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Simulation on the Welding Process of Low-Alloy Steel
by Finite Element Method

by

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the Faculty of Graduate Studies and Research

in partial fulfillment of the requirements for the degree of

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Abstract

After more than 30 years of development, Computational Weld Mechanics (CWM) has made a tremendous progress. The objective of this thesis is to focus on the development of more accurate algorithms that capture more physics while requiring less computer time.

Due to the limited capacity (speed and memory) of computers, simulation of large complex welding structures is usually not satisfactory. This thesis aims at computing physical changes in long welds, especially during the quasi-steady state period.

In this work, a weld pool model is proposed to compute the surface geometry of the molten pool as well as a temperature distribution in the weld pool region. The temperature field in the weld joint is computed by solving a convective-diffusion heat equation, based upon the space-time finite element method which can deal with both transient and steady state. The model for evolution of microstructures in low-alloy steels is implemented for both an Eulerian formulation and a Lagrangian formulation. The results from the microstructure analysis, such as specific volume and phase fractions, can be used in stress analysis to capture the effects of volume change during phase change on the stress states. In thermal-stress analysis, a flow tube model, which possesses features from both the Lagrangian formulation and the Eulerian formulation, is developed to predict the steady-state stress and displacement fields in the weld joint domain. A thermal-elasto-viscoplastic constitutive relationship, with

consideration of transformation plasticity, is applied.

All these analyses are coupled by data flows to incorporate interactions between the thermal, mechanical and metallurgical processes present in the welds. The input data for the analysis included geometry, material properties, initial temperature field, initial microstructure states, base metal and filler metal compositions, initial stress and strain states, and boundary conditions appropriate for the problem analyzed. Numerical results are compared with experimental, analytic or other numerical results.

To my parents,
my wife, Yiwen
and my daughter, Tianyu

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Nomenclature

Γ	Boundary of the domain
Φ	Distribution function
ϕ	Isotropic function
Ω	Space domain
α	Diffusivity or Coefficient of linear thermal expansion
σ	Surface tension
$\boldsymbol{\sigma}$	Cauchy stress
σ_Y	Flow stress
ϑ	Ionization parameter
ρ	Density
θ	Inclination angle or Test function
τ	Time in reference time element
$\boldsymbol{\tau}$	Kirchhoff stress
$\underline{\tau}$	Principal Kirchhoff stresses
χ	Basis function for reference time element
ξ, η, ζ	Local coordinate system
ξ	Vector of internal variables
φ	Basis function in space
φ, χ	Map of the motion of a body

λ	Basis function for space-time element
λ_k	Eigenvalue
$\dot{\epsilon}$	Logarithmic strain rate
$\bar{\epsilon}$	Logarithmic stretch tensor
λ_c	Coefficient of convective heat transfer
λ_r	Coefficient of heat radiation
ψ	Free energy function
$\Delta\gamma$	Kuhn-Tucker variable
η	Viscosity
μ	Shear modulus
κ	Bulk modulus
A	Area
A_1	Lower critical temperature
A_3	Upper critical temperature
$\mathcal{B}$	Reference configuration
$\mathbf{B}$	Physical gradient operator
B_r	Effective rate coefficient
BS	Bainite start temperature
$\mathbf{C}$	Right Cauchy-Green strain tensor
$\mathcal{D}$	Dissipation function

E	Reference spatial element
$\mathbf{E}$	Elastic domain
$\mathbf{F}$	Deformation gradient tensor
G	Grain size index number
H	Hardness
I	Time interval
J	Jacobian matrix for spatial element
$\mathbf{J}$	Jacobian matrix for space-time element
K	Hardening function
$\mathbf{K}$	Tangent stiffness matrix
L	Distance
$\mathcal{L}$	Lie derivative
MS	Martensite start temperature
P	Pressure
$\tilde{P}_{arc}$	Equivalent arc pressure
$\wp$	Space-time nodes in the physical element
PS	Pearlite start temperature
Q	Heat source
Q_n	Space-time domain boundary
R	Transitional resistance

R_0	Modified Bessel function of second kind and zero order
$\mathfrak{R}$	Space-time reference element
$\mathbf{R}$	Orthogonal rotation tensor or Basis function vector in space
$\nabla \mathbf{R}$	Gradients of Basis function over space
S	Space-time domain
$\mathbf{S}$	Space-time element basis vector or Vector space of symmetric 3×3 tensors
T	Temperature field or Reference element in time
$\mathbf{T}$	Surface traction
∇T	Temperature gradient over space
T_{evap}	Evaporation temperature
T_{liq}	Melting temperature
TS	Precipitate dissolution temperature
$\mathbf{U}$	Symmetric right (material) stretch tensor
$\mathbf{V}$	Symmetric left (spatial) stretch tensor
$\mathbf{V}^*$	Nodal velocity field
V_c	Cooling rate
W	Space-time domain for discretization
X	Volume fraction
$\mathbf{a}$	Elastic moduli in principal stress space, consistent algorithmic moduli
b	Heat transfer coefficient

$\mathbf{b}$	Left Cauchy-Green strain tensor
$\mathbf{b}^e$	Elastic left Cauchy-Green strain
c_p	Specific heat
ds	Space increment
dt	Time step size
e_{ij}	Green-Lagrange strain component
f	Weight fraction
$\mathbf{f}$	Body force or Nodal force vector
g	Acceleration due to gravity
h	Height, thickness
k	Thermal conductivity or Time length
$\vec{n}, \mathbf{n}$	Normal unit vector
$\dot{q}$	Thermal flux density
q	Heat transferred from heat source to plate
$\mathbf{q}$	Hardening parameters
r	Radius
$\mathbf{s}$	Deviatoric stress tensor
t	Time
Δt	Physical time interval length
$\mathbf{u}$	Velocity field

$\nabla \mathbf{u}$	Displacement gradient over space
v	Velocity of the moving heat source
$\mathbf{v}$	Normalized eigenvector
v_{ms}	Specific volume
x, y, z	Cartesian coordinate system

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Chapter 1

Introduction

1.1 General View of the Welding Phenomena

Welding is one of the most important methods of joining components which are made of metallic materials. A weld can be simply described as a region of bonding between adjacent parts. It is desired that the mechanical, metallurgical and chemical properties of the weld should be identical or superior to those of the parts being joined.

The technological core of most welding processes is the melting of the surfaces to be joined, either with or without filler metal, followed by subsequent solidification during cooling. In any welding process that is being used, generation of heat is involved. The direct addition or indirect evolution of heat is the key for the welding

processes, but it is also the source of many of the welding engineer's problems, such as loss of strength, hot or/and cold cracks, distortion, and so on.

For fusion welding, by applying concentrated energy sources locally at the joint, the adjacent surfaces and the filler metal added between them are melted and joined together in the solidification process. The localized heat input causes a thermal cycle which results in:

1. The formation of a weld pool;
2. The initiation of hot cracks mainly in the partly molten zone;
3. The microstructural changes in the heat-affected zone of the base metal;
4. The generation of residual stresses and distortion in the whole structure often resulting in negative effects on strength.

The origin of welding residual stresses and welding distortion is the concentrated heat input that is the characteristic of welding processes. The temperature fields during welding are extremely heterogeneous and transient. At temperatures above the melting point the base metal and filler metal fuse and metallurgical processes evolve in the weld pool. In the weld pool and adjacent regions, the metal melts, solidifies and recrystallizes. Additional microstructural transformations take place during heating and cooling. The temperature field, therefore, drives the welding residual stresses not only directly through the thermal strains, but also indirectly

through the transformation strains that accompany the changes in microstructure states. In addition, the stress-strain relationship is a function of temperature and microstructure state.

The reliability of the design of a welded structure is assessed primarily on the basis of welding residual stress analysis, whereas feasibility of manufacture is assessed primarily on the basis of welding deformation analysis. The results of such analysis have to be compared with corresponding limit values (strength values and dimensional tolerances). Suggestions for improvements and possibilities for optimization of design, materials and manufacturing are derived from comparative analyzes.

The process of welding a structure follows these stages:

- Structural design - specifies the geometry and material for each of the parts to be welded, the location of each weld, the loads and service conditions that the joint must withstand.
- Weld procedure design - specifies the parameters of the welding procedure for each pass in a weld joint: weld process type, consumables, current, voltage, welding speed, preheat and post heat.
- Weld production design - specifies the sequence of weld joints in a structure, the start and end of each weld, the fixturing to be used.

The computation process has to be designed so that the information flow between

these stages is continuous and complete.

In order to design and fabricate a quality welded structure, it is essential to have an adequate design, a proper selection of materials, adequate equipment and proper welding procedures, skilled workmanship and strict quality control. With the development of computer technology, numerical analysis becomes a powerful tool to help people to understand, design and predict welded structures. One of the prevailing numerical methods is the finite element method (FEM).

1.2 FEM Simulation of Welding

Due to their huge capability to store, manage and process large amounts of data, computers have become necessary engineering tools, which allow data and computation to be processed in a cost and time efficient way. Modeling and simulation have become an essential stage in the design process of many engineering applications. With the aid of computer simulation, welding engineers can reduce the costs and time in testing process or establish optimum welding conditions.

Before the 1980s, when the finite element method (FEM) became popular for thermal analysis in welds, the transient temperature field in welds was usually not predicted, while some researchers [25][26] computed the steady state temperature field by solving the heat equation for moving heat sources. Today, with the help of powerful computers, FEM is widely used for simulating the transient temperature

fields in welds. The transient Lagrangian formulation allowed complex geometry, and non-linear equations. Many successful 3-dimensional transient analyses on welds have been reported using Lagrangian FEM formulations [16][43].

Finite element techniques permit complex geometry and temperature dependent material properties to be taken into account. Various welding processes can be simulated by changing the welding procedure parameters (such as preheat conditions, heat input, weld type, welding speed, and imposed cooling patterns, etc.) and materials.

In large welded structures the temperature field varies dramatically from huge temperature change around the weld pool to basically no temperature change in the area further than a certain thermal distance away from the weld pool (depending on thermal diffusivity and welding speed). For a pure thermal analysis, only a relatively small region near the weld needs to be analyzed. Therefore the part of the structure that has little or no change in temperature during welding can be excluded from the solving domain. In contrast, in a thermal-stress analysis, the complete structure being welded is in quasi-static equilibrium and the stresses generated by the welding process will travel through the entire structure. If the whole welded assembly is not included in the stress analysis, it is difficult to define boundary conditions to account for the parts not included in the domain.

During the welding process, there exist many complex physical, chemical and metallurgical phenomena. An ideal simulation will consider each of these phenomena

in relation with the others. However, this will make the simulation very complicated and, at present, difficult to achieve. A practical approach is to make some reasonable simplifications, and gradually enrich it according to computer capacity, mathematical models, software and data available.

One of the ways to simplify the simulation is to decompose the whole welding process into several problems, deal with each problem at a time, but connect and couple them by data flows. For computational welding mechanics, the following topics should be considered:

- weld pool model for the geometry and temperature distribution of a weld pool;
- thermal analysis for heat transfer;
- phase transformation analysis for microstructure evolution;
- stress analysis for plastic deformation, residual stress and distortion.

Figure 1.1 describes the coupling between the different problems in the simulation of welding. The dominant couplings in welding are shown with bold lines and the secondary couplings are shown with dotted lines. The effect of temperature on the microstructure and thermal stress is dominant. Also, phase transformations can dominate the stress analysis [16][43].

Details of data flows are explained as follow:

Figure 1.1: Data flows between different problems in welding analysis.

- Process 1 passes the heat input calculated from the weld pool model to the thermal analysis.
- Some weld pool models may need the temperature field or boundary conditions from the thermal analysis that could be done in process 2.
- Process 3 passes the temperature field from thermal analysis to microstructure evolution because it depends on temperature history.

- Each phase transformation can have an associated latent heat that could go from microstructure evolution to thermal analysis by process 4.
- The results of microstructure evolution, such as material properties (specific volume, yield stress and Young's modulus, etc.) and phase fractions, need to be passed to stress analysis by process 5.
- Process 6 could be needed if microstructure evolution depends on the mechanical deformation or stress field (stress-dependent phase transformation. SDPT).
- Process 7 passes the temperature field from thermal analysis to stress analysis to account on the thermal expansion.
- The displacement field or deformed geometry and, in some cases, the heat (energy) generated by plastic deformation as a heat source could be passed from stress analysis to thermal analysis by process 8.

When the data flows from one problem to another problem, if the meshes of the two problems are the same, data just need to be copied. If the meshes of the two problems are different, data need to be interpolated.

1.3 Layout of Thesis

This thesis is divided into six chapters in total. Following this brief introduction, Chapter 2 presents a weld pool model which considers both the heat distribution and geometry. Correctness of heat input, i.e., the incoming heat distribution, is critical for the thermal analysis. It can be expected that different shapes of the weld pool surface and different flux distribution will result in different temperature contours, microstructures, as well as strain and stress distributions in the final weldment. The model computes the surface geometry of molten pool, as well as the thermal flux and arc pressure distributed over the weld pool. With the thermal flux distribution as a boundary condition, an energy equation is solved for the temperature field in the weld pool region.

Chapter 3 presents a space-time FE Method to solve the convection-diffusion thermal equation with temperature dependant material properties. A quasi-steady state temperature field can be obtained by running a transient analysis until it approaches the steady state.

Chapter 4 presents an algorithm to simulate phase transformations and microstructure evolution in low-alloy steels. The history dependent parameters (grain size and fraction of each phase) are integrated along flow lines in space that is equivalent to integrate material points in time. The data structure has the option to create flow lines by extracting temperature-time data for each material point in the domain from

either a transient Lagrangian formulation or an Eulerian formulation.

Chapter 5 presents the FEM algorithms for both 3D transient stress analysis by a Lagrangian formulation and 3D quasi-steady state stress analysis by an Eulerian formulation. Both formulations use the same constitutive (stress-strain) relation that is intended to deal with thermal-elasto-viscoplastic, large deformation (finite strain) and phase transformation phenomena. The quasi-steady state solution could provide a trial solution for a transient stress analysis.

Chapter 6 presents conclusions of this thesis, and outlines suggestions for future work.

The analytical solution in this thesis is generated with Mathematica software.

Chapter 2

The Weld Pool Model

2.1 Introduction

In an arc weld, a highly localized concentrated energy input fuses the filler metal and nearby base metal to form a weld pool. The shape and temperature distribution of a weld pool are dependent on the type of welding processes, welding parameters (welding velocity, diameter of wire, wire feed rate, voltage, current density, angle of workpiece inclination, etc.), and the weld materials.

One of the major challenges of computational weld mechanics is to simulate the geometry and temperature distribution of a weld pool accurately and efficiently.

There are several approaches to model the effects of the heat source on a weld pool. One of the simple ways is to prescribe either the thermal flux or power den-

sity distribution, or the temperature distribution in the weld pool by a distribution function that intend to model the heat input. Some examples are the double-ellipsoid model provided by Goldak et al. [21] for most realistic welds with simple shapes, and the compound-ellipsoid model by Gu et al. [22] for a more complicated shape which can occur in a submerged arc weld. These models are convenient, accurate, efficient and flexible in an application as long as the geometry of the surface of the molten pool does not need to be considered.

The energy transport (heat flow) is influenced not only by the content of enthalpy, but also by the deformation of the weld pool, especially the deformation of the surface. For some applications, such as welding a pipe, or a workpiece with very large inclination angle (such as vertical or overhead), the weld pool will be heavily deformed, due to gravity. In such cases, the weld pool analysis should consider the geometry of the surface.

In this chapter, a model based on the force balance among gravity, arc pressure and surface tension, that predicts both the temperature distribution in the weld pool and the surface geometry of the molten pool, is presented that can deal with many different welding application.

