research needs, and the questions and issues related to heat source–metal interaction. The need for an improved fundamental understanding in the following areas was discussed.

3.1. Methodologies to determine the energy reaching the surface of the weld pool

Of the various factors that affect the pool size and shape, the energy distribution on the weld pool surface is perhaps most important. In arc welding, the geometry of the electrode,

its distance from the weld pool surface, and the deformation of the surface affect the energy distribution. In laser welding, the attenuation of beam energy by the plasma significantly affects the amount of energy reaching the weld pool surface [24, 25]. Furthermore, the beam energy is scattered by the particles of condensed matter near the weld pool surface. For laser beam welding, the attenuation of the beam energy due to electron–photon interaction has been studied [24, 25], and a reasonable understanding exists for the estimation of the energy loss. However, the energy loss due to scattering by liquid or solid particles is difficult to estimate.

3.2. The geometry of the 'free' weld pool surface

Deformation of the free surface has been recognized as an important parameter that controls the energy reaching the surface. Since the solidified surface of the weld pool does not provide an accurate description of the free surface deformation during welding, both numerical calculations [18–20, 26, 27] and experimental work [28] have been adapted to understand the nature of the weld pool surface. The results of both the experimental and the theoretical work indicate that the deformation of the free surface geometry depends on the welding process, the welded material, and the variables used. Furthermore, the surface is often pulsating in nature. No straightforward, simple model exists that can predict the deformation of the weld pool free surface for a given set of conditions.

3.3. An improved understanding of metal vaporization

In the recent past, there has been a growing recognition that the vaporization of alloying elements can significantly change the composition of the weld metal and the weld properties, and it is a major problem in the welding of many important engineering alloys. Furthermore, the vaporization of toxic elements from the weld pool affects workplace safety. Significant progress has been made in understanding the alloying element vaporization rates during welding through experiments [29–33] and modeling [34–37]. As a result, it is now possible to calculate vaporization rates (figure 3) in systems where the rates are not affected, in a major way, by the presence of a plasma. The role of the welding plasma on alloying element vaporization rate is not well understood.

3.4. Laws governing the partitioning of hydrogen, nitrogen, and oxygen between the weld pool and its environment

The dissolution of nitrogen, oxygen, and hydrogen in the weld pool affects weldment properties. When a metal is exposed to a pure diatomic gas such as hydrogen, the equilibrium concentration of the species in the metal is proportional to the square root of its partial pressure at any given temperature. This relation, known as Sievert's law, is widely used for the calculation of solute concentrations in metals in equilibrium with diatomic gases. However, such estimations are not useful for most welding processes. Near the weld pool surface, besides common diatomic molecules, excited molecules, atoms, and ions are also present within the gas plasma. As a result, the interstitial concentrations in the weld metal are significantly higher than those calculated from Sievert's law [38–43]. The presence of excited neutral atoms, ions, and electrons [44, 45] precludes any simple extension of the well established formal treatment of gas–metal systems to welding. A general principle for understanding the partitioning of nitrogen, oxygen, and hydrogen between the weld pool and its environment remains to be developed [46]. Apart from the improved fundamental understanding of the dissolution process, such a principle can serve as a basis for science based control of weld metal composition and properties.

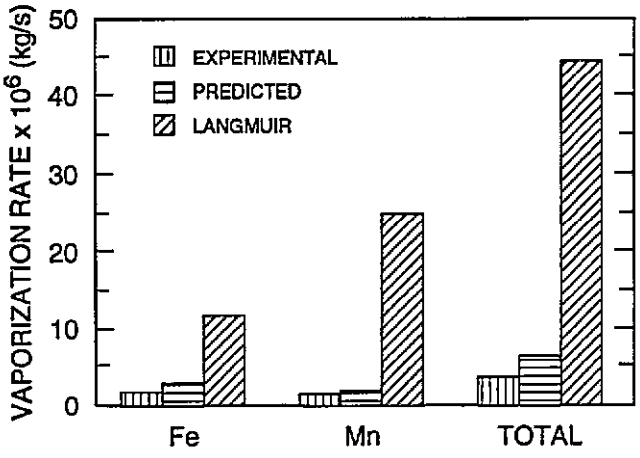

Figure 3. Using the equations of conservation of mass, energy, and momentum in both the gas phase and in the liquid weld pool, the vaporization rates of the alloying elements can be accurately determined. Simple calculations using the Langmuir equation predict high values of vaporization rates. (After [37].)

3.5. Thermophysical and other data relevant to welding

A database of high-temperature materials processing was developed, to a large extent, to understand the manufacture and the subsequent processing or use of metals and alloys. Unlike welding, these operations are carried out at temperatures close to the melting points of the metals. Furthermore, in most thermomechanical processing, the processing environment does not contain a plasma. In contrast, in many welding operations, the peak temperature in the weld pool can be very close to the boiling point of the metal and the weld metal is surrounded by a plasma. Thermophysical data for such high-temperature systems are scarce, if available at all. Thus, an in depth understanding of the behavior of the welding process through modeling is often impeded by the lack of appropriate thermophysical data [47].

3.6. The role of plasma

Since a gas plasma often surrounds the metal during high-energy-density beam processing, the chemical nature of the metal surface is significantly different from that of most other metallic surfaces commonly encountered in the extraction and refining processes. This difference can lead to a lowering of both the interfacial tension [48] of metals and alloys and the vaporization rates of the metallic constituents of the alloys [33] in plasma environments. The transformation of ordinary molecular species to excited neutral atoms and ions in the plasma leads to significant differences in reactivity and enhanced solubility of various species in the metals (figure 4). The uniqueness and complexity of the physicochemical phenomena in welding, and especially the presence of plasma, often preclude meaningful straightforward application of the knowledge of other materials processing operations to understand welding.

