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**COUPLING MICROSTRUCTURE TO HEAT TRANSFER
COMPUTATION IN WELD ANALYSIS**

by

Paramjeet Khoral

B.Eng., University of Delhi, 1984

**A thesis submitted to the Faculty of Graduate
Studies and Research in partial fulfillment
of the requirements for the Degree of**

Master of Engineering

**Department of
Mechanical and Aerospace Engineering
Carleton University
Ottawa, Ontario
Canada**

October, 1989

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Acceptance Sheet

The undersigned recommends to the Faculty of Graduate Studies and Research, acceptance of the thesis: *Coupling Microstructure to Heat Transfer Computation in Weld Analysis*, submitted by Paramjeet Khoral, in partial fulfillment of the Degree of Master of Engineering.

Thesis Supervisor

Chairman
Department of Mechanical
& Aerospace Engineering

Abstract

An algorithm developed by Watt et al to compute the weld microstructure is implemented in this thesis. This algorithm tracks the thermal cycle at any point in the heat-affected zone and predicts the transient and final microstructure. The austenite grain growth is determined by using Ashby's grain growth relationship. Austenite decomposition to its daughter products (ferrite, pearlite and bainite) is determined by Kirkaldy's decomposition kinetics. The ordinary differential equations, which simulate these decomposition reactions, are solved by an adaptive ordinary differential equation integration routine with automatic error checking. The formation of martensite is computed by a algebraic equation taken from the work of Koistinen and Marburger. The hardness throughout the heat-affected zone is predicted by using the rule of mixtures. A three dimensional finite element thermal analysis program is used to model the thermal cycle in the heat-affected zone. The microstructure algorithm is coupled with the heat transfer program to compute the transient microstructure. Contours of phase fractions, e.g., martensite, austenite grain size and hardness, are displayed with three dimensional graphics. The results of this model are compared with the experimental results of a bead-on-plate weld.

Dedication

To my Parents

Acknowledgment

I would like to express my sincerest appreciation and gratitude to Prof. John A. Goldak, my thesis supervisor, for his constant guidance and encouragement throughout the course of this work, as well as in the preparation of this thesis. I would also like to thank Prof. Malcolm Bibby for his suggestions during the course of this research. I also gratefully acknowledge the financial assistance provided by the Department of Mechanical and Aerospace Engineering, Carleton University. Lastly, I would like to thank Kevin Haaland, Maoshi Gu and Dan Downey for their help in structuring the program.

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List of Symbols

- A - property of the precipitate
- A_1 - lower critical temperature (°C)
- A_3 - upper critical temperature (°C)
- Al - aluminum (wt. %)
- As - arsenic (wt. %)
- a - stoichiometry constant for precipitate
- B - property of the precipitate
- B_r - effective rate coefficient
- B_S - bainite start temperature (°C)
- b - stoichiometry constant for precipitate
- C - carbon (wt. %)
- C_α - carbon content of ferrite (wt. %)
- C_C - concentration of non-metal in precipitate (wt. %)
- C_{eut} - carbon content of eutectoid alloy (wt. %)
- C_γ - carbon content of austenite (wt. %)
- C_M - concentration of metal in precipitate (wt. %)
- Cr - chromium (wt. %)
- Cu - copper (wt. %)
- D - diffusion parameter
- FEA - finite element analysis
- g - grain size (μm)
- G - ASTM grain size index
- GMA- gas metal arc welding
- H - hardness (VPN)
- H_B - hardness of bainite (VPN)
- H_{FP} - hardness of ferrite, pearlite and austenite mixture (VPN)

H_M	- hardness of martensite (VPN)
HAZ	- heat-affected zone
k	- grain growth constant
MS	- martensite start temperature (°C)
Mn	- manganese (wt. %)
Mo	- molybdenum (wt. %)
N	- nitrogen (wt. %)
Ni	- nickel (wt. %)
ODE	- ordinary differential equation
P	- phosphorus (wt. %)
q/v	- heat input (J / m)
Q	- activation energy for grain growth (Cal / mole)
R	- universal gas constant (Cal / mole k)
S	- sulphur (wt. %)
Si	- silicon (wt. %)
T	- temperature (°C)
TS	- precipitate dissolution temperature (°C)
T_L	- liquidus temperature (°C)
T_M	- melting point temperature (°C)
T_o	- ambient temperature (°C)
TP	- peak temperature (°C)
T_S	- solidus temperature (°C)
T_1	- temperature at the start of the time step (°C)
T_3	- temperature at the end of the time step (°C)
T_B	- temperature at the boundary of the region (°C)
$\dot{T}$	- cooling rate within a time step (°C / sec)
t	- time (sec)
t_1	- time at the start of the time step (sec)
t_3	- time at the end of the time step (sec)
t_B	- time at the boundary of the region (sec)