2.2 The Hydrostatic Surface Tension Model

The physical phenomena in and around the weld pool during welding are very complicated. The simplification made in this model is based on the following assumptions:

- The influence of the fluid flow in the molten pool on the heat flow can be neglected;
- The weld pool is considered to be in a quasi-steady state;
- The pool surface is assumed to be in a static equilibrium with respect to gravity, arc pressure and surface tension. The influence of buoyancy and the electromagnetic force are disregarded.

2.2.1 The Intensity Distribution

Conventionally, the heat flow density (flux) transferred from the welding arc to the weld pool is assumed to follow a Gaussian distribution curve [4]. Weiss [23] argues that for high surface deformation, a Gaussian distribution will lead to large errors because it does not include the effect of arc deflection. He proposed a model which depends on the electrical resistance in the plasma of the arc. This model is applicable to both small and large deformation of pool geometry. The corresponding distribution function is:

$$\Phi(x, y, z, T) = \exp\left(-\frac{R^2 - R_{min}^2}{R_{max}^2 - R_{min}^2}\right) \quad (2.1)$$

where R is the electrical resistance on a line from the electrode tip to a point on the weld pool surface with temperature (x, y, z, T) . The value of R can be estimated as:

$$R(x, y, z, T) = \begin{cases} L \left(1 - \vartheta \frac{T - T_{liq}}{T_{evap} - T_{liq}} \right) & \text{if } T > T_{liq} \\ L & \text{if } T \leq T_{liq} \end{cases}$$

where L is the distance between the electrode and pool surface. T is the temperature field. T_{liq} is melting temperature, and T_{evap} is evaporation temperature. ϑ is a scalar between 0.0 and 1.0, which is related to ionization conditions.

The thermal flux and pressure distribution caused by the arc can be defined as:

$$\dot{q}_{arc} = \dot{q}_{max} \Phi(x, y, z, T) |\vec{n}_{surf} \cdot \vec{n}_{arc}| \quad (2.2)$$

$$P_{arc} = P_{max} \Phi(x, y, z, T) |\vec{n}_{surf} \cdot \vec{n}_{arc}| \quad (2.3)$$

The maximum values $\dot{q}_{max}$ and P_{max} are determined based on the consideration that the surface integral of heat flux on the effective area of the arc should be equal to the total heat input, while the surface integral of pressure over the effective area of the arc should be equal to the total force caused by the interaction between the arc and weld pool. $\vec{n}_{surf}$ is the unit vector normal to the pool surface, and $\vec{n}_{arc}$ is the unit vector with the direction from electrode tip to the pool surface. Here, the equivalent arc pressure could be defined as:

$$\bar{P}_{arc} = \frac{\int_{\Gamma} P_{arc} d\Gamma}{A} \quad (2.4)$$

where Γ represents the effective surface on which arc interacts with weld pool and A

is the area of this surface.

$$A = \int_{\Gamma} d\Gamma$$

2.2.2 The Heat Flow in the Weld Pool

Figure 2.1: Domain and boundary conditions for weld pool problem.

A convection-diffusion heat transfer equation is used to solve the temperature field in the weld pool region. It is convenient to choose a coordinate system fixed to the

heat source (electrode). The governing equation is:

$$\rho c_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) - \nabla(k \nabla T) = Q \quad (2.5)$$

where T is temperature field. ρ and c_p are mass density and specific heat at constant pressure, respectively. k is the thermal conductivity. Q is a heat source term. Figure 2.1 shows the domain and boundary conditions for the heat flow analysis in the weld pool region. Γ_0 is the inlet surface, normally it is a Dirichlet BC. Γ_1 is the flux BC, which represents heat input. Γ_2 is the top surface, which is usually set to a convection BC that includes radiation effects. Γ_3 is the bottom surface that is set to convection BC. Γ_4 is the side surfaces, which can be Neumann BC or Dirichlet BC depending on the problem. Γ_5 is the outlet surface on which a flux BC is normally applied. The details of thermal analysis are discussed in Chapter 3.

2.2.3 The Force Equilibrium on Surface

For the formation of the molten pool surface, a static force balance in the normal direction is assumed over the surface among arc pressure, surface tension and hydrostatic pressure. So, for each point on the surface, we have:

$$P_\sigma - P_a + P_h + P_0 = 0 \quad (2.6)$$

with:

$$\begin{aligned}
P_\sigma &= \sigma(T) \left(\frac{1}{r_1} + \frac{1}{r_2} \right) \\
P_a &= P_{max} \Phi(x, y, z, T) |\vec{n}_{surf} \cdot \vec{n}_{arc}| \\
P_h &= -\rho g h
\end{aligned}$$

where h is the height of a surface point with respect to the reference point. The constant P_0 is the Lagrange multiplier that enforces mass conservation between the filler metal added and the reinforcement. When the workpiece is inclined, the hydrostatic pressure can be specified as:

$$P_h = -\rho g z \cos \theta + \rho g x \sin \theta \quad (2.7)$$

where θ is the inclination angle.

2.3 Numerical Implementation

The thermal flux and pressure distribution equations 2.2-2.3, heat transfer equation 2.5 and force balance equation 2.6 can be numerically solved iteratively over the updated domain geometry. The algorithm for solving the coupled thermal and surface problem is outlined below:

1. Initialize the problem, including the temperature field and geometry;
2. Solve the temperature field by using the double ellipsoid Dirichlet temperature model to obtain a trial solution;

3. Go into iterative loop, inside the loop, we do:
  - (a) Solve the thermal flux and pressure distribution equations;
  - (b) Solve the heat equation by applying the thermal flux computed above to get the temperature field;
  - (c) Solve the force balance for surface, and update the mesh, i.e., the weld pool free surface;
  - (d) Compare the result (surface geometry and temperature field) with the criteria, and decide whether to exit the loop or go back to the beginning of the loop;
4. Output the temperature field and mesh.

2.4 Tests and Results

The weld pool model is tested on a flat weld pool mesh (Figure 2.2) to simulate the formation of weld pool surface and temperature distribution on the upper side of a horizontal workpiece. The influence of arc pressure and angle of workpiece inclination is investigated. Then, the model is also applied to a butt weld and an edge weld, the results of which are used in Chapter 3.

Figure 2.2: Mesh for weld pool problem.

2.4.1 Influence of Arc Pressure

The surface geometry is greatly influenced by the amount of arc pressure. To confirm this, tests were run with different arc pressures, while keeping the other parameters constant. Here the equivalent arc pressure $\tilde{P}_{arc}$, which is defined in equation 2.4, is used for comparison. The welding velocity $v = 0.005 \text{ m/s}$. The material is a low alloy steel, and heat input $Q = 2250 \text{ J/s}$. Figure 2.3 and Figure 2.4 show the effect of arc pressure. The larger the arc pressure, the larger the molten pool surface deformation. It is noticed that within the molten pool region (temperature $\geq 1700 \text{ K}$) and the region around it, the temperature distribution is quite different. But for the region

away from the molten pool, the temperature distribution is similar, provided the heat inputs and materials are the same.

Figure 2.3: Influence of arc pressure - a 3D view.

Figure 2.4: Influence of arc pressure - a 2D view in mid-y plane.

2.4.2 Influence of Workpiece Inclination Angle

Figure 2.5: Influence of workpiece inclination angle.

Inclination of the workpiece also alters the molten pool surface deformation (Figure 2.5), through the hydrostatic pressure term (equation 2.7) due to gravity. The material is low alloy steel. Different inclination angles result in different molten pool

shape and different temperature distributions in the weld pool region. It is also interesting to note that downward welding needs lower heat inputs, and upward welding needs higher heat inputs. This agrees with welding practice.

2.4.3 Butt Weld

A weld pool domain of size $0.01\text{ m} \times 0.024\text{ m} \times 0.038\text{ m}$ is a sub-domain cut from a butt weld thermal problem with size of $0.019\text{ m} \times 0.100\text{ m} \times 0.250\text{ m}$. The material is a low alloy steel. The equivalent arc pressure $\hat{P}_{arc} = 500\text{ Pa}$ and heat input $Q = 1900\text{ J/s}$. The welding velocity $v = 0.002\text{ m/s}$. The inlet surface is set to be a Dirichlet boundary condition, with Dirichlet temperature $T_{in} = 300\text{ K}$. The outlet surface is set to be a flux boundary condition. The flux data is from the thermal results of the larger domain by domain decomposition. The upper and bottom surfaces are natural convection boundary conditions. The side surfaces are Dirichlet boundary conditions, with the temperature values from the thermal results of the larger domain by domain decomposition. The molten zone shape and temperature distribution is shown in Figure 2.6 and Figure 2.7. The results here will be used in the following chapter.

Figure 2.6: Weld pool thermal result of a butt weld.

Figure 2.7: Weld pool cross section of a butt weld.

2.4.4 Edge Weld

A weld pool domain of size $0.020\text{ m} \times 0.0127\text{ m} \times 0.038\text{ m}$ is a sub-domain cut from an edge weld thermal problem with size of $0.0508\text{ m} \times 0.0127\text{ m} \times 0.334\text{ m}$. The material is a low alloy steel. The equivalent arc pressure $\hat{P}_{arc} = 500\text{ Pa}$ and the heat input $Q = 1875\text{ J/s}$. The boundary conditions are similar to the previous butt weld test. But there are two differences. Instead of a Dirichlet boundary condition, a natural convection boundary condition is applied to the side surfaces. The bottom surface now is set to be Dirichlet boundary condition, with the temperature field from the thermal results of the larger domain by domain decomposition. The welding velocity $v = 0.005\text{ m/s}$. The temperature distribution is shown in Figure 2.8. The results here will be used in the following chapter.

Figure 2.8: Weld pool thermal result of an edge weld.

Chapter 3

Space-Time Thermal Analysis

3.1 Introduction

In the welding processes, the temperature fields during welding are extremely heterogeneous and transient. The temperature of base metal is normally about 300 K, while the local maximum temperature in the fusion zone (FZ) is well above the melting temperature (normally above 2500 K in the case of steel). In this temperature range, the filler metal and base metal in the weld pool melt, solidify and recrystallize. Meanwhile, microstructural transformations take place in the heat-affected-zone (HAZ) during the thermal cycle. Therefore, the temperature field determines the welding residual stress and distortion not only directly through the thermal strains, but also indirectly through the transformation strains that accompany the changes in

microstructure and the temperature dependence of material properties such as yield stress.

Early attempts to deal with the analysis of thermal processes during welding were provided by Rykalin [25] and Rosenthal [26], who independently developed an analytic solution, that is based on an Eulerian formulation, to solve the heat equation for moving heat sources. Their solution then became the primary analytical method for computing the steady state temperature fields in welds. However, there are some limitations in their analytical solutions: (1) geometry and heat input models are usually simplified; (2) material property values normally are assumed temperature independent; (3) heat transfer and heat radiation from the surface to the ambient environment are often neglected.

Since the 1970s, with the advancement of computer technology, the finite element method (FEM) became popular for computing the transient temperature fields in welds. The transient Lagrangian formulation allowed analysis of complex geometry as well as non-linear equations. Many successful 2-dimensional and 3-dimensional transient analyzes of welds have been developed [14][15][16]. Two-dimensional programs are usually based on simplified geometry and capable of computing stresses under plane stress or plane strain conditions, while three-dimensional programs can deal with more realistic and complex thermal stress analysis.

To simulate the temperature field of a weldment by using the Lagrangian formu-

lation, however, there are three major concerns:

- A fine discretization of space is required to accommodate properly the sharp temperature gradient around the heat source, particularly at the leading edge. This normally requires a very fine mesh near the weld pool. In a Lagrangian formulation, we usually need to change the mesh dynamically while the heat source moves [17].
- A fine discretization of time is required to lessen the effect of “spot welding”. This means many steps that will consume a huge amount of computing time. For a medium sized weld, it may take days, or even weeks, to analyze a weld on a personal computer.
- Due to the complexity and cost of changing the geometry or mesh between time steps to accommodate the added filler metal, the addition of filler metal is usually ignored in current Lagrangian FEM formulations. However, the filler material can significantly alter the cooling rate and temperature distribution near the weld pool by releasing a large amount of enthalpy during solidification. Therefore, it is important in the subsequent microstructure and thermal stress analyzes.

To overcome these difficulties, Gu [18] proposed a transformed Eulerian formulation to compute the steady state temperature field in welds. However, like the

Rosenthal solution, it is then limited to: (1) steady state, (2) constant thermal properties and, (3) nearly prismatic domains with constant cross-section and prismatic axis in the direction of welding.

In this chapter, a nonlinear, transient, three-dimensional FEM analysis with temperature dependant material properties is presented by using a space-time FEM element to solve the convection-diffusion thermal equation. Normally we apply this analysis for the weld pool region. A quasi-steady state can be obtained by running a transient analysis until it approaches the steady state. It can be expected that the nonlinear solver in the Lagrangian frame would converge more rapidly if the solution of the current analysis is used as the first approximation.

3.2 Space-time Finite Element Method

3.2.1 Solution in Time

For time dependent or evolution problems (such as the heat equation), the finite element method was used to formulate the solution in physical space. To obtain the solution over a range of time, a finite difference scheme can be used. The finite-difference schemes available for the time-dependent heat problem can be grouped in two categories: *explicit schemes* and *implicit schemes*. Each method has its own advantages and disadvantages. For example, the equations derived from the explicit

method are simple to solve, but their solution is stable only for sufficiently short time steps. If the space step ds is chosen very small to improve the accuracy of the calculations, the computational problem becomes very expensive because the time step dt must be chosen very small to satisfy the stability conditions. On the other hand, the implicit method offers coupled equations that are more expensive to solve, but their solution is not limited by stability criteria. Their solution is limited by accuracy requirements.

To accommodate the added filler metal and the moving weld pool during the welding processes, we use the finite element method in both the space and time domain. The main reason for using a space-time finite element lies in the difficulty of using the classical finite difference approach in cases where the domain undergoes large deformation, the domain changes in time, or the domain includes a moving interface or a free boundary [19].

3.2.2 Formulation of Space-time Finite Elements

For the space-time continuum domain, if we treat space and time equivalently, the idea of discretizing this continuum by use of space-time finite elements comes naturally. However, due to the fact that information is transferred from earlier to later times, we do not need to have a global coupling of the variables in time dimension, but still we wish to retain the standard step-wise approach from finite differences. Actually, we

can use a continuous Galerkin method for discretization in space and a discontinuous method for discretization in time, by using an arbitrary polynomial order [27].

Let $0 = t_0 < t_1 < t_2 < t_3 < \dots < t_N = T$ be a sequence of times and a partition of the time interval $[0, T]$, and let $\Omega(t)$ be a space domain that can change from one time-step to another. A space-time “slab” $S_n = S(t_n)$ is defined as the set of all ordered pairs $\{x, y, z, t\}$, with $(x, y, z) \in \Omega(t)$ and t in the interval $I_n = [t_n, t_{n+1}]$, of length $k_n = t_{n+1} - t_n$; if Ω has no dependence on t , then this is the Cartesian product, that is, $S_n = \Omega \times I_n$. The union of all the slabs makes the whole space-time domain $\Omega \times I$.