3.7. Modeling for control

On a more practical side, several broad issues related to modeling for control were discussed. The implementation of adaptive control in welding would involve sensing and control of

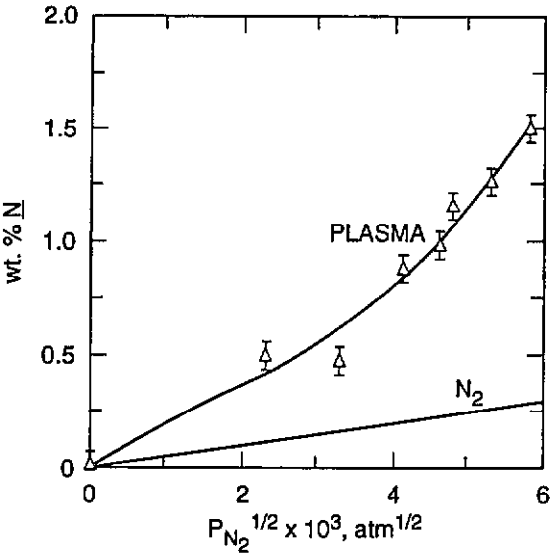

Figure 4. Enhanced solubility of nitrogen in niobium at 2243 K in low-pressure plasma. In pure diatomic nitrogen, nitrogen solubility obeys Sieverts' law. However, in a plasma environment containing molecular, atomic, and ionic nitrogen, the solubility is significantly higher than that in pure diatomic nitrogen. (After [43].)

the heat source position, weld pool temperature, weld penetration, defect formation, and, ultimately, control of microstructure and properties [22]. Some examples of intelligent control include the developments of a connectionist fuzzy logic system for welding control [49] and multioutput process dynamics [50]. It was pointed out that several process and subprocess models are now available for the control of electrode feed [51–55], and for determining the properties of the welds [56]. The available process models include distributed parameter models, lumped parameter models with some physical insight, and process models with linear systems or neural networks. In particular, applications of the neural networks were discussed [57]. It was felt that process models need to be developed further since these models are primary candidates for technology transfer to improve the quality and productivity of welding operations. Most of the comprehensive phenomenological process models require extensive computer time and cannot be used for real time applications. However, large models can be used to calibrate the computationally simpler real time control models. Appropriate reduction of the essence of phenomenological models to help in the development of the process control models through appropriate collaboration was stressed.

4. Weld solidification microstructure

Microstructures that develop in the fusion zone of the weld depend strongly upon the shape of the melt pool and can ultimately influence any solid state transformations that may subsequently occur during cooling. They also play a major role in defect formation such as microporosity or hot cracking. In this sense, they are an important step in any welding process prediction. The fundamental aspects associated with solidification microstructures are many: heterogeneous nucleation of grains in the bulk of the liquid, epitaxial growth

of columnar grains from the mushy zone, the growth selection process, growth kinetics, preferential growth directions of dendrites, microsegregation, coarsening, and competition between phases and/or between growth morphologies. All of these are intimately related to the alloy being investigated and, more specifically, to its phase diagram. Diffusion of solute elements in the liquid and solid phases, capillarity, and attachment kinetics are also important phenomena. In order to determine within the fusion zone the volume fractions of stable and metastable phases, the grain structure, the microstructural features (primary and secondary dendrite arm spacings, eutectic spacing), the local inhomogeneities of solute concentration, etc, it is essential to couple all of these microscopic phenomena with the thermal history of the weldment.

The solidification theories and models developed for rapid solidification processes (atomization, melt spinning, laser treatment, etc) have improved considerably over the last decade. They are becoming of great value for welding. Four contributions related to solidification microstructures in welding have been presented at this workshop: one was related to microsegregation, and the others dealt with grain structure formation.

4.1. Nucleation

The formation of equiaxed grains in the bulk of the liquid is desirable for the final mechanical properties of the weld since it decreases both the anisotropy associated with columnar grains and the segregation in the centre line plane [58]. Equiaxed grains can form according to two different mechanisms: they can nucleate on foreign substrates (heterogeneous nucleation in the bulk of the liquid or at a free, oxidized surface) or they can start to grow from fragments of dendrites detached by convection. With the first mechanism, the addition of an inoculant, such as TiB_2 for aluminium alloys or TiN for stainless steel, can promote equiaxed grain nucleation, as shown in figure 5.

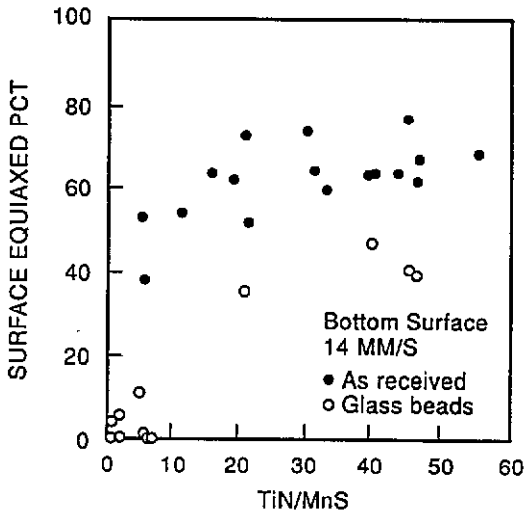

Figure 5. The fraction of equiaxed grains formed in a stainless steel weld as a function of the relative amount of TiN versus MnS. (After [58].)

The theory of heterogeneous nucleation on a foreign substrate has been developed by Turnbull [59]. However, it is difficult to apply to engineering alloys for several reasons

[60]. Therefore, the modeling of equiaxed solidification microstructures usually relies on a nucleation site density, rather than a nucleation rate, whose parameters must be determined from experimental observations. Similar remarks apply to heterogeneous nucleation, which might occur at a boundary such as the mold surface of a casting or the free, oxidized surface of the weld pool.