V	- vanadium (wt. %)
V_1	- cooling rate at 700 °C (°C/h)
v	- welding velocity (mm / sec)
W	- tungsten (wt. %)
X	- phantom phase fraction
X_A	- fraction of austenite
X_B	- fraction of bainite
X_F	- fraction of ferrite
X_{FE}	- equilibrium fraction of ferrite
X_M	- fraction of martensite
X_P	- fraction of pearlite
X_{PE}	- equilibrium fraction of pearlite
α	- thermal diffusivity (m^2/s)
λ	- thermal conductivity (J / m s °C)
η	- arc efficiency
ρ	- density (g/cm^3)
$\tau_{8/5}$	- cooling time from 800 - 500 °C (sec)
ΔT	- undercooling (°C)

Chapter 1

Introduction

One of the most widely used method for joining metal in engineering is fusion welding. The progress made in the chemical and oil industry, aerospace, shipbuilding, structures, etc. heavily relies on reliable welds. Potential losses and risk to human life involved in weld failure have resulted in stringent material and welding process control requirements.

The energy of fusion welding causes a thermal cycle that drives the austenite grain growth and microstructural changes in the low alloy steel weld heat-affected zone. A large grain size along with transformation products such as martensite and bainite renders the base metal structurally weak. In addition these hard and brittle products can make the weld sensitive to stress and corrosion and can also lead to formation of stress induced cold cracks.

The fusion welding causes melting and bonding of base metal. A number of distinct zones are formed by the fusion welding as shown in Figure 1. The fusion zone is the area from the centerline of the weld to the solid-liquid transition zone. In this zone base metal fuses with the molten electrode filler metal and solidifies. The solid-liquid transition zone is a narrow band surrounding the fusion zone. On the inner side of this band the peak temperature during weld thermal cycle goes above the liquidus line and on the outer side temperature remains below the solidus line. The heat-affected zone (HAZ) which is the most critical area, ranges from the solid-liquid transition zone on its inner edge to the unaffected base metal on its outer edge. The HAZ can be subdivided into four distinct regions as shown in Figure 1. The size of the grains and microstructure varies in the HAZ according to the peak temperature. The width of the HAZ varies from 0.1 to 1.5 cm depending

Figure 1 - Schematic Representation of Various Zones in the Fusion Welding

on the welding process and its parameters. In the HAZ temperature variation is sufficient to alter the microstructure. During heating, the microstructure in the HAZ gets partially or fully austenitized as temperature goes above the lower critical temperature (A_1) and upper critical temperature (A_3) line. In the recrystallized zone new and fine austenite grains are formed. In the grain growth zone austenite grains begin to grow. On cooling austenite decomposes to its daughter products as shown in Figure 2. Ferrite, pearlite and bainite are formed by nucleation and growth. This physical phenomenon of austenite decomposition is modelled by ordinary differential equations. These equations describe both nucleation and subsequent growth of austenite daughter products.

In equilibrium conditions, the microstructure is ferrite and pearlite as shown in Figure 2E. Figure 2D shows the formation of martensite and retained austenite in prior pearlite colonies in partially transformed region. In the grain refining and grain growth region, as the peak temperature goes up the prior pearlite colonies expand while being austenitized. On cooling austenite decomposes to martensite as shown in Figure 2B and 2C. The presence of hard and brittle martensite can result in severe deterioration of the HAZ mechanical properties.

There are number of factors which influence the microstructure of the HAZ.

- The decomposition products of austenite depends on carbon content and alloy content of the steel. The higher carbon content favours the formation of hard and brittle products such as bainite and martensite. The lower and upper critical temperature, liquidus and solidus line, and other transformation temperatures are function of carbon and alloy content of the steel. Steels with different alloying contents can have absolutely different microstructure after the a same welding process with same parameters.
- In the modern microalloyed steels, austenite grain growth phenomenon is controlled by grain growth retarding precipitates. In order to com-

Figure 2 - Microstructure in Various Zones (from Sindo Kou,
Welding Metallurgy, John Willey & Sons, 1987, p. 330)

pute the final grain size the effect of these precipitates must be taken into account. The size of austenite grains has a significant effect on the the rate of austenite decomposition reactions. Therefore in order to predict final microstructure of the HAZ, austenite grain size must be computed accurately.