Let E be the 3-dimensional reference spatial element, the vector of basis function $\mathbf{R}(\xi, \eta, \zeta)$ and its gradients $\nabla \mathbf{R}(\xi, \eta, \zeta)$ will be:

$$\mathbf{R}(\xi, \eta, \zeta) = [\varphi_1(\xi, \eta, \zeta), \varphi_2(\xi, \eta, \zeta), \dots, \varphi_m(\xi, \eta, \zeta)] \quad (3.1)$$

$$\nabla \mathbf{R}(\xi, \eta, \zeta) = \begin{bmatrix} \frac{\partial \varphi_1(\xi, \eta, \zeta)}{\partial \xi} & \frac{\partial \varphi_2(\xi, \eta, \zeta)}{\partial \xi} & \dots & \frac{\partial \varphi_m(\xi, \eta, \zeta)}{\partial \xi} \\ \frac{\partial \varphi_1(\xi, \eta, \zeta)}{\partial \eta} & \frac{\partial \varphi_2(\xi, \eta, \zeta)}{\partial \eta} & \dots & \frac{\partial \varphi_m(\xi, \eta, \zeta)}{\partial \eta} \\ \frac{\partial \varphi_1(\xi, \eta, \zeta)}{\partial \zeta} & \frac{\partial \varphi_2(\xi, \eta, \zeta)}{\partial \zeta} & \dots & \frac{\partial \varphi_m(\xi, \eta, \zeta)}{\partial \zeta} \end{bmatrix} \quad (3.2)$$

Let $T = [\tau^1, \tau^3]$ be the *reference* element in time. Assume that the time basis is nodal and linear. In this case, χ^1 and χ^3 are the linear basis functions, while τ^1 and τ^3 are reference nodes. Let $|T| = |\tau^3 - \tau^1|$ be the length of the time interval in

reference time element, then, the time basis functions are:

$$\chi^1(\tau) = (\tau^3 - \tau) / |T|$$

$$\chi^3(\tau) = (\tau - \tau^1) / |T|$$

$$\frac{d\chi^1(\tau)}{d\tau} = -1/|T|$$

$$\frac{d\chi^3(\tau)}{d\tau} = 1/|T|$$

Let $\mathfrak{R}$ be the space-time reference element $\mathfrak{R} = E \times T$, then, the basis is:

$$\lambda_{ij}(\xi, \eta, \zeta, \tau) = \varphi_i(\xi, \eta, \zeta) \chi^j(\tau), \quad i = 1, \dots, m; \quad j = 1, 3 \quad (3.3)$$

for $(\xi, \eta, \zeta) \in E$ and $\tau \in T$. The space-time node (ξ, η, ζ, τ) ranges over $\mathfrak{R}$. Now define the space-time element basis matrix:

$$\mathbf{S}(\xi, \eta, \zeta, \tau) = \underbrace{[\chi^1(\tau) \mathbf{R}(\xi, \eta, \zeta) \quad \chi^3(\tau) \mathbf{R}(\xi, \eta, \zeta)]}_{1 \times 2m} \quad (3.4)$$

Now, the space-time nodes in the physical element $\wp$ are given by:

$$\begin{bmatrix} x_1^1 \\ y_1^1 \\ z_1^1 \\ t^1 \end{bmatrix}, \begin{bmatrix} x_2^1 \\ y_2^1 \\ z_2^1 \\ t^1 \end{bmatrix}, \dots, \begin{bmatrix} x_m^1 \\ y_m^1 \\ z_m^1 \\ t^1 \end{bmatrix}, \begin{bmatrix} x_1^3 \\ y_1^3 \\ z_1^3 \\ t^3 \end{bmatrix}, \begin{bmatrix} x_2^3 \\ y_2^3 \\ z_2^3 \\ t^3 \end{bmatrix}, \dots, \begin{bmatrix} x_m^3 \\ y_m^3 \\ z_m^3 \\ t^3 \end{bmatrix}.$$

where $(x_i^j, y_i^j, z_i^j, t^j) \in \wp$, with $i = 1, \dots, m; \quad j = 1, 3$ is the i th nodal position at time

j . The mapping from $\mathfrak{R}$ to the physical element $\wp$ is then given by

$$\begin{bmatrix} x(\xi, \eta, \zeta, \tau) \\ y(\xi, \eta, \zeta, \tau) \\ z(\xi, \eta, \zeta, \tau) \\ t(\tau) \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^m (\lambda_{i1}(\xi, \eta, \zeta, \tau)x_i^1 + \lambda_{i3}(\xi, \eta, \zeta, \tau)x_i^3) \\ \sum_{i=1}^m (\lambda_{i1}(\xi, \eta, \zeta, \tau)y_i^1 + \lambda_{i3}(\xi, \eta, \zeta, \tau)y_i^3) \\ \sum_{i=1}^m (\lambda_{i1}(\xi, \eta, \zeta, \tau)z_i^1 + \lambda_{i3}(\xi, \eta, \zeta, \tau)z_i^3) \\ t^1 + (\Delta t)(\tau - \tau^1) \end{bmatrix} \quad (3.5)$$

where $\lambda_{ij}(\xi, \eta, \zeta, \tau)$ is the basis function of the space-time element defined in equation 3.3. Δt is the physical time interval length of the current physical interval $[t^1, t^3]$:

$$\Delta t = t^3 - t^1.$$

Suppose there is a mesh Π_n on $\Omega(t_n)$, consisting of spatial elements. The mesh Π_n might be newly constructed on each time step, or it might (if Ω is independent of t) be the same mesh each time. We then construct space-time elements by extruding the nodes of Π_n along velocity vectors $\mathbf{V}_i^*$ defined at each node (x_i, y_i, z_i) , on the time interval I_n . The $\mathbf{V}_i^*$ can be chosen according to the characteristic of the problems. One common choice is to take the $\mathbf{V}_i^*$ to be, on each interval I_n , some constant-in-time approximation to the fluid velocity on the interval. Although the velocity field $\mathbf{V}^*(x, y, z, t)$ can be defined on $\Omega(t)$, but in fact it is only needed at the nodes [28].

Now suppose we have a time-dependent velocity field $\mathbf{V}^*(x, y, z, t)$ defined on the physical domain. Its nodal values on a particular element at time t are given by a $3 \times m$ matrix

$$\mathbf{V}(x, y, z, t) = [\mathbf{V}_1^* \mathbf{V}_2^* \dots \mathbf{V}_m^*] = \begin{bmatrix} v_{1x} & v_{2x} & \dots & v_{mx} \\ v_{1y} & v_{2y} & \dots & v_{my} \\ v_{1z} & v_{2z} & \dots & v_{mz} \end{bmatrix}$$

We will usually take $\mathbf{V}_i^* = [v_{ix}, v_{iy}, v_{iz}]^T$, $i = 1, 2, \dots, m$ to be constant in time on each time interval $[t_n, t_{n+1}]$, but there is nothing in the definition that requires this.

If we consider the spatial nodes in the physical element at any time in interval $[t^1, t^3]$ be advected from time t^1 under the velocity field $\mathbf{V}^*$, then the space-time nodes can be given by:

$$\begin{bmatrix} x(\xi, \eta, \zeta, \tau) \\ y(\xi, \eta, \zeta, \tau) \\ z(\xi, \eta, \zeta, \tau) \\ t(\tau) \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^m \varphi_i x_i^1 + (\Delta t)(\tau - \tau^1) \sum_{i=1}^m \varphi_i v_{ix} \\ \sum_{i=1}^m \varphi_i y_i^1 + (\Delta t)(\tau - \tau^1) \sum_{i=1}^m \varphi_i v_{iy} \\ \sum_{i=1}^m \varphi_i z_i^1 + (\Delta t)(\tau - \tau^1) \sum_{i=1}^m \varphi_i v_{iz} \\ t^1 + (\Delta t)(\tau - \tau^1) \end{bmatrix} \quad (3.6)$$

where $\varphi_i = \varphi_i(\xi, \eta, \zeta)$, $i = 1, 2, \dots, m$ is the basis function of the space element defined in equation 3.1. This mapping has the characteristic that any points in the reference element with the same time τ will be mapped to the points in the physical element

with the same time t . The Jacobian matrix is:

$$\mathbf{J}(\xi, \eta, \zeta, \tau) = \begin{bmatrix} x_\xi & x_\eta & x_\zeta & x_\tau \\ y_\xi & y_\eta & y_\zeta & y_\tau \\ z_\xi & z_\eta & z_\zeta & z_\tau \\ t_\xi & t_\eta & t_\zeta & t_\tau \end{bmatrix} = \begin{bmatrix} x_\xi & x_\eta & x_\zeta & x_\tau \\ y_\xi & y_\eta & y_\zeta & y_\tau \\ z_\xi & z_\eta & z_\zeta & z_\tau \\ 0 & 0 & 0 & t_\tau \end{bmatrix} \quad (3.7)$$

where the subscripts mean partial derivatives. The determinate of the Jacobian matrix is:

$$\det(\mathbf{J}) = t_\tau \det \begin{bmatrix} x_\xi & x_\eta & x_\zeta \\ y_\xi & y_\eta & y_\zeta \\ z_\xi & z_\eta & z_\zeta \end{bmatrix}$$

where t_τ is a scalar. We can also write the Jacobian matrix by substituting equation 3.6 to 3.7:

$$\mathbf{J} = \begin{bmatrix} J(\xi, \eta, \zeta) + (\Delta t)(\tau - \tau^1) \mathbf{V} \nabla \mathbf{R}(\xi, \eta, \zeta)^\top & (\Delta t) \mathbf{V} \mathbf{R}(\xi, \eta, \zeta)^\top \\ 0 & \Delta t \end{bmatrix} \quad (3.8)$$

where $J(\xi, \eta, \zeta)$ is the spatial element Jacobian at time t_1 ,

$$J(\xi, \eta, \zeta) = \begin{bmatrix} \sum_{i=1}^m \frac{\partial \varphi_i}{\partial \xi} x_i^1 & \sum_{i=1}^m \frac{\partial \varphi_i}{\partial \eta} x_i^1 & \sum_{i=1}^m \frac{\partial \varphi_i}{\partial \zeta} x_i^1 \\ \sum_{i=1}^m \frac{\partial \varphi_i}{\partial \xi} y_i^1 & \sum_{i=1}^m \frac{\partial \varphi_i}{\partial \eta} y_i^1 & \sum_{i=1}^m \frac{\partial \varphi_i}{\partial \zeta} y_i^1 \\ \sum_{i=1}^m \frac{\partial \varphi_i}{\partial \xi} z_i^1 & \sum_{i=1}^m \frac{\partial \varphi_i}{\partial \eta} z_i^1 & \sum_{i=1}^m \frac{\partial \varphi_i}{\partial \zeta} z_i^1 \end{bmatrix}$$

and where $\nabla \mathbf{R}(\xi, \eta, \zeta)$ is a $3 \times m$ matrix defined in equation 3.2.

3.3 Convection-Diffusion Equations

3.3.1 Problem Definition

The general convection-diffusion heat transfer (transport) equation, with divergence free velocity field, will be:

$$\begin{aligned}\rho c_p(T_t + \mathbf{u} \cdot \nabla T) - \nabla(k \nabla T) &= Q \\ T_t + \mathbf{u} \cdot \nabla T - \alpha \Delta T &= f\end{aligned}\tag{3.9}$$

where T is temperature field. T_t represent partial derivative of T with respect of time t , $\mathbf{u}$ is the given convective velocity field, and $\alpha = k/\rho c_p$ is diffusivity, where ρ and c_p are mass density and specific heat at constant pressure, respectively. k is the thermal conductivity. Q is a heat source term and $f = Q/(\rho c_p)$.

The initial condition can be expressed as:

$$T(x, y, z, 0) = T_0(x, y, z) \quad (x, y, z) \in \Omega \tag{3.10}$$

where Ω is the physical domain. The boundary conditions depend on α . In the case of pure convection, $\alpha = 0$, the boundary condition becomes a condition on the inflow boundary:

$$T = g \quad \text{on } \Gamma^{in}$$

If $\alpha > 0$, the boundary conditions are:

$$\begin{aligned}
T &= g && \text{on } \Gamma^D \\
\alpha \nabla T \cdot \mathbf{n}(x, y, z) &= h && \text{on } \Gamma^N
\end{aligned}$$

where $\mathbf{n}(x, y, z)$ is the outward normal at point (x, y, z) on boundary Γ^N .

3.3.2 Stepping Equation

As mentioned earlier, we do not want to have a global coupling of the variables in the time dimension because information is transferred from earlier to later times. We use a step-by-step procedure to get the solution in space-time domain. In each time step, we solve one space-time “slab”.

The temperature field T defined on a space-time slab S_n can be written as $T(x, y, z, t)$, where $(x, y, z) \in \Omega(t)$ and t is in the interval I_n . The time-derivative and the spatial gradient can be written as T_t and $\nabla_x T = \nabla T$. The solution is defined on each slab S_n . The boundary of $\Omega(t)$ is denoted by $\Gamma(t)$, and is a union of a Dirichlet part $\Gamma^D(t)$ and a Neumann part $\Gamma^N(t)$. Denoted by Q_n the space-time boundary consists of all ordered pairs $\{x, y, z, t\}$, with $(x, y, z) \in \Gamma(t)$ and t in the interval I_n . This is a subset of the boundary of S_n , which excludes the spatial end-faces. Similarly we have Q_n^D and Q_n^N . In a pure advection problem, with given velocity field $\mathbf{u}$, $\Gamma^N(t)$ is empty, and $\Gamma^D(t)$ consists of the inlet boundary, which is

$$\Gamma^{in}(t) = \{ (x, y, z) \in \Gamma(t) \mid \mathbf{u}(x, y, z) \cdot \mathbf{n}(x, y, z) < 0 \}.$$

We use W_n to denote the space-time “slab” corresponding to the chosen discretization on S_n . W denotes the whole space-time domain on which the space of test functions θ is defined, i.e., $\theta \in W$ and $\theta|_{S_n} \in W_n$. As usual, T must satisfy the Dirichlet conditions and θ must satisfy the homogeneous Dirichlet conditions.

The space-time FE method may now be formulated as follows [27]: for $n = 0, 1, \dots, N$, find $T \in W_n$ such that

$$\begin{aligned} \int_{S_n} (T_t + \mathbf{u} \cdot \nabla T)(\theta + \delta[\theta_t + \mathbf{u} \cdot \nabla \theta]) dx dy dz dt + \int_{S_n} \alpha' \nabla T \cdot \nabla \theta dx dy dz dt \\ + \int_{\Omega(t_n)} (T_n^+ - T_{n-1}^-) \theta_n^+ dx dy dz = \int_{S_n} (f(\theta + \delta[\theta_t + \mathbf{u} \cdot \nabla \theta]) dx dy dz dt \end{aligned} \quad (3.11)$$

Here

$$\theta_n^\pm = \lim_{s \rightarrow 0^\pm} \theta(t_n \pm s)$$

and

$$\delta = \frac{C}{\|\mathbf{u}\|} \max \left(h - \frac{\alpha}{\|\mathbf{u}\|}, 0 \right)$$

where $\|\mathbf{v}\| = (1 + (\mathbf{u}^x)^2 + (\mathbf{u}^y)^2 + (\mathbf{u}^z)^2)^{1/2}$. $C \simeq 1$ and h is a measure of the local mesh size (e.g., the average element diameter). Note that data are transferred from one slab to the next via a built-in L_2 -projection in the jump term

$$\int_{\Omega(t_n)} (T_n^+ - T_{n-1}^-) \theta_n^- dx dy dz$$

Furthermore, let r be a measure of the size of the residual on S_n :

$$r = \left(\frac{|T_n^+ - T_{n-1}^-|}{(t^{n+1} - t^n)} + |T_t + \mathbf{u} \cdot \nabla T| \right) / \max_{S_n} |T|,$$

where the terms in the numerator apparently represent L^2 norms over $\Omega(t_n)$ and S_n , respectively. Then

$$\alpha' = \max(\alpha, Ch^2r).$$

3.3.3 Initial and Boundary Conditions

The initial condition for thermal analysis depend on the welding process: with or without pre-heating, single- or multi-pass, and so on. Normally, for a single-pass weld without pre-heating, the initial temperature field will be set to a constant value equal to the temperature of the surrounding medium.