Although the problem of heterogeneous nucleation is greatly reduced in welding, due to the epitaxial growth at the fusion line, there are, nevertheless, several issues which need to be addressed in the future. In particular, the effect of convection on promoting the formation of nuclei by dendrite fragmentation is an open issue [61].

4.2. Growth kinetics

The theories of dendrite and eutectic solidification are now rather well established and are applied in the modeling of casting and welding processes [62]. Although these theories were first developed for the growth of binary alloys at low solidification rate, they have been recently extended to multicomponent systems [63, 64] and to rapid solidification conditions [65, 66]. Such theories enable us to predict the undercooling at which the eutectic interface or the dendrite tips are growing, the spacing of the eutectic lamellae, and the radius of curvature of the dendrite tips. This later value is not of paramount importance *per se* since the final secondary dendrite arm spacing is dictated by Ostwald ripening [67] and the primary trunk spacing is a geometric mean between the dendrite tip radius and a thermal length [68] (i.e., a length given by the ratio $\Delta T_0/G$, where ΔT_0 is the solidification interval of the alloy and G is the average thermal gradient across the mushy region). Nevertheless, growth kinetics models are essential to predict the competition between dendritic and eutectic growth (coupled zone) [69] or between columnar and equiaxed microstructures, i.e., columnar to equiaxed transition (CET) [70], or between different phases [63]. A good example of phase competition is provided by the solidification of Fe–Ni–Cr alloys, whose primary solidification into ferrite or austenite has been shown to be dependent upon the growth rate [63]. At the relatively high growth rates encountered in welding, especially with lasers, the growth kinetics of the dendrite tips can also account for the increased solute concentration measured at the cell cores [71–74]. As an example, figure 6 shows the concentration profile of copper measured along a line in an Al–1.1% Cu electron beam welded specimen [74]. The minimum concentration in this profile, which is measured near the center of the cells, is already above the value predicted from the equilibrium phase diagram, and is indicative of significant undercooling during solidification.

4.3. The preferential growth direction of dendrites

In situ observations of the solidification of organic transparent analogs [75] and metallography observations of metallic alloys [76] clearly show that dendrites preferentially grow along ⟨100⟩ crystallographic directions. The epitaxial growth of dendrites during welding of austenitic Fe–Ni–Cr single crystals provides a very good example of this growth anisotropy, as shown in figure 7 [64]. The preferential growth directions of dendrites have a direct influence on the branching mechanisms of dendrite arms and are the basic mechanism by which grains are selected in any solidification process.

4.4. Microsegregation and the phase diagram

The access to calculated multicomponent phase diagrams is now made easier thanks to the development of large software packages [77] and to international cooperation. Using such programs, the liquidus and the solidus surfaces of a multicomponent alloy can be

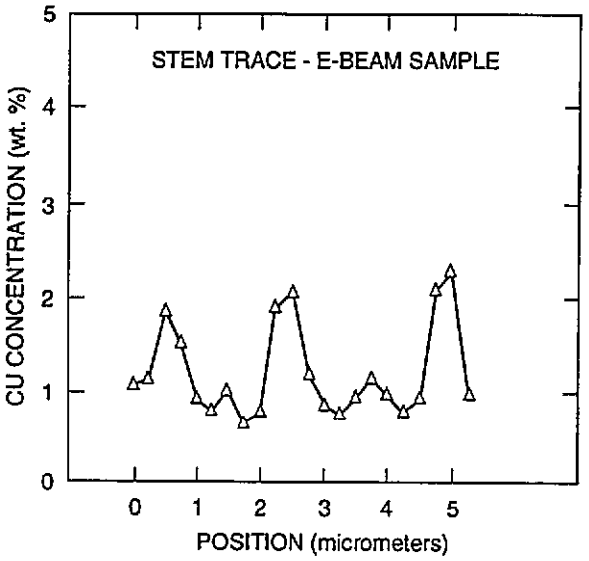

Figure 6. The concentration profile measured along a line in an Al–1.1% Cu electron beam welded specimen (welding speed 3.2 cm s^{-1}). (After [74].)

computed for the primary solidification range. This input is needed in order to calculate the partitioning of the various solute species and the solidification path of the alloy (i.e., the relationship between the volume fraction of solid and the temperature). Most of the existing microsegregation models use the approximation that, on a local scale, solute is completely mixed with the liquid phase whereas some solute diffusion might occur in the solid [62]. The backdiffusion problem, originally derived by Brody and Flemings [78], for a parabolic growth law, has recently been solved analytically [79]. Several numerical solutions have also been developed in order to take into account the coarsening of the dendrite arms, multicomponent alloys, non-constant solute diffusion coefficients, and a non-parabolic growth law [80, 81].

The major limitation of all of these models is that they consider backdiffusion in one dimension only. Therefore, it is a crucial point to decide whether such calculations should be performed with the primary or the secondary spacings. (The first situation would apply to cellular structures, whereas the second one is relevant for dendritic solidification.) Another difficulty arises at high solidification rates since these models neglect any undercooling associated with solute diffusion in the liquid (i.e., any undercooling of the dendrite/cell tips, see figure 6). When predicting solute concentration profiles, it is important to account for backdiffusion and solid state transformations that might occur after solidification has been completed. This is particularly true for the case of steel, for which the austenite–ferrite transformation plays a major role [81].