- In the case of high energy input welds, the HAZ spends more time above the precipitate dissolution temperature. This leads to formation of larger austenite grains (up to ASTM 0) and makes the grain growth zone wider. On rapid cooling, austenite transforms to martensite and bainite. This type of coarse grained structure with hard and brittle decomposition products reduces fracture toughness and fatigue resistance.
- Cooling rate also affects the decomposition products of austenite as can be seen from the continuous cooling transformation (CCT) diagram shown in Figure 3. This CCT diagram is plotted by the data obtained from end-quench hardenability tests. These results can also be applied for welding because the cooling conditions in these cases are similar. A fast cooling rate shown by Curve A leads to formation of martensite but as the cooling rate reduces as shown by Curves B, C, and D, other transformation products, ferrite, bainite and martensite, are formed.

All this makes the prediction of the HAZ microstructure complex and difficult. The HAZ is the most sensitive area of the weld joint and the mechanical properties of the joint depend on its grain size and austenite transformation products. The hydrogen embrittlement along with residual stresses (produced by thermal and transformation strains) can develop cracks in the HAZ as shown in Figure 4. This can make structures fabricated by welding unreliable in service. The hardness of the HAZ is a measure of tensile strength of the steel and also gives an indication of the degree of embrittlement. For low-alloy high-strength steels, a hardness of

Figure 3 - Continuous Cooling Diagram (from R.D. Stout and W.D. Doty, *Weldability of Steels*, Welding Research Council, 1971, p. 84)

over 350 VPN in HAZ is considered harmful.

All these arguments indicate that predicting microstructural changes induced by the severe weld thermal cycle would help to predict the reliability of the weld joint. Several models have been proposed to predict the microstructure of the HAZ. A group of researchers [1-4] have attempted to predict the hardness distribution in the HAZ without taking into account the phases present in the microstructure.

Figure 4 - Cracks Developed in the Heat-Affected Zone
(from K.G. Richards, *Weldability of Steel*, The Welding
Institute, Cambridge, 1976, p.14)

The details of their calculations vary, but all are based on the hypothesis that the unknown hardness at some point in the HAZ can be predicted by matching that point with either a cooling rate at some temperature, or cooling time between two temperatures, on a sample piece of the same steel previously tested under known conditions. There is no direct calculation of metallurgical reaction rates. These

calculations do not include the effects of austenite grain size and peak temperature achieved.

Another approach to the HAZ microstructure prediction has been proposed by Ashby and Easterling et al [5-7]. The austenite grain size and final amount of martensite can be obtained from the plot of cooling time (time to cool from 800 to 500°C) and peak temperature. Transformation rates for ferrite, pearlite, bainite and martensite are calculated using the carbon equivalent index. The weld thermal cycle is predicted by using a modified version of Rosenthal's [8] analytical equation. The austenite grain growth calculation is based on a simplified kinetic equation. In their analysis they also proposed a relation for precipitate dissolution temperature which takes into account the retarding effect of nitrides and nonferrous carbides on grain growth. The drawback of this model is the weakness of the Rosenthal equation, which assumes that thermal conductivity and specific heat of the material are independent of temperature. But these material properties are temperature dependent as shown by Moore et al [9]. This leads to significant errors in temperature distribution in the HAZ predicted by Rosenthal equation. The calculation procedure used to estimate the austenite decomposition products is also very crude.

A third set of workers have modified Kirkaldy's hardenability algorithm [10-13] to predict the microstructure of the HAZ. This algorithm can be used to isolate the individual effects of weld process parameters. It also highlights the effect of austenite grain growth on the HAZ microstructure. This group of researchers [14-16] have shown that the hardenability algorithm proposed by Kirkaldy can predict the resultant microstructure of the HAZ quite accurately. The main draw back in their [14-16] computation is use of inefficient integration techniques to solve the austenite decomposition relationships. This problem limited accuracy and made their algorithm CPU intensive and costly.