The boundary conditions are the conditions of heat input or dissipation at the boundary surfaces of the welds. Three types of boundary conditions occur in the thermal analysis of welding process: (1). Dirichlet BC (isothermal boundary condition), the temperature is prescribed; (2). Neumann or flux BC, the heat flow density is prescribed; (3) Robin or convection BC, the heat transfer to the surrounding medium is proportional to the difference between surface temperature and the surrounding medium temperature.

3.3.4 Melting and Solidification

In the molten pool region, the filler metal and base metal will first melt when heating, then solidify when cooling. Latent heat should be considered in the thermal analysis

for the weld process. An enthalpy method is used for melting and solidification. In this case, the specific enthalpy increment is used to compute residual. The heat transfer equation (eqn. 3.9) could be written as:

$$\dot{h} + \mathbf{u} \cdot \nabla h - \nabla(k \nabla T) = Q$$

where h is the specific enthalpy.

3.4 Tests and Results

3.4.1 One-Dimensional Transient Conduction Problem

Consider a semi-infinite one-dimensional bar with $0 \leq x < \infty$. The bar is initially at a constant temperature T_0 throughout, when suddenly (at time $t = 0$) the end at $x = 0$ is changed to T_f , and set as a Dirichlet BC. If its side surfaces have zero Neumann BC (zero flux), then, the transient temperature distribution can be written as:

$$\frac{T - T_f}{T_0 - T_f} = \text{erf} \left(\frac{x}{2\sqrt{\alpha\tau}} \right)$$

where T is the temperature at point x for time $t = \tau$. This test is designed to test the transient term and diffusion term of the energy equation (equation 3.9).

The numerical test was performed on a bar mesh with the size of $1\text{ m} \times 0.01\text{ m} \times 0.01\text{ m}$. To accommodate a sharper temperature gradient, a finer grid was used at

Figure 3.1: Bar mesh for the one-dimensional transient conduction problem.

the $x = 0\text{ m}$ end (Fig. 3.1). The material is a low-alloy steel, with the diffusivity $\alpha = 1.13 \times 10^{-5}\text{ m}^2/\text{s}$. The initial temperature $T_0 = 300\text{ K}$. The Dirichlet temperature at $x = 0\text{ m}$ is $T_f = 400\text{ K}$.

Both analytic and numerical results are shown in Figure 3.2. It can be seen that the numerical results agree very well with the analytic results.

3.4.2 Moving Line Heat Source in the Infinite Plate

The widely used analytic model to simulate a butt weld on a thin plate is the moving line heat source in the infinite thin plate [2][4]. The line-type heat source moves at constant speed in the infinitely extended thin plate. Because of the small thickness of

Figure 3.2: The analytic and numerical results for one-dimensional transient conduction problem.

the workpiece, temperature variations in the thickness direction are assumed negligible. As such it can be treated as a two-dimensional problem. The analytic solution for a steady state temperature distribution T in the plate was provided by Rykalin [25]:

$$T - T_0 = \frac{q}{h2\pi k} e^{-vx/2\alpha} R_0 \left(r \sqrt{\frac{v^2}{4\alpha^2} + \frac{b}{\alpha}} \right) \quad (3.12)$$

where T_0 is the initial temperature, q is the heat transferred from heat source to plate,

Figure 3.3: Mesh for moving line heat source in the infinite plate problem.

h is the thickness of the plate, k is the thermal conductivity, v is the velocity of the moving heat source, α is the thermal diffusivity. R_0 is modified Bessel function of second kind and zero order. b is a heat transfer coefficient defined as:

$$b = 2(\lambda_c + \lambda_r)/(\rho c_p h)$$

where λ_c is the coefficient of convective heat transfer, λ_r is the coefficient of heat radiation, ρ is the density, and c_p is the mass-specific heat capacity.

The numerical test was performed on a mesh with the size of $0.24\text{ m} \times 0.672\text{ m} \times 0.003\text{ m}$. The line source is represented by a cylinder with radius $r = 0.0001\text{ m}$. The finer grid is used near heat source to accommodate a sharper temperature gradient

Figure 3.4: Temperature field for moving line heat source in the infinite plate problem.

(Fig. 3.3). The heat from line source $q = 3900 \text{ J/s}$, and the velocity of the moving heat source $v = 0.002 \text{ m/s}$. The thermal diffusivity $\alpha = 1.13 \times 10^{-5} \text{ m}^2/\text{s}$ and heat transfer coefficient $b = 0.00377$. The inlet Dirichlet temperature is 300 K .

The FEM thermal result is shown in Fig. 3.4. To check the validation, a comparison of FEM results with the analytic solution (eqn. 3.12) is made (Fig. 3.5 - Fig. 3.6). A very good agreement between the numerical results and analytic results is observed.

Figure 3.5: Longitudinal temperature distribution for moving line heat source in the infinite plate problem.

Figure 3.6: Transverse temperature distribution for moving line heat source in the infinite plate problem.

3.4.3 Butt Weld

Figure 3.7: Mesh for butt weld thermal analysis.

A thermal analysis of a butt weld was performed on a mesh 0.01 m thick, 0.12 m wide and 0.25 m long (Fig. 3.7). The coordinates are x : the thickness direction; y : the lateral direction; and z : the longitudinal direction. The moving mesh is fixed with the heat source with the welding speed at 0.002 m/s in $-z$ -direction. The center of the weld pool is 0.025 m from the leading edge. The material is low-alloy steel with temperature-dependent properties. The inlet surface is a Dirichlet boundary condition, with the Dirichlet temperature $T_{in} = 300\text{ K}$. The outlet surface is a zero flux boundary condition. The other four surfaces are a natural convection boundary

condition. The heat source is provided by the hydrostatic surface tension weld pool model discussed in Chapter 2. The temperature field from the weld pool analysis (Figure 2.6 and Figure 2.7) is used as a Dirichlet temperature in the weld pool region. After 30 time steps, with each time step size 4 seconds, the temperature field reaches a quasi-stationary state. The steady state results of this test (Fig. 3.8 - Fig. 3.9) will be used to analyze microstructure evolution and stresses.

Figure 3.8: Top view of temperature distribution for a butt weld thermal analysis.

Figure 3.9: Temperature distribution at the mid-plane for a butt weld thermal analysis.

Chapter 4

Microstructure Evolution

Many mechanical properties of metals, such as hardness, ductility and strength, are sensitive to their microstructural state. People can, to some extent, control the properties through purposely changing the microstructure, to provide the best service. However, it is not uncommon that many manufacturing processes may produce unfavorable microstructures, that will greatly reduce the reliability and performance of the product. In welding, undesirable microstructural changes can result in cracks, loss of strength, and even failures.

Heat flow can strongly affect phase transformations during welding and the resultant microstructure and properties of the weldment. The energy input of fusion welding causes a short-time thermal cycle, which will be the dominant factor that affects evolution of the microstructural state of a metal. It is the peak temperature,

the time at that temperature and the heating and cooling rate in the thermal cycle that controls the phase transformations and microstructural changes.

Each material point in the weldment will experience its own thermal cycle. Actually, we are just interested in the points that are in or near the fusion zone and heat-affected zone that actually undergo phase transformation and microstructure change. In this Chapter, an algorithm is presented to simulate the phase transformation and microstructure change for low-alloy steels.

4.1 Thermal Cycle and Microstructure Evolution

4.1.1 Thermal Cycle and Transformation Temperatures

In fusion welding, the base metal is melted on the surface and together with the filler metal, forms the fusion zone of the weld seam. Adjacent to the weld seam are several layers with different microstructural states. Figure 4.1 shows a number of distinct zones that are formed by the fusion welding of low-alloy steels. The fusion zone (FZ) is the area where base metal fuses with the molten electrode filler metal and solidifies. It ranges from the centerline of the weld to the partially melted zone (PMZ), also called the solid-liquid transition zone. This is a narrow band surrounding the fusion zone. This zone is characterized by the peak temperatures between the liquidus line and solidus line of the alloy. The heat-affected zone (HAZ) ranges from the partially

melted zone on its inner edge to the unaffected base metal on its outer edge.

Figure 4.1: Peak temperature profile and microstructural zones of low-alloy steel, and iron-carbon binary diagram; modified after Radaj [4].

The HAZ, normally varies from 0.1 to 1.5 cm in width, is the area where the peak temperatures are not high enough to melt but are high enough to cause significant microstructural changes. For low alloy steel, this zone is characterized by peak tem-

peratures between the melting temperature and the temperature that is slightly above the lower critical temperature A_1 . A typical HAZ of low alloy steel can be subdivided into three distinct regions (Fig. 4.1): grain-coarsening region, grain-recrystallization region and partial recrystallization region. Among these regions, the size of the grains and microstructure varies according to the peak temperature. The grain-coarsening region is subjected to a peak temperature well above the upper critical temperature A_3 line, thus allowing austenite grains to grow. The grain-recrystallization region is subjected to a peak temperature just above A_3 , thus allowing austenite grains to nucleate but not grow large. While cooling, such austenite grains will decompose into small grains of daughter products, such as ferrite, pearlite, bainite and/or martensite phases. The partial recrystallization region is subjected to a peak temperature between the lower critical temperature A_1 and upper critical temperature A_3 . In this region, pearlite grains transform to austenite, and expand slightly into the ferrite grains during heating, and then decompose into very fine grains of daughter products during cooling.

The partially melted zone and the grain-coarsening region within the heat-affected zone are the most critical part of the weld, because some unfavorable microstructural states may appear there. Strength and ductility may be reduced to the extent that cracks may occur during or after welding. Also, the presence of hard and brittle martensite can result in severe deterioration of the HAZ mechanical properties.

Figure 4.2: Thermal cycle and transformation temperatures for low-alloy steel.

A typical thermal cycle in the HAZ is characterized by a steep rise over time from room temperature or pre-heated temperature to the peak temperature followed by a flatter drop (Fig. 4.2). Along the thermal cycle, there are several critical temperatures that determine the microstructural transformations:

- A_1 is the lower critical temperature, which indicates the beginning of austenization while heating slowly, or the beginning of the austenite decomposition to pearlite when cooling slowly.
- A_3 is the upper critical temperature. When the temperature goes above A_3 ,

the equilibrium microstructure change for low-alloy steels will be from ferrite to austenite. When cooling slowly, A_3 is the temperature that austenite begins to decompose to ferrite.

- TS is the precipitate dissolution temperature. Some alloy elements, such as niobium (Nb), vanadium (V), and titanium (Ti), are strong carbide and nitride formers. The carbide or nitride precipitates will hinder the movement of austenite grain boundaries, thus making grain growth difficult. Above this temperature, the precipitates become unstable and dissolve. Theory predicts and experiments confirm that the austenite grain growth will be difficult while the carbide or nitride precipitates are present, that is below TS on heating.
- PS is the start temperature for the austenite decomposition to pearlite while cooling. When cooling slowly, PS is equal to A_1 .
- BS is the start temperature for the austenite decomposition to bainite while cooling.
- MS is the start temperature for the austenite decomposition to martensite while cooling.

These microstructural transformation temperatures are functions of the carbon and alloy contents of the low alloy steel. Steels with different alloy contents may have very different microstructural states even though they follow the same thermal cycle.

The temperature A_1 and A_3 are associated with equilibrium states, that is, very slow heating or cooling rates are required. But in welding, the heating and cooling rate are relatively large. In such case, the kinetics of phase transformation should be considered. The equilibrium state will be a reference for computing the driving force of phase transformation, i.e., the system always strives to achieve local equilibrium, but the rate at which it moves toward equilibrium is determined by kinetics.

4.1.2 Austenite Decomposition

In welding, the phase transformations while cooling, mainly the austenite decomposition, are the most interesting, because they determine the microstructure state, mechanical properties (such as hardness) and residual stress in the final weldment. While cooling, austenite (γ -phase) will transform to ferrite (α -phase), pearlite, bainite and martensite, depend on the alloy composition, current microstructure state and cooling rate.

The phase transformations of austenite to ferrite and austenite to pearlite are governed by nucleation and growth mechanism which generally depends on thermal diffusion of atoms, and the free energy change. The phase transformation of austenite to martensite is governed by a shear mechanism which does not depend on diffusion. While the phase transformations of austenite to bainite may be regarded as a martensite-like transformation involving the diffusion of carbon atoms [37]. In

other words, the free energy for the transformation to bainite and martensite has a significant contribution from elastic strain energy.

The physical phenomenon of austenite growth and austenite decomposition can be modeled by ordinary differential equations (ODE). This was originally developed by Watt, et al. [35] and enhanced by Khoral [36]. These equations describe both nucleation and subsequent growth of austenite decomposition products (except martensite).

The general reaction rate can be computed as [36]:

$$\frac{dX}{dt} = B_r(G, T) X^m (1 - X)^n \quad (4.1)$$

where X is the volume fraction of the decomposition product. $B_r(G, T)$ is an effective rate coefficient, which is a function of the austenite grain size index number G and temperature T . t is the time. m and n are empirical coefficients.

Details of the microstructural transformation temperatures and various decomposition reaction equations are given by Khoral [36] and Goldak [38].

4.1.3 Hardness

Because hardness is intimately related to strength and ductility, it is a very good measure to indicate the susceptibility of a weldment to cracks or other failures. For low alloy high strength steel, the HAZ is susceptible to cracking if the hardness is larger than 350 VPN (Vickers Pyramid Number). The hardness at any material point

in the weld joint can be calculated using the rule of mixtures, based on the volume fractions of ferrite, pearlite, bainite, martensite and austenite. The rule of mixtures for hardness can be expressed as follows [39]:

$$H = H_M X_M + H_B X_B + H_{AFP} X_{AFP} \quad (4.2)$$

where H is the final hardness H_M and X_M are the hardness and volume fraction of martensite, H_B and X_B are the hardness and volume fraction of bainite, H_{APF} and X_{AFP} are the hardness and volume fraction of ferrite-pearlite-austenite mixture.

The equations to calculate the hardness for different phases proposed by Maynier et al [40] are:

$$H_M = 127 + 949C + 27Si + 11Mn + 8Ni + 16Cr + 21 \log V_c \quad (4.3)$$

$$H_B = -323 + 185C + 330Si + 153Mn + 65Ni + 144Cr + 191Mo \\ + [89 + 53C - 55Si - 22Mn - 10Ni - 20Cr - 33Mo] \log V_c \quad (4.4)$$

$$H_{AFP} = 42 + 223C + 53Si + 30Mn + 12.6Ni + 7Cr + 19Mo \\ + [10 - 19Si + 4Ni + 8Cr + 130V] \log V_c \quad (4.5)$$

All the compositions are in weight percent ($wt\%$). V_c is the average cooling rate from $800^\circ C$ to $500^\circ C$. Equation 4.3 - 4.5 are only valid for low carbon, low alloy steels [32][36].

4.1.4 Density and Specific Volume

Density of a multi-phase system is a function of temperature, chemical composition, and fractions of each phase. Specific volume is defined as volume per unit mass. It is the reciprocal of the density. By the rule of mixtures, the specific volume of a multi-phase system can be computed as:

$$v_{ms} = \sum_i (f_i v_i)$$

where f_i and v_i represent the weight fraction and specific volume of the single phase i , respectively. The specific volume of a single phase is the reciprocal of the density of this phase:

$$v_i = \frac{1}{\rho_i}$$

Here is a list of density of phases that may exist in low alloy steel [34][38]:

1. Density of ferrite phase:

$$\rho_{\alpha}(T, \%C = 0) = 7875.96 - 0.297T - 5.62 \cdot 10^{-5}T^2$$

$$\rho_{\alpha}(T, \%C) = \rho_{\alpha}(T, \%C = 0)(1 - k_{\alpha}\%C)$$

where $k_{\alpha} = 2.62 \cdot 10^{-2}$, and $\%C$ represent carbon content in the phase (in weight percentage).