4.5. Phenomena at high solidification rates

As mentioned earlier, important deviations may occur at high solidification rates [82]. With the solutal undercooling increasing with velocity, the concentration in the central part of the dendrite will deviate from the value expected from the phase diagram. Other effects may also become important: curvature effects, solute trapping, kinetics of atom attachment, temperature dependence of the diffusion coefficient, etc. Since the first

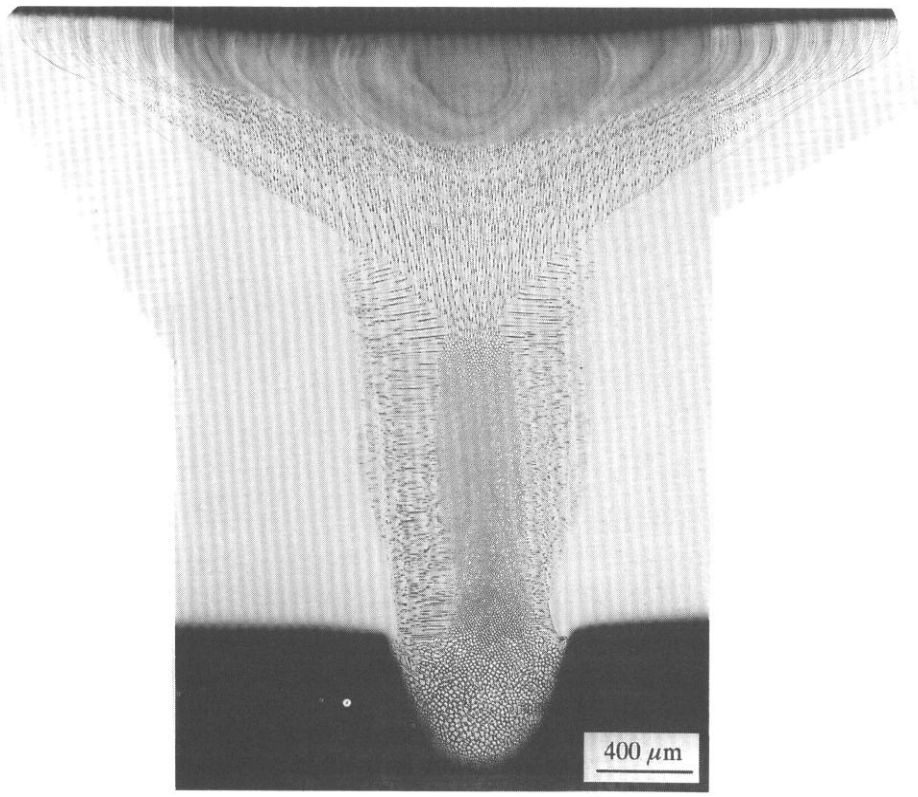

Figure 7. A transverse section micrograph of an Fe–15% Ni–15% Cr austenitic single crystal autogenously electron beam welded. The top surface is (001) and the weld was made along a [100] direction. As can be seen from their appearance, the dendrite trunks can grow along the [100], [010], or [001] crystallographic directions. The transitions between these various dendrite morphologies have been analyzed in terms of the weld pool shape, preferential growth directions and minimum undercooling of the dendrites. (After [64].)

prediction of the absolute stability limit by Mullins and Sekerka [83], it has been shown that a microsegregation free planar front structure can indeed be produced at high solidification rates [71, 73, 82]. Before reaching such a limit, new microstructures or phases can form. Among these, band structures have been observed for both hypo-eutectic and eutectic alloy compositions [71, 73]. It has also been observed that, at the large growth rate encountered in laser remelting, equiaxed grains could form ahead of the undercooled columnar front of Al–Si hypereutectic alloys [84] (see figure 8). The shape of these 'equiaxed' grains (i.e., formed by nucleation in the bulk of the liquid), which is more elongated in the transverse direction of the heat source, has been explained recently [85]. Rapid solidification of hypereutectic Al–Be alloys results in the formation of ultrafine Be particles. A model of the macroscopically steady state but microscopically oscillatory motion of the solidification front has been proposed [86].

4.6. Modeling of grain structure formation

Over the last few years, probabilistic modeling of grain structures has emerged in the field of castings [87–91]. Such techniques are very valuable since they allow for direct

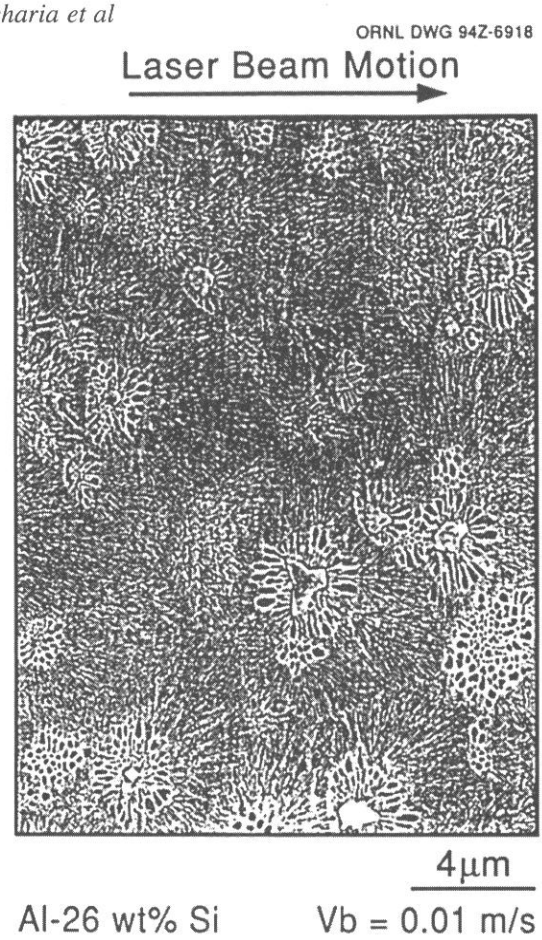

Figure 8. The equiaxed grain structure of a laser treated Al–26 wt% Si specimen showing fine primary silicon crystals surrounded by α-Al cells/dendrites and the eutectic matrix. The specimen was treated at $v_b = 500$ mm s^{-1}. (After [84].)

visualization of grain structure and prediction of the extension of the columnar zone, the impingement of the equiaxed grains, and the CET. The models [87–89] were based on Monte Carlo techniques, which were originally developed for grain growth and recrystallization (Potts model) [92]. They lacked a sound physical background since they did not consider specifically the growth kinetics of dendrites or eutectics and the preferential ⟨100⟩ growth directions of the dendrite trunks. More recently, cellular automata techniques have been able to include such physical mechanisms [90, 91]. A coupling of such models with finite-element heat flow calculations can then predict grain structures in realistic situations [93, 94]. As an example, in figure 9, the grain structure observed in an Al–7% Si ingot, which has been directionally solidified against a copper chill, is compared with the grain structure computed with a coupled finite-element–cellular automata technique [93]. Although the cellular algorithm is still two dimensional, it illustrates what can be done for the prediction of the CET in castings. Figure 10 shows grain structure resulting from a simulation of welding polycrystalline sheet metal [94]. The base metal grains were computed by allowing 1500 randomly placed seeds to grow until they impinged each other, following which the epitaxial growth of fusion zone solidification structure was simulated. The curvature of the grains resulting from competitive growth is evident in the calculated result.