The object of this thesis is to predict transient and final microstructure of

heat-affected zone using the algorithm developed by Watt et al [15-16]. This work uses automatic error checking and adaptive ordinary differential equation integration routines developed at Lawrence Livermore National Laboratory [17] to solve austenite decomposition equations. The problem of starting the non-isothermal austenite decomposition has also been solved in this work. The microstructure algorithm has also been coupled with the three dimensional finite element heat transfer program developed by Goldak et al [18-19] to predict the transient microstructure of the HAZ. This coupled program provides a powerful tool for weld process selection and control.

The thesis organisation is as follows:

- **Chapter 2** - The theory of Watt et al [15-16] microstructural model is presented in this chapter. This chapter presents discussion about transformation reactions according to different zones of the thermal cycle. All the governing equations of the model are discussed in this chapter.
- **Chapter 3** - The computer implementation of the algorithm is discussed in this chapter. The starting condition for isothermal and non-isothermal transformation of austenite to ferrite and use of ODE solvers is also presented in this chapter
- **Chapter 4** - The results of the present algorithm are compared with the experimental results of Ion [21] in this chapter.
- **Chapter 5** - This chapter presents discussion about the present work and suggestions for the future development in this area at Carleton.
- **Chapter 6** - The final conclusions are presented in this chapter.

Chapter 2

Theory of the Microstructural Model

The microstructure model presented in this chapter has been developed by Watt et al [15-16]. It tracks the thermal cycle for various computations. For the present work it is assumed that temperature-time history of the weld is known. It is computed by using three dimensional finite element heat transfer program developed by Goldak et al [18- 19]. The welding process parameters along with natural and essential boundary conditions are submitted to the heat transfer program and it produces the temperature-time history throughout the fusion and heat-affected zone.

The algorithm for metallurgical kinetics is divided into two distinct sections. The first section deals with the calculations of various critical temperatures and constants. They depend on material composition and are independent of thermal cycle. The second section computes the evolution of various transformation reactions which are dependent on thermal cycle.

2.1 The Base Material Dependent Properties

The various microstructural transformation temperatures are function of carbon and alloy content of the low alloy steel. This section of the model computes all the parameters which are dependent on composition of the base metal and are independent of temperature-time history of the HAZ.

For low alloy steel, the liquidus and solidus temperature can be determined as a function of carbon content [20].

$$T_L = 1530.0 - 80.581C \quad (2.1)$$

$$T_S = 1527.0 - 181.356C \quad (2.2)$$

where

C - is the carbon content of the steel

T_L - is the liquidus temperature of the steel in °C

T_S - is the solidus temperature of the steel in °C

As the peak temperature goes above the solidus temperature melting begins and if the temperature goes above the liquidus temperature then the material is totally liquid. The present thesis work is limited to the HAZ of the weld and in this zone the temperature is always below the solidus temperature.

In the modern microalloyed steels, austenite grains are pinned by carbide/nitride precipitates. These precipitates retard the grain growth. A recent development in the steels is precipitates (TiC) which are theoretically stable up to the melting temperature of the steel. Ashby/Easterling [5-7] presented a modified relationship to calculate the precipitate dissolution temperature. This relationship takes into account the effect of these grain growth retarding precipitates and is given as:

$$TS = \frac{B}{A - \log[C_m^a C_c^b]} \quad (2.3)$$

where

A & B are constants that depend on the precipitate species

C_m & C_c are concentration of metal (Nb, Ti, V etc.) and non metal (carbide, nitride or boride) in precipitate respectively

a & b are stoichiometry constants

The concentrations are in wt % and temperature is in degree Kelvin. For the present work the steel is microalloyed by niobium (Nb) and the precipitate is niobium carbide (NbC). The value of different constants for NbC precipitate are as follows[21]:

Table 2-1: Various Constants of the Precipitate

A	B	a	b
3.11	7520.0	1.0	1.0

The upper critical temperature (A_3) depends on the carbon content of the steel as shown in the iron-carbon phase diagram Figure 5. The most accurate representation for the A_3 line is given by Kirkaldy and Baganis [13]. But this can not be used in the computer model because of the difficulty involved in inverting this relation for use in the lever law. To avoid this difficulty an alternative relation proposed by Leslie [22] is used in this algorithm.

$$A_3(^{\circ}\text{C}) = 912 - 200\sqrt{C} - 15.2\text{Ni} + 44.7\text{Si} + 104\text{V} + 315\text{Mo} + 13.1\text{W} \\ - (30\text{Mn} + 11\text{Cr} + 20\text{Cu} - 700\text{P} - 400\text{Al} - 120\text{As} - 400\text{Ti}) \quad (2.4)$$

where the composition are in wt %.