2. Density of austenite phase:

$$\rho_{\gamma}(T, \%C = 0) = 8099.79 - 0.506T$$

$$\rho_{\gamma}(T, \%C) = \rho_{\gamma}(T, \%C = 0)(1 - k_{\gamma}\%C)$$

where $k_{\gamma} = 1.46 \cdot 10^{-2}$.

3. Density of liquid steel:

$$\rho_L(T, \%C = 0) = 8319.49 - 0.835T$$

$$\rho_L(T, \%C) = \rho_L(T, \%C = 0)(1 - k_L\%C)$$

where $k_L = 1.0 \cdot 10^{-2}$.

4. Density of cementite:

$$\rho_{CM}(T) = 7686.45 - 6.63 \cdot 10^{-2}T - 3.12 \cdot 10^{-4}T^2$$

5. Density of martensite & bainite:

$$\rho_M(T = 20^{\circ}C, \%C) = \frac{2 \times 0.055847}{(2.86 - 0.0131579\%C)^2(2.86 + 0.118421\%C)10^{-30}N}$$

$$\rho_M(T, \%C) = \rho_M(T = 20^{\circ}C, \%C) - 0.297T - 5.62 \cdot 10^{-5}T^2$$

where $N = 6.023 \times 10^{23}$ is Avagadro's number.

4.2 Framework for Software Design

To predict the microstructural changes for one material point (e.g., at a Gauss point or a node in a Lagrangian formulation), we must follow the temperature and microstructural state history of this material point. The software has the option to

extract temperature-time data for each material point in the domain from either a transient Lagrangian formulation or along a flow line in an Eulerian formulation. Based on the temperature-time data, microstructure evolution can be evaluated.

Figure 4.3 is a schematic diagram of the software design for microstructure evolution. The phase diagram class keeps binary (or pseudo-binary) equilibrium phase diagrams, such as Fe-C, Al-Si, and Cu-Zn phase diagram. It provides equilibrium phases, their fractions and transformation lines. For low alloy steel, a pseudo Fe-C binary phase diagram is very useful. The C content or equivalent C content [7] is defined here to represent the alloy.

The alloy class keeps all the information about a particular alloy. An object of the alloy class will contain the chemical composition of an alloy, the transformation temperatures, current microstructure state and material properties. The microstructure state may contain temperature, enthalpy, pressure, phase fractions, grain sizes and other information.

An object of microstructure driver will have the kinetic phase transformation equations. It obtains the thermal cycle information from an energy solver and computes the microstructure evolution. The results will be output for visualization, or for further use by the stress solver.

Figure 4.3: Software design for microstructure evolution

4.3 Simulation

For the purpose of this test, the chemical compositions chosen for both base metal and filler metal are listed in Table 4.1.

Table 4.1: Chemical composition of the low-alloy steel analyzed.

Materials	Chemical Composition (wt%)									
	C	Si	Mn	P	S	Al	Nb	N	Cu	Mo
Base Metal	0.12	0.16	0.91	0.002	0.005	0.04	0.021	0.011	0.12	-
Filler Metal	0.10	0.6	0.95	-	-	-	-	-	-	0.5

4.3.1 One Material Point Test

A simple test with only two elements (Fig. 4.4) was created to verify the algorithm and test the software efficiently. Because the whole domain has the same temperature at any time, it can be regarded as one material point. There are five cases. They have the same initial temperature (300 K), heating rate (700 K/s) and peak temperature (1700 K), but have different cooling rates (Fig. 4.5). The initial austenite grain sizes are all set to $10\mu\text{m}$. The chemical composition for this test is the base metal from Table 4.1.

Figure 4.4: Two-element mesh for tests.

4.3.1.1 Phase Transformation

Due to different cooling rates, the microstructure evolution, while cooling, behaves quite differently for the five cases.

- Case 1: The cooling rate is -700 K/s . Because of the very high cooling rate, most of the austenite phase changes to martensite. There are also some ferrite, bainite and residual austenite phases (Fig. 4.6). The final hardness is $HV371$.
- Case 2: The cooling rate is -233.3 K/s . At this cooling rate, the majority of the final phase is the ferrite phase, with some bainite, martensite and residual austenite phases (Fig. 4.7). The final hardness is $HV193$.

Figure 4.5: Temperature profile of five test cases during cooling.

- Case 3: The cooling rate is -100 K/s . The final phases are ferrite and bainite phases (Fig. 4.8). The final hardness is $HV145$.
- Case 4: The cooling rate is -35 K/s . The final phases are ferrite and bainite phases (Fig. 4.9). The final hardness is $HV139$.
- Case 5: The cooling rate is -10 K/s . The final phases are ferrite and pearlite phases, with very little bainite phase (Fig. 4.10). The final hardness is $HV120$.

Figure 4.6: Phase fractions at cooling rate = -700 K/s .

Figure 4.7: Phase fractions at cooling rate = -233.33 K/s .

Figure 4.8: Phase fractions at cooling rate $\dot{T} = -100\text{ K/s}$.

Figure 4.9: Phase fractions at cooling rate $\dot{T} = -35\text{ K/s}$.

Figure 4.10: Phase fractions at cooling rate = -10 K/s .

During the thermal cycle, the austenite grains grow mainly depending on the time the material point stays above the A_3 temperature (or more precisely, T_S temperature). Figure 4.11 shows the austenite grain growth during cooling for different cases: at the peak temperature, they have the same grain size ($\sim 20\mu\text{m}$). With different cooling rates, the final austenite grain size varies from $25\mu\text{m}$ in case 1 to $162\mu\text{m}$ in case 5.

Figure 4.11: Austenite grain growth for five test cases.

4.3.1.2 Dilatometer Curve of thermal strain and transformation strain

A dilatometer is used to determine the thermal expansion coefficient of a material while heating or cooling. Microstructural transformations in the solid state are usually studied by dilatometry. When a phase transformation takes place, if the new phase occupies a different volume than the old phase, the transformation strain and the thermal strain of the phases will add, and a discontinuity will be observed in the thermal strain vs. temperature curve.

A test, which simulates the dilatometer curve of the low-alloy steel during thermal cycles, is presented here to test the algorithm developed in this work. The specific volume results from the phase transformation test are used to solve the displacements on the two element mesh which can deform freely but without rigid body modes. Dilatometer curves for the low alloy steel with different cooling rates are shown in Fig. 4.12. While heating, the A_1 - A_3 transformation temperature region is marked as a discontinuity. While cooling, depending on the cooling rate, the transformation temperature differs.

Figure 4.12: Dilatometer curve for a low-alloy steel.

4.3.2 Butt Weld

The domain (Fig. 4.13) needed for microstructure analysis is much smaller than that for thermal analysis, because phase transformations only take place in the fusion zone, partially melted zone, and heat-affected zone. The microstructures were computed for the quasi-steady state temperature field obtained from Chapter 3 (Fig. 3.8-Fig. 3.9) by data mapping. The welding speed was 0.002 m/s . The chemical compositions for the test is based on Table 4.1 for filler metal and base metal. To make sure the phase transformation is completed, the mesh should be long enough so that the maximum temperature in the downstream outlet surface is below 500 K .

Figure 4.13: Mesh for microstructure evolution.

Figure 4.14: Phase fractions in the downstream outlet surface.

The microstructure results for the butt weld test are shown in Figure 4.15 and Figure 4.14. The hardness in the downstream outlet surface is in Figure 4.16.

Figure 4.15: Bird's eye view of the microstructure evolution in the weld pool region.

(a). liquid phase; (b). ferrite (delta) phase; (c). austenite phase.

Figure 4.16: Hardness profile in the downstream outlet surface.

Chapter 5

Stress Analysis

The prediction of residual stresses are very important because these stresses can reduce the usefulness of the object by altering the performance. Because of the extreme complexity involved in the numerical stress analysis, even with the super-powerful computers available today, it seems that some kinds of simplification are necessary to carry out an application-oriented FEM simulation of a weld process.

The reduction of the transient process to a quasi-stationary (steady state) process is one of such simplification. It is based on the fact that in many welds there exists small transient regions at the start and end of the weld pass where the thermal and stress histories differ from those in the middle part because of transients caused by turning the heat source on and off or by the presence of the plate ends. These regions are known as the end transients. These end-transients are purely a 3D phenomenon.

For a long weld, a quasi-steady state solution of the stress field can be found that is a useful approximation of the real stress field over most of the middle part of the weld joint. Only at the starting and stopping end of the weld is the stress field substantially different from the quasi-steady state middle part. For a one-meter butt weld, the region of end-transients are about 15 *cm* on both ends [42]. So, for long welds, the quasi-steady state assumption for the middle part is reliable. It is also very practical because many real welds are often several meters in lengths. The stress field in fusion welding basically has the following features:

- The stress field is driven by the thermal cycle. A good thermal analysis is critical for stress analysis.
- In stress analysis, the plastic deformation should be considered. The mechanical properties are both temperature and deformation-history dependent.
- Phase transformations occur during the welding process. The effects of such transformations should be included to predict the stress state, and the final residual stress.

To simulate a complete weld, a combination of the transient Lagrangian formulation with the quasi-steady state Eulerian formulation is desirable. The whole weld workpiece or weld joint domain will be analyzed by the Lagrangian formulation. But for the middle part, based on the quasi-stationary assumption, we can use an Eule-

rian formulation to carry out a stress analysis which is focused just on the weld pool region. The results from the quasi-steady state stress analysis can be used as a trial solution for the transient stress analysis using Lagrangian formulation. There are two advantages to using the results from the Eulerian stress analysis: (1). It greatly reduces the number of non-linear iterations. (2). it can use a larger time step without the “spot” welding effect, because the quasi-steady state analysis results contains the deformation history and the evolution of internal variables.

In this Chapter, the FEM algorithms are presented for 3D transient stress analysis by a Lagrangian formulation, as well as 3D quasi-steady state stress analysis based on a flow tube model. Both analyses use the same constitutive (stress-strain) relation that is intended to deal with thermal-elasto-viscoplastic, large deformation (finite strain) and phase transformation phenomena.

5.1 Deformation Gradient

During the welding process, the material points in the workpiece experience large displacements, large strains, thermal expansion/shrinkage, plastic deformation and phase changes. Large residual stresses often exist in the workpiece after welding. Weld deformations are often very large, so large in fact that the change in shape can usually be clearly visible to the eye. Infinitesimal strain measures can cause large errors in the residual stress analysis for welds [43]. Finite strain measurements have

to be used in the residual stress and deformation analysis for welds.

In a large deformation analysis, special attention must be given to the fact that the configuration of the body is changing continuously. This change in configuration can be dealt with in an elegant manner by defining a key quantity, the deformation gradient and appropriate stress and strain measures as functions of time.

By introducing a reference configuration, any configuration in the deformation process can be expressed in that reference configuration. Let $\mathcal{B}$ denote the reference configuration of a body, and $\mathcal{B}'$ denote the current configuration at time t . We can define:

$$\mathcal{B}' = \varphi(\mathcal{B}, t) \quad (5.1)$$

where φ is the map of the motion of a body. If X is a point in the reference configuration $\mathcal{B}$, and x is a point in current configuration $\mathcal{B}'$, at time t , then:

$$x = \varphi(X, t)$$

and the inverse map is χ , such that:

$$X = \chi(x, t)$$

A fundamental measure of the deformation of the body is given by the deformation gradient, at any time t , defined as:

$${}^t\mathbf{F} \equiv \mathbf{F}(X, t) = \frac{\partial \varphi(X, t)}{\partial X} = \nabla_0 \varphi \quad (5.2)$$

The deformation gradient tensor describes both the rotation and stretch in the neighborhood of a material point that the body experiences during the deformation. The tensor $\mathbf{F}$ can, by polar decomposition, be expressed as the product of a rotation tensor with a stretch tensor:

$$\mathbf{F} = \mathbf{R}\mathbf{U} \quad (5.3)$$

or

$$\mathbf{F} = \mathbf{V}\mathbf{R} \quad (5.4)$$

where $\mathbf{R}$ is the orthogonal rotation tensor, $\mathbf{U}$ is the symmetric right (material) stretch tensor, and $\mathbf{V}$ is the symmetric left (spatial) stretch tensor. For the purpose of calculation, we may define two more tensors:

$$\mathbf{C} = \mathbf{F}^T \mathbf{F} = \mathbf{U}^T \mathbf{U} = \mathbf{U}^2 \quad (5.5)$$

$$\mathbf{b} = \mathbf{F} \mathbf{F}^T = \mathbf{V} \mathbf{V}^T = \mathbf{V}^2 \quad (5.6)$$

where $\mathbf{C}$ is the *right Cauchy-Green strain tensor*, and $\mathbf{b}$ is the *left Cauchy-Green strain tensor*.

By choosing a proper reference configuration, and by mapping material points in any of the other configurations to the reference configuration, it is possible to obtain the deformation gradient tensor between any two deformed configurations. Let ${}^i\mathbf{F}$ be the deformation gradient from the reference configuration to $\mathcal{B}^i$, and ${}^{i-1}\mathbf{F}$ be the deformation gradient from the reference configuration to $\mathcal{B}^{i-1}$. Then, a relative defor-

mation gradient tensor, ${}_{i-1}^i\mathbf{F}$, between a configuration at time i and a configuration at time $i - 1$ will be:

$${}_{i-1}^i\mathbf{F} = {}^i\mathbf{F}(X) {}^{i-1}\mathbf{F}(X)^{-1} \quad (5.7)$$

Any constitutive model requires that the stress and strain must be work-conjugate each other, i.e., the measurements of the stress and strain must be in the same configuration and their inner product should equal work or the strain energy density. Several valid measurements of stress-strain rate pairs are listed below:

- The first Piola-Kirchhoff stress, which is non-symmetric, is work-conjugate to the rate of the deformation gradient $\dot{\mathbf{F}}$. They are both measured in the initial undeformed geometry.
- The second Piola-Kirchhoff stress is work conjugate to the material strain rate tensor $\dot{\mathbf{E}}$ and often deals with large displacement, large rotation problems in total Lagrangian formulation. This is because they are all measured in the initial undeformed geometry. The material strain rate tensor can be expressed in indicial notation as:

$$\dot{\mathbf{E}} = \frac{1}{2}\dot{\mathbf{C}} = \frac{1}{2}(\dot{\mathbf{F}}^T \mathbf{F} + \mathbf{F}^T \dot{\mathbf{F}})$$

- The Cauchy (or true) stress is work conjugate with the logarithmic (also called Hencky or true) strain rate $\dot{\epsilon}$. The Cauchy stress is measured in the final

deformed geometry. The logarithmic strain will be defined in the following section.

For large strain inelastic analysis in an updated Lagrangian formulation, logarithmic strain and Cauchy stress measures are recommended [8][43]. They argue that (1). They have physical meaning and most engineers are familiar with the concept of true strain. (2). The yield condition, constitutive relation, flow rule, and hardening rule are written in terms of the true stresses.

For computational convenience, another true stress tensor, the Kirchhoff stress $\boldsymbol{\tau}$ is introduced. Like the Cauchy stress, it is a spatial symmetric tensor field. It is related to the Cauchy stress $\boldsymbol{\sigma}$ by:

$$\boldsymbol{\tau} = J\boldsymbol{\sigma}$$

where $J = \det(\mathbf{F})$ is the Jacobian.

5.2 Constitutive Relations

The stress-strain (constitutive) relations reflects the material response to the strain at the current configuration. In a numerical approach, the material relationships are used at two points of the solution process [8]: (1) the evaluation of the stresses which are used in the calculation of the nodal point force vectors and the nonlinear strain

stiffness matrices, (2) the evaluation of the tangent stress-strain matrices which are in the calculation of the linear strain stiffness matrices.

It is imperative that the stresses be evaluated with high accuracy since otherwise the solution will not converge to the correct solution, and it is also important that the stiffness matrices be truly tangent matrices since otherwise, in general, the convergence rate will be slower than necessary. The evaluation of the stresses and the tangent stress-strain matrix is performed at each element integration point for each Newton-Raphson iteration. Hence, it is imperative that these computations be performed as efficiently as possible.