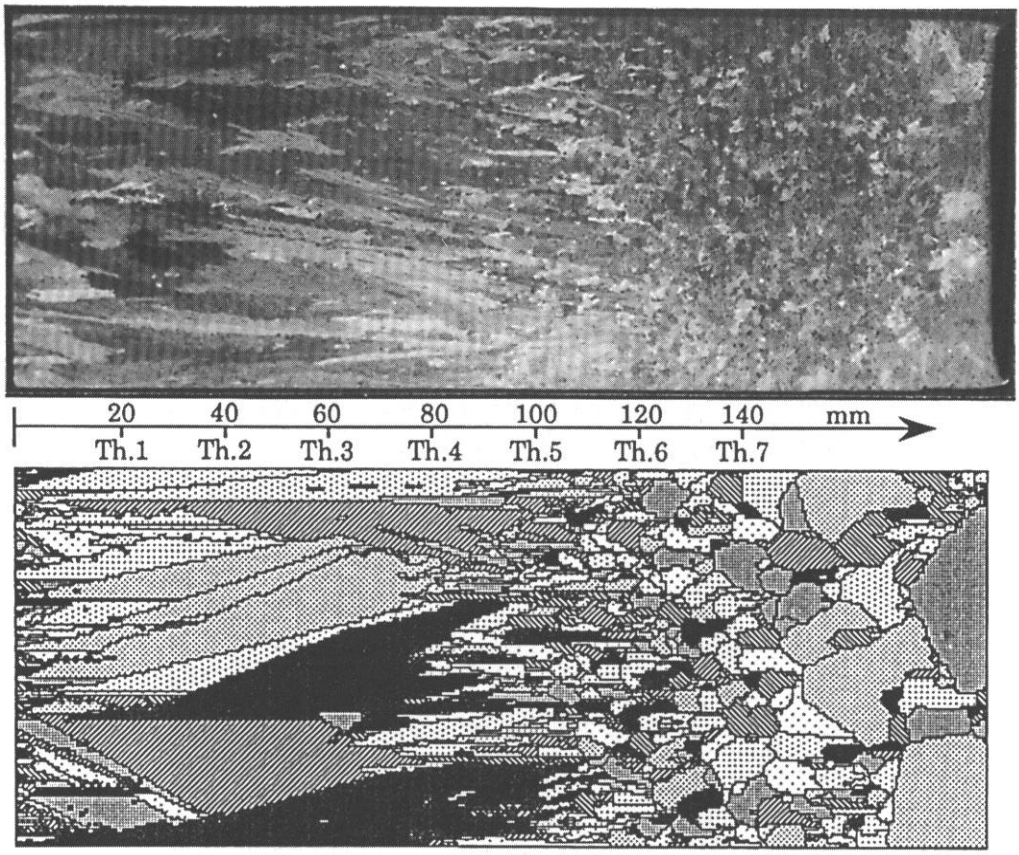

Figure 9. (a) Experimental and (b) simulated grain structure in a directionally solidified Al–7% Si ingot. (After [93].)

5. Phase transformations

Microstructure modeling has its foundations in thermodynamics. Phase parameters, calculated with the use of assessed thermodynamic data, are combined with kinetic theory and routinely applied towards the understanding of weld phenomena in multicomponent alloys, particularly steels [95–110]. The state of weld microstructure models is summarized in figure 11. Microstructure modeling of low-alloy steels will be emphasized here, although the principles can be readily applied to other systems.

The fusion and heat affected zones of welds represent distinct regions from the point of view of phase transformation theory. For the fusion zone, it is possible to model the development of microstructure (figure 10) in steel welds as a function of alloy chemistry (C, Mn, Si, Ni, Mo, Cr, V, O, Ti, Al, B, etc in any reasonable combination) and joint design [108]. The microstructure in this case represents phase fractions, distributions, chemistries, and the sequence of evolution in time. The phases of concern are allotriomorphic ferrite, Widmanstatten ferrite, bainite, acicular ferrite, martensite, and retained austenite. Some calculations can also be carried out on the constitution of non-metallic particles that are entrapped during solidification [108, 111, 112]. Mechanical properties can also be predicted to some extent, although toughness cannot even be estimated.