The lower critical temperature (A_1) or pearlite start temperature is also dependent on the composition of the low alloy steel and is given as [23]:

$$A_1(^{\circ}\text{C}) = 723 - 10.7\text{Mn} - 16.9\text{Ni} + 29\text{Si} + 16.9\text{Cr} + 290\text{As} + 6.4\text{W} \quad (2.5)$$

As the weld cools and the temperature drops below the bainite start temperature (BS), the formation of pearlite and ferrite stops and the austenite decomposition to bainite starts. The bainite start temperature is given as [10]:

$$BS(^{\circ}\text{C}) = 656 - 58\text{C} - 35\text{Mn} - 75\text{Si} - 15\text{Ni} - 34\text{Cr} - 41\text{Mo} \quad (2.6)$$

On rapid cooling of the weld, austenite in the heat-affected zone starts decomposing into martensite. This transformation starts below the martensite start temperature, which is given as [23]:

$$MS(^{\circ}C) = 561 - 474C - 35Mn - 17Ni - 17Cr - 21Mo \quad (2.7)$$

The carbon content of eutectoid alloy is also a constant for a particular low alloy steel and is given by the following relations [22]:

$$C_{eut} = \frac{[\phi_1 - \phi_2 - A_1]^2}{203^2} \quad (2.8)$$

$$\phi_1 = 910 - 15.2Ni + 44.7Si + 104V + 315Mo + 13.1W \quad (2.8a)$$

$$\phi_2 = 30Mn + 11Cr + 20Cu - 700P - 400Al - 120As - 400Ti \quad (2.8b)$$

All these parameters given by equations (2.1) to (2.8) are used to divide the HAZ thermal cycle into eight distinct regions as shown in Figure 5. At a specific point in the HAZ if the temperature is known and its thermal history is also known then with the help of these regions and their specific reaction kinetics its transient microstructure and hardness can be obtained.

2.2 Modelling of the Phase Transformations

Phase transformations taking place in the HAZ during the weld thermal cycle can be divided into two sections a) transformations which take place during heating and b) transformations which take place during cooling.

Transformation on Heating

2.2.1 Initialization of Ferrite and Pearlite

This region spans from room or pre-heat temperature to the lower critical temperature (A_1). In this region, the microstructure is assumed to be in equilibrium and is a mixture of ferrite and pearlite. The volume fraction of ferrite and pearlite is given by the lever law:

- a) Schematic cross-section of weld identifying the HAZ and fusion zone
 b) Iron-Carbon phase diagram identifying critical temperatures
 c) Thermal cycle identifying the regions for implementing the microstructure algorithm

Figure 5

$$X_F = \frac{C - C_{eut}}{C_\alpha - C_{eut}} \quad (2.9)$$

$$X_P = 1 - X_F \quad (2.10)$$

where

X_F - is the fraction of ferrite

X_P - is the fraction of pearlite

C - is the carbon content of steel

C_{eut} - is the carbon content of the eutectoid

C_α - is the carbon content of ferrite

The carbon content of ferrite below A_1 is given by an empirical relation assuming linear decrease from eutectoid value to a value of zero at room temperature (20°C) [14].

$$C_\alpha = \frac{T - 20.0}{A_1 - 20.0} (0.105 - 115.3 \times 10^{-6} \times A_1) \quad (2.11)$$

2.2.2 Austenitization

As the temperature in the HAZ exceeds the A_1 line during heating, pearlite colonies transform to austenite. The intercritical region or partially transformed region of the HAZ is the region where temperature varies between A_1 and A_3 . As the peak temperature goes towards A_3 , the austenite content increases under near equilibrium conditions. Because of the very high heating rate in the welds α phase is not likely to get superheated substantially before $\alpha \Rightarrow \gamma$ phase transformation takes place. These superheating effects are small and they are transitory as long as material gets austenitized before grain growth begins. Hence the superheating has little effect on final microstructure. In the partially transformed region this may not be true but the effect due to superheating is of the second order and

is not taken into consideration [15]. Under equilibrium conditions the amount of austenite and ferrite is given as:

$$X_F = \frac{C - C_\gamma}{C_\alpha - C_\gamma} \quad (2.12)$$

$$X_A = 1 - X_F \quad (2.13)$$

where

X_A - is the fraction of austenite

C_γ - is the carbon content of the austenite

C_α - is the carbon content of ferrite

The carbon content of austenite can be obtained by rearranging equation (2.4).