Prediction of the stress, strain and displacement fields in a weld requires a constitutive model that deals with thermo-elasto-viscoplastic deformation. Traditional models decompose the total strain rate $\dot{\epsilon}^{tot}$ into the elastic $\dot{\epsilon}^{el}$, viscoplastic $\dot{\epsilon}^{vp}$, and thermal $\dot{\epsilon}^{th}$ strain rate. When dealing with phase transformations, extra terms: namely, $\dot{\epsilon}^{TrV}$, the volume change rate associated with the transformation, and $\dot{\epsilon}^{TrP}$, the transformation plasticity strain rate are introduced.

$$\dot{\epsilon}^{tot} = \dot{\epsilon}^{el} + \dot{\epsilon}^{vp} + \dot{\epsilon}^{th} + \dot{\epsilon}^{TrV} + \dot{\epsilon}^{TrP} \quad (5.8)$$

The constitutive equations describing inelastic materials invariably depend upon the path followed to reach a given state of deformation and stress. It is therefore essential to be able to closely follow this path in order to accurately obtain current

stress values. This is implemented by taking a sufficient number of load increments, which may be related to an artificial or real time parameter.

For large strain inelastic analysis, up to the late 80's, an integration process was used from the state at time t to the current strain state, based on the rate model [43]. Using a rate-type formulation, rates of stress, strain, and rotational effects are integrated, which leads to additional numerical errors and, for an accurate solution, requires significantly smaller solution steps than are needed in a total strain formulation. Simo [44] and other workers [8] proposed a finite strain analysis procedure that is formally similar to the well-established infinitesimal strain analysis procedure. An important feature of the infinitesimal strain analysis procedures is that these formulations are total strain and not rate-type formulations. That is, the equations of equilibrium are written for time $t + \Delta t$ and the total strain for that time is calculated.

A natural approach based on micromechanical observations for large strain elastoplasticity is based on the hyperelastic material description with the product decomposition of the deformation gradient into elastic and plastic parts. Such an approach also lends itself to a total formulation that is a natural extension of the infinitesimal strain formulation.

The constitutive relation used in this thesis is based on Simo's model [44][45]

5.2.1 The Thermal-Elasto-Viscoplastic Finite Strain Model

A convex elastic domain $\mathbf{E}$ which is specified by a smooth yield criterion in stress space could be defined as:

$$\mathbf{E} = \{(\boldsymbol{\tau}, \mathbf{q}) \in \mathbf{S} \times R^m \mid \phi(\boldsymbol{\tau}, \mathbf{q}) \leq 0\} \quad (5.9)$$

where $\mathbf{S}$ is the vector space of symmetric 3×3 tensors, and $\mathbf{q}$ is a m -dimensional vector of hardening parameters. $\phi()$ is a scalar-valued isotropic function. Here, $\boldsymbol{\tau}$ is interpreted as the Kirchhoff stress tensor.

It is assumed that for any material point, at any instant in the motion, the deformation gradient can be factored into an elastic and plastic deformation by using the multiplicative decomposition:

$${}^t\mathbf{F} = {}^t\mathbf{F}^e {}^\tau\mathbf{F}^p \quad (5.10)$$

For conceptual understanding, we may write the above equation as:

$${}^t\mathbf{F} = {}^t\mathbf{F}^e {}^\tau\mathbf{F}^p.$$

Hence, we can interpret it in a way that the total deformation is obtained by first applying the plastic deformation which takes place from the original to the hypothetical configuration (corresponding to τ) by ${}^\tau\mathbf{F}^p$. Then, the elastic deformation occurs with ${}^t\mathbf{F}^e$, the deformation gradient which is thought to be from the relaxed configuration τ to final time t , and therefore stresses are measured using the elastic strain increment

from this deformation gradient. The relaxed hypothetical configuration (corresponding to τ) can be obtained by unloading the material from the current configuration to a state of zero stress in such a way that no inelastic process takes place.

It is also assumed that there is a free energy function ψ which represents the stored energy resulting from elastic deformation. Isotropy implies that ψ depends on $\mathbf{F}^e$ only through the corresponding elastic left Cauchy-Green strain:

$$\psi = \psi(\mathbf{b}^e, \xi).$$

where ξ denotes the vector of (strain-like) internal variables conjugate to $\mathbf{q}$ in the sense that:

$$\mathbf{q} = -\partial_\xi \psi(\mathbf{b}^e, \xi).$$

we also have a dissipation function $\mathcal{D}(x, t)$, a spatial scalar field, defined as

$$\mathcal{D} = \boldsymbol{\tau} \cdot \dot{\boldsymbol{\varepsilon}} - \frac{d}{dt} \psi(\boldsymbol{\varepsilon}^e, \xi)$$

Clearly, for elastic deformation, $\mathcal{D} = 0$, and for inelastic deformation, the inequality $\mathcal{D} \geq 0$ is a consequence of the second law [48]. The simplest model describing the evolution of plastic flow is obtained by postulating maximum dissipation of the flow. Simo [44] provided the evolution equations for viscoplasticity as:

$$-\frac{1}{2} \mathcal{L}[\mathbf{b}^e] = \Delta \gamma \partial_{\boldsymbol{\tau}} \phi(\boldsymbol{\tau}, \mathbf{q}) \mathbf{b}^e \quad (5.11)$$

$$\dot{\xi} = \Delta \gamma \partial_{\mathbf{q}} \phi(\boldsymbol{\tau}, \mathbf{q}) \quad (5.12)$$

$$\Delta \gamma = g(\phi(\boldsymbol{\tau}, \mathbf{q})) \Delta t / \eta \quad (5.13)$$

where $\mathcal{L}[\mathbf{b}^e]$ is referred to as the Lie derivative of $\mathbf{b}^e$, $\Delta\gamma$ is the plastic consistency parameter (or Kuhn-Tucker variable) that indicates whether yielding has occurred. η is viscosity. Δt is the time step size. $g(x)$ is a penalty function, which for one special case can be defined as:

$$g(x) = x^+ = \max(x, 0)$$

Now, we can apply the theory to a specific case: if the function ϕ , which constrains the elastic domain, is defined by the Von Mises yield criterion, with the flow rule given by 5.11 - 5.13, we can immediately obtain the J_2 flow theory for finite strain.

As in small strain plasticity, it is always assumed that the J_2 plastic deformation is incompressible; hence,

$$\det(\mathbf{F}^p) = \det(\mathbf{C}^p) = 1.$$

5.2.1.1 Thermal Strain

The thermal strain is connected with the temperature change in a body. It is reversible and, for polycrystalline metals, isotropic. The expression is:

$$\dot{\epsilon}^{th} = \alpha \dot{T} \mathbf{I} \quad (5.14)$$

where α is the coefficient of linear thermal expansion, normally a temperature-dependent property. $\mathbf{I}$ is a 3×3 identity matrix here.

One important consideration here is that the thermal strain and the strain from the displacement can be incompatible [16] if the same mesh and element basis functions

are used for both thermal and stress analysis. To solve this problem, methods of selective reduced integration are often used on the dilatation components of strain to alleviate the inconsistency. In this thesis, quadratic elements are used for the stress analysis, while linear elements are used for the temperature field.

5.2.1.2 J_2 Flow Theory for Finite Strain with Principal Components

One of the simplest possible constitutive models that works well for many metals is the Von Mises plasticity theory. Von Mises plasticity with linear isotropic hardening is defined by a yield surface Φ , which is a function of true (Kirchhoff) stress $\boldsymbol{\tau}$ and a hardening parameter given by the Von Mises equivalent plastic strain ξ (internal variables). For finite strain, Simo [44] suggests using the principal Kirchhoff stress, so the yield function becomes:

$$\hat{\phi}(\boldsymbol{\tau}, \xi) = \|\text{dev}(\boldsymbol{\tau})\| - \sqrt{\frac{2}{3}} K(\xi) \quad (5.15)$$

where $\boldsymbol{\tau} = [\tau_1, \tau_2, \tau_3]^T$ is the vector of 3 principal components and $\text{dev}(\boldsymbol{\tau})$ is the deviatoric part of $\boldsymbol{\tau}$ defined as:

$$\text{dev}(\boldsymbol{\tau}) = \boldsymbol{\tau} - \frac{1}{3} \text{Tr}(\boldsymbol{\tau}) \mathbf{I}$$

while $K(\xi)$ is a hardening function. If it is assumed to be linear in ξ , the hardening function will be:

$$K(\xi) = \sigma_Y + K' \xi$$

The spectral decomposition is used to obtain the principal strains and stresses, which should be commute with each other (i.e., they have the same eigenvectors). Now, we defined the logarithmic elastic stretch tensor $\tilde{\varepsilon}^e$ and logarithmic stretch tensor $\tilde{\varepsilon}$ as:

$$\tilde{\varepsilon}^e = \frac{1}{2} \log(\mathbf{b}^e) \quad (5.16)$$

$$\tilde{\varepsilon} = \frac{1}{2} \log(\mathbf{b}) \quad (5.17)$$

Suppose $(\lambda_k^e)^2$ and $\mathbf{v}_k$ are the eigenvalues and normalized eigenvectors of $\mathbf{b}^e$, then, we can write:

$$\mathbf{b}^e = \sum_{k=1}^3 (\lambda_k^e)^2 (\mathbf{v}_k \otimes \mathbf{v}_k) \quad (5.18)$$

$$\tilde{\varepsilon}^e = \sum_{k=1}^3 \log(\lambda_k^e) (\mathbf{v}_k \otimes \mathbf{v}_k) \quad (5.19)$$

$$= \sum_{k=1}^3 \varepsilon_k^e (\mathbf{v}_k \otimes \mathbf{v}_k) \quad (5.20)$$

where ε_k^e is the principal strains of $\tilde{\varepsilon}^e$, and can be expressed as: $\varepsilon_k^e = \log(\lambda_k^e)$. Because they commute, the stress will be:

$$\boldsymbol{\tau} = \sum_{k=1}^3 \tau_k (\mathbf{v}_k \otimes \mathbf{v}_k) \quad (5.21)$$

here τ_k is the principal Kirchhoff stresses. Because of isotropy, the trial elastic strain $\mathbf{b}_{tr}^e$ commutes with $\mathbf{b}^e$, so we can write:

$$\mathbf{b}_{tr}^e = \sum_{k=1}^3 (\lambda_{trk}^e)^2 (\mathbf{v}_k \otimes \mathbf{v}_k)$$

Now, the flow rule (5.11 - 5.13) becomes:

$$\varepsilon_k^e = \varepsilon_{trk}^e - \Delta\gamma \partial_{\tau_k} \hat{\phi}(\tau_1, \tau_2, \tau_3, \mathbf{q}) \quad (5.22)$$

$$\xi = \xi_n + \Delta\gamma \partial_{\mathbf{q}} \hat{\phi}(\tau_1, \tau_2, \tau_3, \mathbf{q}) \quad (5.23)$$

$$\Delta\gamma = \dot{\phi}(\tau_1, \tau_2, \tau_3, \mathbf{q}) / [(\eta/\Delta t) + 2\mu + \frac{2}{3} K(\xi)] \quad (5.24)$$

If a trial elastic strain $\mathbf{b}_{tr}^e$ causes an elastic deformation, then, we have $\Delta\gamma = 0$. If plastic deformation occurs, $\Delta\gamma > 0$, and the radial-return algorithm will be needed to solve for $\Delta\gamma$.

5.2.1.3 Radial-Return Algorithm

Radial return mapping algorithms are widely used in many commercial finite element softwares. The technique is remarkably simple. Within a typical time step, one first computes a trial elastic state for prescribed strain increments by ignoring plastic flow. Then, the actual stress is defined as the closest-point projection of the trial state onto the elastic domain in the natural norm defined by the complementary (Helmholtz) energy. This projection is computed locally at each quadrature point of a typical finite element and depends exclusively on the functional form adopted by the yield criterion in stress space.

For J_2 flow theory, the return mapping algorithm boils down to the classical radial return method [46][47]. Here, the solution is obtained by radially scaling the deviatoric trial stress onto the Mises yield surface.

Suppose we know the balanced stress and internal variables at the end of the last time step, then for a trial elastic state, we can compute the new equilibrium stress for a new time step. The algorithm will be:

1. Compute the trial principal logarithmic stretches and trial principal stress:

$$\varepsilon_{trk}^3 = \log(\lambda_{trk}^3)$$

$$\underline{\boldsymbol{\tau}}_{tr}^3 = \mathbf{a} \underline{\boldsymbol{\varepsilon}}_{tr}^3$$

where $\mathbf{a}$ is the constant 3×3 matrix of elastic moduli in principal stress space:

$$\mathbf{a} = 2\mu[\mathbf{I} - \frac{1}{3}(\underline{\mathbf{1}} \otimes \underline{\mathbf{1}})] + \kappa(\underline{\mathbf{1}} \otimes \underline{\mathbf{1}})$$

here μ is the shear modulus, κ is the bulk modulus, and $\underline{\mathbf{1}} = [111]^T$.

2. Compute the deviatoric trial stress:

$$\underline{\mathbf{s}}_{tr}^3 = dev(\underline{\boldsymbol{\tau}}_{tr}^3)$$

3. Test for trial load:

$$\hat{\phi}_{tr}^3 = \|\underline{\mathbf{s}}_{tr}^3\| - \sqrt{\frac{2}{3}K(\alpha^1)}$$

If $\hat{\phi}_{tr}^3 \leq 0$, then $\Delta\gamma = 0$. Otherwise, go to the “Radial Return” step solve for $\Delta\gamma$.

4. Radial Return: The algorithmic loading condition $\hat{\phi}_{tr}^3 > 0$ implies that $\Delta\gamma > 0$, and the consistency condition $\hat{\phi}^3 = 0$ yields the following scalar equation which

defines $\Delta\gamma$ during plastic loading:

$$\hat{\phi}_{tr}^3 - g^{-1}(\eta\Delta\gamma/\Delta t) - 2\mu\Delta\gamma - \sqrt{\frac{2}{3}}[K(\alpha^1 + \sqrt{\frac{2}{3}}\Delta\gamma) - K(\alpha^1)] = 0 \quad (5.25)$$

Having evaluated $\Delta\gamma$, set the unit normal to the Mises cylinder in principal stress space:

$$\underline{\mathbf{n}} = \underline{\mathbf{s}}_{tr}^3 / \|\underline{\mathbf{s}}_{tr}^3\|$$

5. Update stress and internal variables:

$$\begin{aligned} \underline{\mathbf{s}}^3 &= \underline{\mathbf{s}}_{tr}^3 - 2\mu\Delta\gamma \underline{\mathbf{n}} \\ \alpha^3 &= \alpha^1 + \sqrt{\frac{2}{3}}\Delta\gamma \\ \underline{\boldsymbol{\tau}}^3 &= \underline{\boldsymbol{\tau}}_{tr}^3 - 2\mu\Delta\gamma \underline{\mathbf{n}} \\ \underline{\boldsymbol{\varepsilon}}^{e3} &= \mathbf{a}^{-1}\underline{\boldsymbol{\tau}}^3 \end{aligned}$$

5.2.1.4 Tangent Modulus

Prior to the mid 80's, implementations of Newton's method used the standard elasto-plastic moduli obtained by enforcing the consistency condition on the rate model.