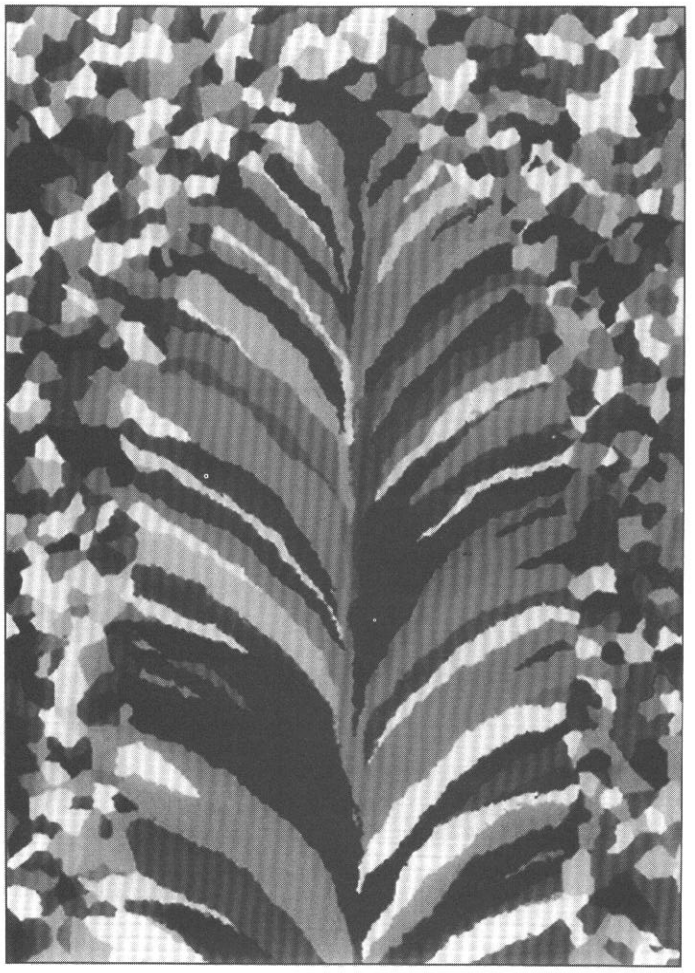

Figure 10. Two-dimensional grain structures calculated for a thin plate welded autogenously with a gas tungsten arc. (After [94].)

The HAZ presents additional problems [100]. There is no accepted method for predicting the transformation behavior during heating, and, therefore, it is usual to assume that equilibrium transformation temperatures actually represent true transformation temperatures with no kinetic effects accounted for other than detailed modeling of particle (carbonitride) dissolution. Thus, for example, full austenitization under these assumptions occurs when the Ae_3 temperature is exceeded. The variation in austenite grain size can be calculated fairly accurately, and subsequent transformation of this austenite is usually treated empirically. Hardness profiles in the HAZ can also be estimated.

There have been many recorded applications of weld microstructure models, both to rationalize existing data [108] and to predict alloys and procedures that would not otherwise have been conceived. Three particular examples of the latter case are (i) deposition of multipass welds (for power plant) in a manner predicted by modeling to lead to an enhanced degree of grain refinement [95, 96, 98]; (ii) the design of a GTAW pulsed welding

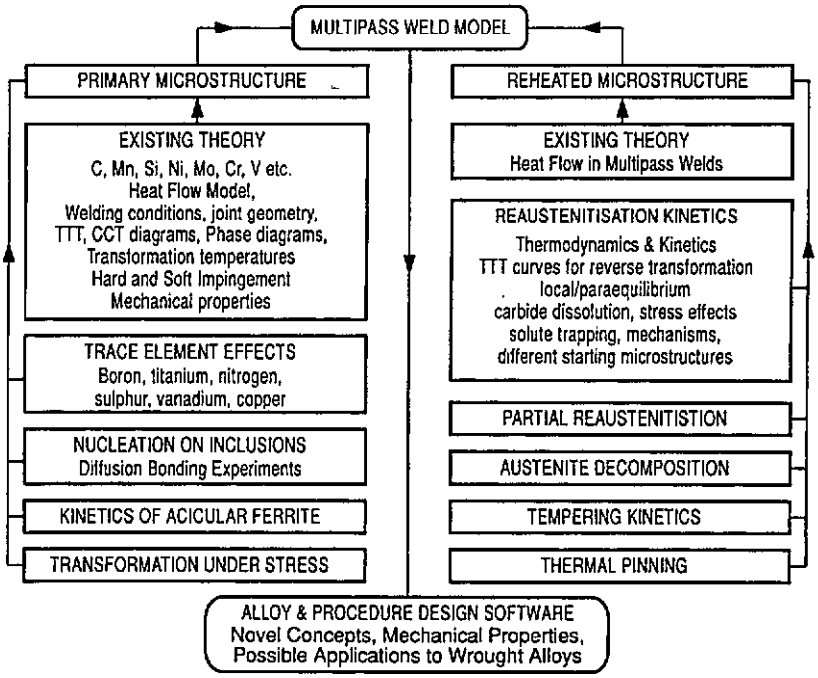

Figure 11. A flow chart illustrating the state of steel weld microstructure models.

technique that eliminates the need for postweld heat treatment [109], and (iii) the design of a mechanically homogeneous high-strength multipass weld deposit [108].

5.1. Treatment of variables

The chemical composition is important for any microstructural model. The influence of many of the elements can be rationalized out of the calculation by estimating the effect of each species on the free energy change for transformation. In steels, manganese, nickel, and chromium fall into that category. However, other elements, such as titanium, oxygen, and boron, have major consequences at very small concentrations. This is because their influence is kinetic. Boron segregates to austenite grain surfaces and influences the heterogeneous nucleation rates. Oxides have a major role in controlling intragranular nucleation. A further effect is diffusion of elements during transformation, in which case their transport properties in particular phases need to be considered.

When considering solid state transformations in welds, it is unlikely that the starting material is chemically homogeneous. Chemical inhomogeneity is currently dealt with by estimating the level of segregation and treating the solute depleted and solute enriched regions separately.

The cooling curve over the temperature range in which transformation occurs (roughly 900–400 °C for steels) needs to be known fairly accurately. This is one of the ways in which the nature of the welding process is accounted for in phase transformation models. Development of the solidification microstructure is the other way in which the process influences the calculation of microstructure. The influence of joint geometry is incorporated into the cooling curve and solidification microstructure and is not otherwise incorporated in any of the models.

The variables listed above are the obvious inputs to any phase transformation model. There are many other inputs that are required in the formulation of the models but need not be specifically considered subsequently. These include thermodynamic data for phase diagram and free energy calculations, diffusion data, rate control decisions, the way in which phase impingement phenomena are handled, parameters for time–temperature–transformation (TTT) diagram calculations, and factors such as the intrinsic contributions to strength and other properties of interest.