$$C_\gamma = \frac{[\phi_1 - \phi_2 - T]^2}{203^2} \quad (2.14)$$

$$\phi_1 = 910 - 15.2\text{Ni} + 44.7\text{Si} + 104\text{V} + 315\text{Mo} + 13.1\text{W} \quad (2.14a)$$

$$\phi_2 = 30\text{Mn} + 11\text{Cr} + 20\text{Cu} - 700\text{P} - 400\text{Al} - 120\text{As} - 400\text{Ti} \quad (2.14b)$$

Above A_1 the carbon content of ferrite is given by the following relation:

$$C_\alpha = 0.105 - 115.0 \times 10^{-6} \times T \quad (2.15)$$

If a point is in the partially transformed region then carbon rich austenite could transform to bainite or martensite upon cooling. The final microstructure therefore consists of hard martensite grains embedded in the soft untransformed ferrite matrix.

As the peak temperature goes above A_3 the remaining ferrite matrix also transforms to austenite. Thermal cycles with peak temperature between A_3 and precipitate dissolution temperature represents the recrystallized zone as shown in

Figure 1. In this region new grains are formed that are smaller in size as compared to the base metal. Austenite grains formed during heating in this zone are pinned by the grain growth retarding precipitate particles. This does not allow newly formed unstable austenite grains to grow. On cooling, the $\gamma \Rightarrow \alpha$ transformation produces a fine grained ferrite and pearlite structure in the recrystallized zone. This final structure depends on welding energy input, plate thickness, steel composition, etc. This zone is quite wide in the case of microalloyed steels because of the effectiveness of carbonitrides in preventing the grain growth at these temperatures.

2.2.3 Austenite Grain Growth

The austenite grains are assumed to be pinned by carbide/nitride precipitates until their dissolution. As the temperature in the HAZ goes above the precipitate dissolution temperature, the precipitates become unstable and they begin to dissolve. The grains produced by recrystallization are very unstable. The fine size of the grains and mechanical unequilibrium between grain boundary tension leads to certain grain boundary energy. As the grain growth retarding precipitate particles dissolve, the grains with more sides begin to swallow grains with less sides as shown in Figure 6, and the grain boundary energy progressively decreases.

It is assumed that grain growth is diffusion controlled and the driving force is the surface energy and it does not require any nucleation. The grain growth equation is given as [5]:

$$\frac{dg}{dt} = \frac{k}{2g} \exp\left(-\frac{Q}{RT}\right) \quad (2.16)$$

where

- g - is the grain size in microns
- k - is the grain growth constant
- Q - is the activation energy for grain growth (cal/mole)

R - is the universal gas constant (cal/mole k)

T - is the temperature in °K

t - is the time in seconds.

Q and k are dependent on the type of precipitate. The austenite grain growth which begins at precipitate dissolution continues up to the peak temperature of the thermal cycle. On cooling grains continue to grow till the temperature reaches the upper critical value (A_3).

Transformation on Cooling

On cooling as the temperature drops below the A_3 line, austenite starts decomposing into its daughter products. These products can vary widely depending on the cooling rate, austenite grain size, alloy content, etc. Watt et al [14-16] have modified Kirkaldy's [10-13] hardenability algorithm and have developed a set of ordinary differential equations which model the austenite decomposition. These equations describe both nucleation and subsequent growth of austenite daughter phases. The general reaction rate can be characterized as

$$\frac{dX}{dt} = B_r(G, T)X^m(1 - X)^n \quad (2.17)$$

where

X - is the volume fraction of the daughter product

B_r - is an effective rate coefficient

G - is the austenite grain size index number

T - is the temperature in °K

t - is the time in seconds

m & n - are semi-empirical coefficients set to less than one to assure convergence

An Array Of Grains Showing The Likely Direction Of Grain Growth

Figure 6

The rate coefficient includes the effects of grain size, amount of austenite supercooling and effect of temperature and alloy elements on diffusion. The details of various decomposition reactions are as follows.