Simo [44] proposed an efficient algorithm to obtain the consistent moduli. The exact closed-form linearization of the return map produces modified elastoplastic moduli, referred to as the consistent algorithmic moduli, which restore the quadratic rate of convergence of Newton's method and results in improved rates of convergence. The algorithmic elasto-visco-plastic moduli $\mathbf{a}^{vp}$ associated with the radial return map

will be explicitly expressed as:

$$\mathbf{a}^{vp} = \kappa \mathbf{1} \otimes \mathbf{1} + 2\mu[\theta(I - \frac{1}{3}\mathbf{1} \otimes \mathbf{1}) - \delta(\mathbf{n} \otimes \mathbf{n})] \quad (5.26)$$

where the coefficients θ and δ are:

$$\begin{aligned} \theta &= 1 - \frac{2\mu\Delta\gamma}{\|\mathbf{s}_{tr}^3\|} \\ \delta &= \begin{cases} \frac{2\mu}{2\mu + \frac{2}{3}K(\alpha)} - (1 - \theta), & \Delta\gamma > 0 \\ 0, & \Delta\gamma = 0 \end{cases} \end{aligned}$$

note that $\mathbf{a}^{vp}$ is a symmetric, 3×3 matrix.

5.2.2 Transformation Plasticity

During welding process, phase transformations often occur, and thus, result in a volume change. Phase transformations can have a significant effect on the residual stress in two ways: volume changes which occur during the phase transformation, and transformation plasticity.

During a phase transformation, in addition to the reversible volume change, some amount of inelastic deformation may be induced if the body has a non-zero stress state, even if the stresses are well below the yield value. This deformation is named transformation plasticity.

Transformation plasticity is irreversible, proportional to the stresses present, and will cease if the transformation ceases. It occurs through the interaction of the stresses

and the volume change during phase transformation. There are two widely recognized mechanisms: (1). The Greenwood-Johnson [49] mechanism: It states that the volume change between the two coexisting phases generates microscopic plasticity in the weaker phase and this permits macroscopic plastic flow in the presence of an applied stress; (2). The Magee [50] mechanism: It states that for a martensitic transformation, as the atoms rearrange themselves, some orientations are preferred due to the presence of stresses, and this affects the overall shape of the body.

Leblond [51] provided a theoretical analysis for transformation plasticity that suggested that transformation plasticity is a consequence of the homogenization process without postulating arbitrary extra plastic strain. He decomposed the traceless plastic strain ϵ^{pl} into two terms: (1). the classical plastic strain ϵ^c which describes the response of the material to variations of the applied stress and/or the temperature; (2). the transformation plastic strain ϵ^{tp} that describes the response of the material to variations of the phase fractions.

Here, we just consider the response of the material to variations of the phase fractions. Oddy [43] proposed, for each time step, explicit expressions for computing the hydrostatic volume change $\Delta\epsilon^{tv}$ and transformation plastic strain increment $\Delta\epsilon^{tp}$ as:

$$\Delta\epsilon^{tv} = \frac{1}{3} \frac{\Delta V}{V} I \quad (5.27)$$

$$\Delta\epsilon^{tp} = \frac{5}{4} \frac{\Delta V}{V} \frac{1}{\sigma_Y} \mathbf{s}(2 - 2z_{(n)} - \Delta z) \Delta z \quad (5.28)$$

where $\Delta V/V$ is the change in specific volume. I is a 3x3 identity matrix, σ_Y is the flow stress in the weaker phase, $\mathbf{s}$ is the deviatoric stress tensor, $z_{(n)}$ is the fraction transformed at the start of the time step and Δz is the amount that transformed during the time step.

The volume change $\Delta \epsilon^{tr}$ can be treated the same way as thermal strain. Here we focus on the transformation plastic strain increment $\Delta \epsilon^{tp}$. During the phase transformation, the stress can change dramatically. If the time step size is too large, using a constant stress can result in two problems: loss of accuracy and numerical instability [54]. To overcome the problems, the normal time step is divided into a number of smaller substeps according to the value of fraction transformed.

For a low-alloy steel, during the thermal cycle of welding, the transformation from austenite to martensite is more important for transformation plasticity based on two facts: (1). significant stresses may be developed before the transformation occurs for low transformation temperature; (2). the volume change is larger (4% compares to 1% for austenite decomposing to ferrite).

5.3 FEM Formulation and Implementation

From conservation of momentum, if we neglect the inertial force term, we obtain a local spatial equilibrium equation for quasi-static state in the current configuration:

$$\nabla \cdot \boldsymbol{\sigma} + \mathbf{f} = 0 \quad (5.29)$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor associated with the current spatial configuration, $\mathbf{f}$ is the body force per unit volume. This equation is valid for both Lagrangian and Eulerian reference frame.

For the FEM formulation, the equilibrium equation 5.29 will be integrated over the physical configuration, or a reference configuration with unique mapping to that physical configuration.

5.3.1 Transient Stress Analysis by Lagrangian Formulation

The Lagrangian formulation or the updated Lagrangian(UL) formulation, which is the one most commonly used in solid mechanics, has dominated computational weld mechanics for more than a decade. To avoid the spot welding effect, as discussed earlier, many small time steps would be necessary.

For an incremental step-by-step analysis, the updated Lagrangian formulation may be more numerically efficient based on the fact that in the total Lagrangian formulation the strain-displacement matrix is more complex [8]. It will be more

convenient to use an updated Lagrangian formulation which updates all static and kinematic variables at the end of every time step.

For the time step from t to $t + \Delta t$, the solution for the discrete time t is assumed to be known and, in fact, is assigned to be the initial condition in the (UL) formulation. The solution for the discrete time $t + \Delta t$ is required. To solve the problem by FEM, the equilibrium conditions of a system of finite elements representing the body under consideration (domain) can be expressed as:

$${}^{t+\Delta t}\mathbf{f}^{int} - {}^{t+\Delta t}\mathbf{f}^{ext} = 0 \quad (5.30)$$

where the left superscript denotes “at time $t + \Delta t$ ”, $\mathbf{f}^{int}$ is the nodal internal force vector that correspond to the element stresses in this configuration and $\mathbf{f}^{ext}$ is the nodal external force vector applied in this configuration. This means that the equilibrium equation 5.30 is evaluated in the configuration at the current time $t + \Delta t$. For each element, the internal and external nodal force vector can be computed as:

$${}^{t+\Delta t}\mathbf{f}_e^{int} = \int_{\Omega^e} {}^{t+\Delta t}\mathbf{B}^T {}^{t+\Delta t}\boldsymbol{\sigma} d\Omega \quad (5.31)$$

$${}^{t+\Delta t}\mathbf{f}_e^{ext} = \int_{\Gamma^e} {}^{t+\Delta t}\mathbf{R}^T {}^{t+\Delta t}\mathbf{T} d\Gamma - \int_{\Omega^e} {}^{t+\Delta t}\mathbf{R}^T {}^{t+\Delta t}\mathbf{f} d\Omega \quad (5.32)$$

where ${}^{t+\Delta t}\mathbf{B}$ and ${}^{t+\Delta t}\mathbf{R}$ are the matrix of symmetric physical gradient operator and matrix of basis functions, respectively. ${}^{t+\Delta t}\mathbf{T}$ is the surface traction exerted on the boundary, Γ , of the domain Ω . The global nodal force vectors are assembled from

element nodal force vectors:

$${}^{t+\Delta t}\mathbf{f}^{int} = \mathbf{\Pi} {}^{t+\Delta t}\mathbf{f}_e^{int} \quad (5.33)$$

$${}^{t+\Delta t}\mathbf{f}^{ext} = \mathbf{\Pi} {}^{t+\Delta t}\mathbf{f}_e^{ext} \quad (5.34)$$

Normally, with the thermal-elasto-viscoplastic finite strain analysis, equation 5.30 is nonlinear. In a displacement-based FEM analysis, by introducing the tangent stiffness matrix $\mathbf{K}$, a linearized matrix equation can be obtained for the time step from t to $t + \Delta t$:

$$\mathbf{K} \mathbf{dU} = {}^{t+\Delta t}\mathbf{f}^{ext} - {}^t\mathbf{f}^{int} \quad (5.35)$$

where $\mathbf{dU}$ is a vector of nodal displacement increment in this time step.

By using the Newton-Raphson iterative scheme, the linearized equation 5.35 is iteratively solved until a solution to the nonlinear problem in equation 5.30 is found.

The equations used in the Newton-Raphson, at iteration k , are:

$${}^{t+\Delta t}\mathbf{K}_{k-1} \mathbf{du}_k = {}^{t+\Delta t}\mathbf{f}^{ext} - {}^{t+\Delta t}\mathbf{f}_{k-1}^{int} \quad (5.36)$$

$${}^{t+\Delta t}\mathbf{dU}_k = {}^{t+\Delta t}\mathbf{dU}_{k-1} + \mathbf{du}_k \quad (5.37)$$

with the initial conditions:

$${}^{t+\Delta t}\mathbf{dU}_0 = 0 \quad (5.38)$$

$${}^{t+\Delta t}\mathbf{K}_0 = {}^t\mathbf{K} \quad (5.39)$$

$${}^{t+\Delta t}\mathbf{f}_0^{int} = {}^t\mathbf{f}_0^{int} \quad (5.40)$$

For each Newton-Raphson iteration, the residual vector

$$\mathbf{r}_k = {}^{t+\Delta t}\mathbf{f}^{ext} - {}^{t+\Delta t}\mathbf{f}_k^{int}$$

and its Euclidean norm are calculated. If the Euclidean norm or energy norm of the residual vector is smaller than a tolerance, or the convergence ratio (the Euclidean norm over a reference number, usually the Euclidean norm of the maximum residual vector of the problem) is smaller than a tolerance, the linearized equation 5.35 is considered to be converged, and thus, the equation is solved. The solution (displacement field) here satisfies the equation of continuity and the Dirichlet BCs. Thus, the stress computed here is called kinematically admissible stress. But, the error between the FEM solution and the exact solution can not be predicted by residual type error estimates.

A more reliable error measurement was implemented based on considering both kinematically admissible stress (KAS) and statically admissible stress (SAS) fields [59][60]. A statically admissible stress field is defined as the stress field that satisfied the static equilibrium conditions in the interior and on the Neumann boundaries of domain. Mashaie [59] pointed out that the difference between the energy norm (defined in strain energy) of the kinematically admissible stress field and that of the statically admissible stress field is an upper bound for the difference between the energy norm of the kinematically admissible stress field and that of the exact solution of the problem.

The statically admissible stress field can be computed from the kinematically admissible stress field, together with enforcing the Neumann constraints.

With the error bound in each element computed, one can efficiently determine when the problem is solved, or where the mesh needs to be refined or coarsened for certain accuracy or efficiency requirements.

5.3.2 Quasi-Steady State Stress Analysis by Eulerian Formulation

A steady state is a physical field (scalar, vector or tensor) that does not change with respect to time in some specific reference frame, i.e., the time derivatives are zero. In the manufacturing industry, a quasi-steady state (quasi-stationary) under a localized load in a certain region (frame) is quite common. Many manufacturing processes, such as sheet rolling, extrusion, wire drawing, continuous casting, laser surface heat treatment, just name a few, contain problems for which at least an approximate steady state (quasi-stationary) phenomenon exists.

In long welds, except at the start and end of a pass, the processes, more or less, approach the steady state of their physical fields in the majority middle parts. The most concerned region in steady-state stress analysis for welding is where the plastic deformation occurs. It is also noticed that the major part of a thermal cycle in the steady state covers a short distance compared to the length of a long weld path. So,

for a nearly prismatic workpiece with prismatic axis in the direction of welding at least near the weld joint, the domain for quasi-steady state analysis can be chosen as a prismatic domain with constant cross-section that only includes the weld pool and the nearby region.

To simulate quasi-steady state phenomenon occurring in the welding process, normally, one chooses the domain to be fixed with respect to the heat source (i.e., an Eulerian frame) and to cover the weld pool region. The material points in the workpiece move relative to the Eulerian frame almost exactly at the welding speed. To include the evolution of deformation-history in the Eulerian formulation for stress analysis, the history-dependent state variables evolve along streamlines [55]. The streamlines are the characteristics of the problem and start from the inlet boundary. Gu [18] proposed a data structure, which is based on a layered-tree structure, to compute and store streamlines. The complicated data structure has the following advantages: (1). The streamlines are calculated one after another in the order from upstream to downstream; (2). For a given point, find the element that contains it; (3). Find all points along a given streamline. There are several drawbacks of the data structure: (1). It will consume CPU time to create the structure and sort data, especially, to locate the elements that contain points on the streamline; (2). It needs memory to store the structure and data; (3). It needs to interpolate and map data, which normally will lose precision.

A new strategy, which uses flow tubes to handle the evolution of variables effectively, is proposed here to simplify the data structure while dealing with the steady state stress analysis.

5.3.2.1 Flow Tube Model

Assume that there exists a coordinate system in space-time. In this coordinate system, we can define flow lines. The flow tube is a mesh structure, which contains a bundle of flow lines, to discretize the space according to the characteristics of the problem (here, along the direction of the moving heat source). If a flow tube is made by an extruded mesh with constant extrusion distance dz , from inlet to outlet, with a sequence of elements labeled $0, 1, 2, \dots, i, \dots, n-1, n$, the material point at the spatial position of Gauss point j in element i at time t_i will be at the spatial position of Gauss point j in element $i+1$ at time t_{i+1} . In fact, the inlet element holds the reference state as well as the initial condition. The history dependent variables evolve as the Lagrangian element and its material points travel down the flow tube.

To compute a quasi-steady state thermal stress solution, elements in each flow tube are integrated in order from inlet to outlet. Integration of the stress model, residual and stiffness for each element takes its initial condition from the upstream element. Nodal temperature is provided to each element by the CD thermal solver. The microstructure solver can provide microstructure information. The first element

has the initial condition which comes from the inlet boundary. For a single weld pass, for simplicity, the initial condition (also the reference state) can be set to zero displacement, zero plastic strain, zero thermal strain and zero stress. However, a more complicated general reference state can be set to the inlet element [56].

To deal with evolution along the flow tube, the relative deformation gradient (defined in 5.7) is used for stress analysis. It is computed from the relative displacement increment by:

$${}_{i-1}^i\mathbf{F} = \mathbf{I} + \nabla D\mathbf{u}(i)$$

where $D\mathbf{u}(i)$ is the relative displacement increment from element $(i - 1)$ to element (i) defined by:

$$D\mathbf{u}(i) = D\mathbf{U}(i) - D\mathbf{U}(i - 1) \quad (5.41)$$

where $D\mathbf{U}(i)$ is the total displacement of nodes in element (i) . It must always be wrt the original mesh (i.e., we can not update coordinates and still use this method to solve for a quasi-steady state stress solution).

By assuming that a trial displacement solution, time dependent temperature and the state of the reference element for each flow tube are given, we march along elements in a flow tube to compute the residual by evaluating the stress model at the Gauss points in each element relative to the previous element, i.e., using ${}_{i-1}^i\mathbf{F}$. This evaluates the stress and the internal variables at each Gauss point in each element along each flow tube. In a quasi-steady state problem, marching along a flow tube is

equivalent to marching in time for material points.

The evaluation of all elements in a flow tube can be viewed as evaluating a single element for as many time steps as there elements in the flow tube. The algorithm always works with a pair of elements, the previous (upstream) element and current element. When it goes to the next element in the flow tube, it should delete the previous element, make the current element the previous element and make the next (downstream) element the current element, i.e., a time step in flow tube i moves from the pair of elements $(i - 1)$ and (i) to the pair of elements (i) and $(i + 1)$. For filler metal added in this weld pass, the first element in a flow tube is expected to have $i > 0$.

Normally, the domain will contain several flow tubes. We need to evaluate each flow tube in turn. Then, we can solve the global equations

$$\mathbf{K} d\mathbf{u} = \mathbf{R}$$

using Newton-Raphson iterations to compute the quasi-steady state displacement and stress where $\mathbf{R}$ is residual. This is a quasi-static analysis, i.e., inertial forces are neglected. The procedure that we have just described can be considered to be one Newton-Raphson iteration. Given the updated displacement field $d\mathbf{U}+ = d\mathbf{u}$, we can solve additional NR iterations to convergence or until some maximum number of NR iterations is reached. In a fully nonlinear context, however, linear displacements will arise again during the Newton-Raphson solution process as iterative increments from

the current position of body until final equilibrium is reached.