5.2. Output

The output is of two kinds, field data and feature data. Field data describe overall parameters such as the volume fraction of a phase, the mean grain size, and so on, whereas feature data deal with size distributions, spatial distributions, etc. In steels, the phases that grow from austenite consist of allotriomorphic ferrite, Wiedmanstatten ferrite, acicular ferrite, bainite, martensite, and retained austenite. When necessary, it is possible to calculate the volume fractions, growth rates, phase chemistries, dimensions, and location in the microstructure to various degrees of accuracy. The time evolution of the microstructure can be assessed.

Mechanical properties such as strength, the components of ductility, and the expected homogeneity in properties can also be estimated. It is interesting that the models are in a state where considerable generalization is straightforward.

5.3. Stress affected transformations and residual stress calculations

Shear stress is not a thermodynamic function of state. However, it can be considered to be so if its magnitude is limited to a value below the yield stress. Stress effects that include plastic deformation must be treated differently since non-conservative effects such as the creation of dislocations and their influence on kinetics and thermodynamics are important. The whole subject is as yet in its infancy, but it is obvious that major progress is now essential in order to estimate both the microstructural development aspects and more macroscopic phenomena such as the origin of residual stresses in welded assemblies or otherwise constrained engineering structures.

Superimposed on these considerations is the fact that stress has two prime influences—it assists or opposes transformation via a mechanical driving force and, in addition, it biases the formation of those crystallographic variants that best comply with the stress. It can therefore have a major effect on the degree of chaos (or organization) in the microstructure, and hence on mechanical properties (e.g., toughness).

Many important phase changes in steel welds involve a displacive mechanism of transformation. The formation of the product phase is accompanied by a change in shape which is an invariant-plane strain (figure 12). This deformation has a large shear component (~ 0.22) in addition to a dilatational strain (~ 0.03). During stress free transformation (even in a single crystal), it is, in principle, possible to form a sufficiently large number of crystallographic variants that the shear terms cancel on a macroscopic scale and can be neglected. Thus, residual stress models that include transformation plasticity can rely only on volume change terms. However, if the microstructure is biased by stress (figure 13), then the shear component of the shape change (a component that is very large) must also be included. This is a major difficulty with current models, which will require focused research.

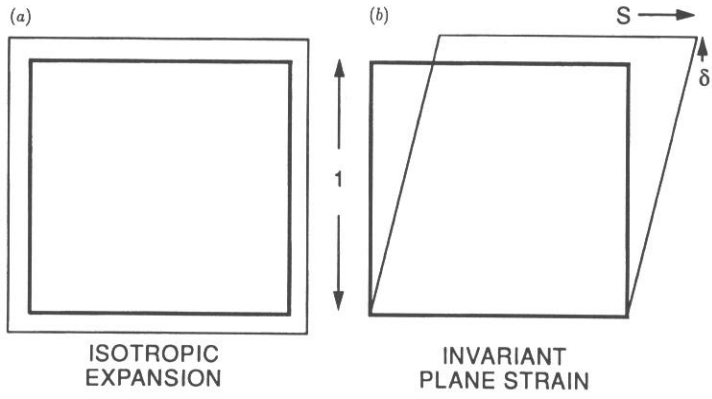

Figure 12. The nature of the shape change accompanying transformations in steels: (a) isotropic expansion in a reconstructive transformation when the product phase is not plate shaped (for example, allotriomorphic ferrite, pearlite); (b) invariant-plane strain shape deformation with a large shear component and a dilatational strain that is not isotropic (for example, Widmanstatten ferrite, bainite, acicular ferrite, martensite).

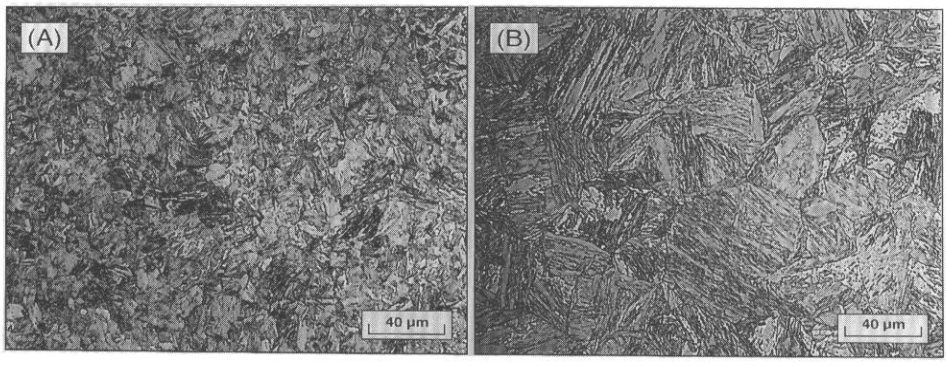

Figure 13. An illustration of how the microstructure is biased during transformation under the influence of an applied stress, in this case a stress of only about 90 MPa [122]. (A) Bainitic transformation without stress; (B) bainitic microstructure developed under the influence of an applied stress, with whole grains of austenite tending to transform into just one variant.

5.4. Austenite formation during cooling

The columnar austenite grain structure that evolves from the corresponding columnar δ-ferrite solidification structure of low-alloy steels has a major effect on the development of subsequent microstructure during weld cooling, yet there is no way of predicting the columnar austenite grain structure. There are clear indications that the crystallographic texture of the base plate has an effect via growth selection during the epitaxial growth of solidified grains. In addition, recent work shows that the columnar grains may coarsen during cooling [113].

It is possible that Monte Carlo simulations of weld solidification could be of importance in explaining the evolution of columnar austenite grain microstructures, in a manner similar to the progress that has been made in modeling solidification microstructures for conventional castings.