5.4 Tests and Results

5.4.1 Transformation Plasticity

The two-element bar test in Chapter 4 (Fig. 4.4) is also used to test the influence of transformation plasticity. The domain is set to be fixed in x-direction at both ends, but can move freely in y- and z-directions. The rigid body mode is constrained to zero (i.e. no free translation and no free rotation). Three cases are compared here: (1). The volume change due to thermal expansion and phase transformation is considered; (2). In addition to the volume change, the transformation plasticity is also considered; (3). The volume change only due to thermal expansion (from data base) is considered for comparison. Because the phase transformations depend on the thermal cycle and alloy composition, the case (in Chapter 4) with cooling rate = $-700K/s$ is considered here. Figure 5.1 plots the specific volume for the test. Figure 5.2 and Figure 5.3 show the results of stress σ_{xx} and effective plastic strain, respectively. It can be seen that the volume changes accompanying the phase transformation will greatly change the stress during the thermal cycle, and will have some influence on the final stress and plastic strain states. It also shows that when transformation plasticity occurs, the effect is very similar to a sharp reduction in the

yield strength.

Figure 5.1: Specific volume for the bar test.

Figure 5.2: Stress results from the bar test.

Figure 5.3: Effective plastic strain from the bar test.

5.4.2 Quasi-Steady State Stress Analysis for an Edge Weld

An edge weld has been performed on a thin bar for steady-state thermal-stress analysis. The mesh size is $0.0508\text{ m} \times 0.00635\text{ m} \times 0.550\text{ m}$ (Fig. 5.4). 20-node brick elements are used for stress analysis. The heat source moves in the negative z-direction. The temperature distribution (Fig. 5.5) for the stress test is computed by the space-time finite element method described in Chapter 3, while the heat input is coming from the weld pool model (Chapter 2) by prescribing the temperature in the weld pool region. The specific volume and phase fraction data are provided by the microstructure model discussed in Chapter 4. The chemical compositions for base metal and filler metal are listed in Table 4.1.

Figure 5.4: Mesh for an edge weld with quasi-steady-state stress analysis.

Figure 5.5: Temperature field of the edge weld test.

The mesh in Figure 5.4 was created by extruding a 2D mesh. So, there exist elements in the upstream of the filler metal in the flow tube, where it supposed to be empty. An “element death” technique is applied here by multiplying a very small number to the element stiffness matrix and residual vector before assembly them to the global ones. The thermal distortion bends the bar into the expected “S” shape in Figure 5.6. The displacements in Figure 5.6 have been magnified 20 times. A full view of effective stress, σ_{xx} , σ_{yy} (transverse) and σ_{zz} (longitudinal) is given in Figure 5.7 - Figure 5.10. The results show that stress in and near the weld pool region changes a lot, and that stress away from the weld pool region changes very little along the flow line.

Figure 5.6: Displacement field of the edge weld test, 20x.

Figure 5.7: Effective stress field of the edge weld test.

Figure 5.8: σ_{xx} field of the edge weld test.

Figure 5.9: σ_{yy} field of the edge weld test.

Figure 5.10: σ_{zz} field of the edge weld test.

Figure 5.11: Effective plastic strain of the edge weld test.

Figure 5.12: The through-thickness average longitudinal stress σ_{zz} vs. distance from welded edge. For the Lagrangian formulation [43], sampling data is from the mid-length of the weld path; For the previous [18] and current steady-state formulation, the data is from the near end of the path.

It is also shown that plastic deformation has only occurred in a small region near the weld pool (Fig. 5.11). Comparing to the measured [3] and previously numerical computed [18][43] stresses, Figure 5.12 shows the computed results of the through-thickness average longitudinal stress σ_{zz} obtained from near end of the weld path. The current computational values fit quite well with the measured and previously computed data.

5.4.3 Quasi-Stress Analysis for a Butt Weld

Butt welds have many industrial applications. Many shell and vessel constructions use this process to join sheet metal (or plates). A 3D quasi-steady state stress analysis was performed on a mesh (Fig. 5.13) with the size of 0.01 m thick, 0.3 m wide and 0.6 m long. The weld line was along z direction. The center of the weld pool was 0.010 m from the inlet edge. The filler metal was included in the domain.

The steady state temperature field and the welding parameters were given in Chapter 3 (Figure 3.8 and Figure 3.9). The microstructure state and specific volume were provided by Chapter 4 (Figure 4.15 and Figure 4.14).

Figure 5.14 and Figure 5.15 shows the displacement field on the full domain. The displacements in Figure 5.15 have been magnified 30 times to show the deformation. A full view of effective plastic strain field and stress fields over the domain are shown in Figure 5.16 and Figure 5.18 - Figure 5.23. Figure 5.16 shows that plastic deformation

Figure 5.13: FEM mesh for quasi-steady state stress analysis.

was only taking place in a narrow range around the seam. Furthermore, Figure 5.17 shows the field of effective plastic strain increment which indicates that plastic deformation really occurs in a very small region around weld pool. More precisely, the test simulates the reheating of a welded plate, due to the fact that the filler metal exists in front of the heat source in the domain.

Figure 5.14: Displacement fields of a butt weld quasi-steady state stress analysis.

(a). Magnitude; (b). X component; (c). Y component; (d). Z component

Figure 5.15: Displacement field of a butt weld quasi-steady state stress analysis, 30x.

Figure 5.16: Effective plastic strain field of a butt weld quasi-steady state stress analysis.

Figure 5.17: Effective plastic strain increment field of a butt weld quasi-steady state stress analysis.

Figure 5.18: Stress σ_{xx} field of a butt weld quasi-steady state stress analysis.

Figure 5.19: Stress σ_{yy} field of a butt weld quasi-steady state stress analysis.

Figure 5.20: Stress σ_{zz} field of a butt weld quasi-steady state stress analysis.

Figure 5.21: Stress σ_{xy} field of a butt weld quasi-steady state stress analysis.

Figure 5.22: Stress σ_{xz} field of a butt weld quasi-steady state stress analysis.

Figure 5.23: Stress σ_{yz} field of a butt weld quasi-steady state stress analysis.

As a comparison, a transient stress (TS) analysis was performed on a mesh with the same 2D cross section (Figure 5.24) as that for the quasi-steady state stress (SSS) analysis. The length of the mesh is 1.0 *m*. Element size along the welding direction was 0.01 *m*. The welding velocity and material were the same as used in quasi-steady state stress analysis.

Figure 5.24: 2D cross section of mesh for both quasi-steady state stress and transient stress analysis.

The displacement field of transient stress analysis, with heat source traveled 0.70 m into the plate from one end, is displayed in Figure 5.25. Based on the quasi-steady state assumption, the middle part (in the block) is comparable with the displacement field from the quasi-steady state stress analysis (5.14).

Figure 5.25: Displacement field from transient stress analysis at time = 350 s.

(the 70th time step in transient stress analysis.)

The displacement and effective plastic strain were compared between quasi-steady state stress analysis and transient stress analysis along the streamlines (flowlines based on the quasi-steady state assumption) which passed through points A, B and C shown

in 2D cross section (Figure 5.24). The results were plotted in Figure 5.26 - Figure 5.29.

Figure 5.26: Comparison of displacement between SSS and TS analyses along stream-line through point A.

The displacement fields of the two stress analyses show similar trends near the weld pool region, which suggests that the displacement field from quasi-steady state stress analysis could be used as a trial solution for transient stress analysis in the middle quasi-steady state portion of a long weld. The effective plastic strain fields of the two stress analyses show some difference.

The most probable reason for the difference between SSS and TS results could be that missing the restraint caused by the material cut-off from the front and rear of

Figure 5.27: Comparison of displacement between SSS and TS analyses along stream-line through point B.

the domain misses some bending moments. Ignoring these bending moments could cause errors, especially near the ends. Also, the inlet and outlet condition may not be applied accurately. For a more accurate quasi-steady state stress analysis, it is suggested that the inlet and outlet boundary conditions (Neumann traction and Dirichlet BC) should come from a transient Lagrangian stress analysis by domain decomposition.

In this test, the domain for quasi-steady state stress analysis contains about 9,000 elements. It took about 20 *minutes* CPU time to solve the problem with 4 NR iteration on a PC. On the other hand, the mesh for transient stress analysis has

Figure 5.28: Comparison of displacement between SSS and TS analyses along stream-line through point C.

about 15,000 elements. If the time step size is 5 s, and 70 time steps are needed to get the results shown in Figure 5.25, then about 20 *hours* CPU time were used for that result on the same PC.

Figure 5.29: Comparison of effective plastic strain between SSS and TS analyses .

5.4.4 A Test to Validate the Quasi-Steady State in the Butt Weld

The quasi-steady state assumption is a key point in this thesis. It will be very important to prove the existence of a quasi-steady state in a long weld. A test was performed on a mesh with the 2D cross section shown in Figure 5.24 and the length was 1.0 *m*. A transient Lagrangian formulation was applied for both the thermal and stress analysis to simulate the welding process. Then, the results around the weld pool region of two time instances in the middle of the process were mapped to an Eulerian frame, and then, compared in that frame.

Figure 5.30 shows temperature fields at two time instances, and Figure 5.31 shows the difference of temperature fields between two time instances. It indicates that very small temperature changes occur around the weld pool region in the Eulerian frame. Specifically, the maximum temperature change is 0.137 *K* and temperature range from 300 *K* to 2500 *K*. The difference of displacement fields at this two time instances in the Eulerian frame are shown in Figure 5.32. The displacement deviation between this two time instances is small in the Eulerian frame. The displacement field at $t = 350$ s (the 70th time step) in Lagrangian frame is shown in Figure 5.25.

Figure 5.30: Temperature fields of the butt weld at two time instances.

(a). $t = 300 \text{ s}$ (the 60th time step), (b). $t = 350 \text{ s}$ (the 70th time step).

Figure 5.31: Difference of temperature fields of the butt weld at two time instances.

Figure 5.32: Difference of displacement fields of the butt weld at two time instances.

It is also very interesting to compare the stress fields of the two time instances. Here, the two most important stress components, transverse stress (σ_{xx}) and longitudinal stress (σ_{zz}) in butt weld, are considered (Figure 5.33 - Figure 5.36). It can be seen that maximum stress $\approx 9 \times 10^8$, and maximum $\Delta\text{stress} \approx 2.7 \times 10^7$ in this Eulerian frame.

It can be seen from the results that the difference of temperature, displacement and stress field between two time instances ($t = 300 \text{ s}$ and $t = 350 \text{ s}$) are quite small, especially in the weld pool region. That means a quasi-steady state was reached in the long butt weld with the same cross section. It is interesting to note that the outlet has larger difference than the inlet. One should be aware that for a complex welded structure, quasi-steady state may not be reached.

This test shows that if a weld reaches a quasi-steady state, the results from the current time step could be used as a trial solution for the next time step in transient stress analysis. This trial solution may be even better than that from a quasi-steady state stress analysis from an Eulerian formulation that was applied for both the thermal and stress analysis to simulate the welding process.

At the leading edge of the weld pool, temperature gradients are often 10^4 K/s (the temperature rises from 700 K to 1700 K in 0.1 s). A Lagrangian time step would like to limit temperature increments to 100 K , i.e., a time step size of 0.01 seconds would be required. A 1 meter weld with a welding speed of 0.01 m/s and welding

time of 100 s would require 10^5 time steps. The cost would be prohibitive. Current practice is to take time steps of about 1 – 5 second (depending on the welding speed) and accept the errors caused by the large time step.

If near steady state behavior could be exploited, the cost could be reduced dramatically. In an Eulerian analysis as done in this thesis, the spatial derivatives with respect to time are never greater than the material derivatives with respect to time in a Lagrangian formulation. In a steady state, the spatial derivatives with respect to time are zero. As a solution approaches a steady state, the spatial derivatives go to zero.

Since the length of a time step is usually limited by the size of the first or second derivatives, a spatial formulation seems to present an opportunity to reduce computer time significantly by taking longer time steps.

Figure 5.33: Transverse stress (σ_{xx}) fields of the butt weld at two time instances.

(a). $t = 300$ s (the 60th time step), (b). $t = 350$ s (the 70th time step).

Figure 5.34: Difference of transverse stress (σ_{xx}) fields of the butt weld at two time instances.

Figure 5.35: Longitudinal stress (σ_{zz}) fields of the butt weld at two time instances.

(a). $t = 300$ s (the 60th time step), (b). $t = 350$ s (the 70th time step).

Figure 5.36: Difference of longitudinal stress (σ_{zz}) fields of the butt weld at two time instances.

Chapter 6

Conclusions and Future Work

Welding plays an important role in manufacture. But difficulties still exist for simulation on the weld process of large welded structures, due to the limitation of computer capacity, lack of proper mathematic models and softwares. This work is devoted to developing some algorithms that try to simulate welding by FEM efficiently and accurately.

The arc welding process for low-alloy steels was considered. The analyses include weld pool surface geometry and temperature field, weld joint temperature field, microstructure evolution in the fusion zone and heat-affective zone, and stress and displacement fields in weldment. All these analyzes were coupled by data flows to interact between thermal, mechanical and metallurgical processes present in the welds. The input data for the analysis included geometry, material properties, initial tem-

perature field, initial microstructure states, base metal and filler metal compositions, initial stress and strain states, and boundary conditions appropriated to the problem analyzed.

The algorithms and software were verified by solving several problems with analytic or experimental results. The accuracy of the computation could be limited by the knowledge of some input data: nonlinear material properties, convection coefficient, Dirichlet displacement and Neumann traction. The main conclusions that can be drawn, based on this work, are the following:

1. The numerical experiments in the weld pool region suggest that the arc pressure and inclination angle of workpiece will influence the shape of the molten pool and thus, the temperature field inside and beside the molten pool.
2. The thermal tests show that the space-time FE method is appropriate to deal with the 3D thermal analysis in the weld joint domain which is fixed with the heat source. It will provide both the transient and quasi-stationary results.
3. Based on the ordinary differential equations governing phase transformation kinetics, the microstructure evolution in the FZ and HAZ, computed based on the thermal history of a material point traveling along a flow line from its upstream inlet to its downstream outlet, gives reasonable results of microstructure states.
4. Volume changes accompanying the phase transformations could greatly influ-

ence the stress state by altering the specific volume and by transformation plasticity.

5. A quasi-steady-state stress analysis based on a flow tube data structure provide an efficient way to compute displacement, stress and strain fields in an Eulerian frame. The displacement field from quasi-steady-state stress analysis could be used as a trial solution for transient stress analysis.
6. The results from stress analysis indicated that plastic deformation occurs only in a small region in and around the weld pool. The rest of the structure only deforms elastically.

There are several opportunities for future work including the following:

1. To simulate the weld pool region completely, fluid flow within the molten pool domain should be considered by solving the Navier-Stokes equation, which may include pressure from the arc, electromagnetic force (Lorentz force), buoyancy force, shear stress caused by arc flow, and shear stress induced by surface tension gradient (Marangoni effect).
2. A model could be established to deal with the microstructure evolution on the filler metal to capture the details (such as solidification and decomposition of austenite to accicular, sideplate or grain boundary ferrite).

3. For the analysis of thermal stress, the whole weld structure should be included in the domain to apply boundary conditions properly. But for a large, complicated weld structures, this could cause difficulties due to the capacity of computer. Domain decomposition algorithm should be applied which should have an appropriate coupling mechanism. Also, it is desired that the transient Lagrangian formulation be combined with the steady-state stress results from an Eulerian frame, with the capacity to allow a larger time step in a Lagrangian formulation.

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