5.5. Austenite formation during heating

The transformations that occur during heating have received relatively little attention; they are of importance in welding because of the development of microstructure during the heating part of the thermal cycle felt by the HAZ. This is partly because transformations during cooling are of greater technological importance, but also because of the complexity of the problem. Modeling a normal TTT diagram requires an input of just the austenite grain structure and the chemical composition. On the other hand, for transformations during heating, the input for a TTT calculation could involve any one of a large number of starting microstructures. In addition to bulk chemistry, it is also necessary to account for the inhomogeneous distribution of elements in the different phases.

5.6. Grain growth in temperature gradients

It has long been known in the welding industry that the gradient in grain size in the HAZ cannot be accurately simulated experimentally because of the so called thermal pinning effect, in which the finer grains away from the fusion boundary restrict the free coarsening of those close to the fusion surface. Monte Carlo methods for grain coarsening seem ideally suited for these purposes. Such methods also have the advantage that they can provide detailed information about the distribution of grain sizes, i.e., field data, which are otherwise less accessible in models based on overall transformation kinetics. Recently, it has been shown that Monte Carlo techniques can be used to simulate the thermal pinning phenomenon in the weld HAZ [114].

5.7. Solid state nucleation kinetics

Solid state nucleation kinetics is an area of major difficulty. Convincing calculations of nucleation rates are not available, and theoretical estimates can be incorrect by some ten orders of magnitude [115]. The output of nucleation theory is extremely sensitive to the inputs (interfacial free energy) and detailed factors, such as crystallographic texture, that affect austenite grain boundary energies are simply not available.

General and partly quantitative thermodynamic criteria are, nevertheless, useful in fixing transformation start temperatures [116]. It is unlikely that theoretical work will help resolve these problems, but detailed experimental measurements of nucleation rates would be extremely useful, provided that variables such as texture and purity can be carefully controlled. In the fusion zone, heterogeneous nucleation on non-metallic particles is of crucial importance. In spite of a huge amount of research on the role of these particles in fixing acicular ferrite formation, a convincing theory on the potency of inclusions is missing. Again, clear experiments, in which the purity of the inclusions is controlled (both in solidification and solid state transformation studies) are needed so that the variety of possible explanations can be examined and incorporated in models. Novel research needs to be initiated on how to add potent nucleants into steel melts (welds) without modification of their nucleation characteristics by reaction with the molten steel. Recently, there has been some work done to model the development of oxide inclusions in low-alloy steel weld metal and to predict the inclusion characteristics [117].

5.8. Monte Carlo techniques

Most current weld microstructure models emphasize field data, i.e., deal with the prediction of volume fractions, mean size, etc. However, there is a need to predict feature data such as a size distribution rather than just a mean size. Monte Carlo techniques [118–120] are well suited for this purpose and should be developed further to converge towards known experimental data.

5.9. Other models

The vast majority of phase transformation modeling for welds is for steels because of their technological importance, their wide use, and the complexity of their transformation behavior (which makes them so useful). There is significant research in progress for aluminium alloys [121] where precipitation hardening is the key modeling challenge. While it is possible to find examples of modeling efforts with other metallic systems, more thought is needed to establish whether more intense activity is necessary. There is no clear identification of the commercial demand for modeling metallic systems other than steels and aluminium alloys.

6. Future needs and recommendations

Modeling, simulation, and high-performance computing have evolved as powerful technologies for understanding the fundamental phenomena in welds. Significant advances have been made in weld process modeling that have provided useful insight into the physics and development of the weld pool. The capability for modeling the 3D heat and fluid flow during welding has been developed. The models have been used to understand the relative importance of buoyancy, electromagnetically, and surface tension driven flow on weld pool development.

Microscopic models that couple the heat flow equations with solidification phenomena have been developed. With the help of powerful computers, such models have now been integrated in sophisticated macro–micro models, which couple the average continuity equations (e.g., heat flow equation) with the microscopic phenomena of grain growth. Using such models, it is now possible to perform *computational metallurgy* and to directly visualize the grain structures obtained under given solidification conditions, including those pertaining to welding. However, there are several approximations or hypotheses behind these models that need to be examined in the future. In particular, most of the models are based upon diffusion (of solute, of heat) and neglect the multiple effects associated with convection. If the modification by natural or surface or electromagnetically driven convection of the thermal field can be accounted for in macroscopic models of solidification, the enhancement of nucleation by dendrite fragmentation, the modification of the dendrite growth kinetics, and the transport of grains by convection can be addressed more accurately. Macrosegregation and freckle formation are additional phenomena that need to be examined and are much more difficult to assess.

There are several potentially applicable mathematical and computational tools that have emerged in recent years. Parallel computing provides important opportunities for modeling welding processes. Increasing the awareness and use of state of the art parallel computation and expertise in the process modeling area are important steps. It is encouraging to see that emerging techniques such as neural networks, cellular automata, and Monte Carlo calculations have already found their use in simulation of welding processes. A strength of these methods is the ease with which they can handle complex non-linear boundary conditions. Furthermore, these techniques map fairly well onto massively parallel computers, providing opportunities for solving some of the challenges described in the earlier sections.

The workshop identified possible mechanisms to develop long-term, multidisciplinary collaborations including the establishment of databases and a repository for models, subroutines, and software packages that are needed to establish effective information exchange within the welding community. The following research issues must be resolved if

there are to be further advances in our fundamental understanding of the complex phenomena that occur during welding: (i) coupled micro–macroscopic modeling of weld fusion zone and HAZ structure; (ii) a database of thermophysical and thermodynamic properties; (iii) thermodynamic modeling of phase transformation behavior in welds, (iv) free surface effects on weld pool development, (v) vaporization kinetics and local thermodynamic equilibrium during plasma metal interactions, (vi) turbulence effects in fluid flow and convective heat transfer, and (vii) convection effects on solute redistribution.

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