2.2.4 Austenite Decomposition to ferrite

The first product to be formed on austenite decomposition is ferrite (it depends on the cooling rate). At temperature lower than A_3 austenite becomes unstable and ferrite begins to form at its grain boundaries. Ferrite forms by nucleation and grows into the austenite grains. The amount of ferrite formed depends on the nucleation rate and the rate at which austenite-ferrite interface advances. The nucleation rate is a function of undercooling below the A_3 line and austenite grain size. For a given temperature, degree of undercooling varies with carbon and alloy content of the steel. Alloys tend to be either ferrite or austenite stabilizers. The carbon content of ferrite is less than 0.0025 wt % and as ferrite precipitates it leaves austenite grains which become rich in carbon. The ferrite matrix is soft, ductile and has a body centered crystal structure.

Kirkaldy and Venugopalan [10] have proposed the following ordinary differential equation (ODE) for the austenite transformation to ferrite:

$$\frac{dX}{dt} = \frac{2^{\frac{(G-1)}{2}} (\Delta T)^3 \exp\left(-\frac{23500}{RT}\right)}{59.6Mn + 1.45Ni + 67.7Cr + 24.4Mo} X^{\frac{2(1-X)}{3}} (1-X)^{\frac{2X}{3}} \quad (2.18)$$

where

G - is the ASTM grain size index number

ΔT - is the undercooling given as ($A_3 - T$)

In equation (2.18), $X^{\frac{2(1-X)}{3}} (1-X)^{\frac{2X}{3}}$ takes into account the rate at which the austenite-ferrite interface area changes.

$$X = \frac{X_F}{X_{FE}} \quad (2.19)$$

where

X_F - is the fraction of ferrite formed

X_{FE} - is the equilibrium amount of ferrite

The value of X_{FE} is updated at each time step as the temperature goes down.

$$G = 1 + 1.44 \left[\ln \left(\left(\frac{25.4}{g} \right)^2 \times 100 \right) \right] \quad (2.20)$$

In equation (2.20), g is the grain size in microns. The formation of ferrite stops as soon as its volume becomes equal to the equilibrium ferrite or if the temperature drops below bainite start temperature.

2.2.5 Austenite Decomposition to Pearlite

As the temperature drops below A_1 , ferrite continues to form governed by equation (2.18). The formation of ferrite stops if it reaches its equilibrium value or if the amount of pearlite formed reaches a value of 0.01 as given by the continuous cooling transformation diagram Figure 3. The formation of pearlite begins as the temperature drops below A_1 . The carbon rich austenite starts decomposing into a laminated eutectoid mixture of ferrite and cementite called pearlite. It is a nucleation and growth transformation and it begins at the austenite grain boundary. If cementite crystals are present in the austenite then they act as nucleus. As the cementite platelet is formed, it depletes the carbon on either side which favours the formation of a ferrite platelet on both sides of cementite as shown in Figure 7. The formation of the ferrite platelet rejects carbon to the γ phase and hence favours the formation of cementite. In this manner the formation of pearlite continues until the bainite start temperature is reached. Spacing between the cementite platelet is reduced at lower transformation temperatures and this

increases the hardness and strength of steel [24,25]. The carbon content of pearlite is high and this makes it harder and stronger as compared to ferrite, but it is less ductile.

Kirkaldy has proposed the following ODE relation for the austenite decomposition to pearlite and it is similar to equation (2.17).

$$\frac{dX}{dt} = \frac{2^{\frac{(G-1)}{2}} (\Delta T)^3 D}{1.79 + 5.42(Cr + Mo + 4MoNi)} X^{\frac{2(1-X)}{3}} (1 - X)^{\frac{2X}{3}} \quad (2.21)$$

where

ΔT - is the undercooling given as $(A_1 - T)$

D is a diffusion parameter and it is given by the following relation:

$$\frac{1}{D} = \frac{1}{\exp\left(-\frac{27500}{RT}\right)} + \frac{0.01Cr + 0.52Mo}{\exp\left(-\frac{37000}{RT}\right)} \quad (2.22)$$

and

$$X = \frac{X_P}{X_{PE}} \quad (2.23)$$

where

X_P - is the fraction of pearlite formed

X_{PE} - is the equilibrium amount of pearlite

The equilibrium value of ferrite is calculated at each time step. Therefore the equilibrium amount of ferrite at any specific temperature is the maximum amount of ferrite which can be formed from austenite. The remaining amount of austenite is available for the formation of pearlite. This allows the value of X_{PE} to be set equal to $1 - X_{FE}$.

2.2.6 Austenite Decomposition to Bainite

Austenite starts decomposing to bainite as the temperature in the HAZ drops

Formation Of Pearlite

Formation Of Upper Bainite

Formation Of Lower Bainite

Figure 7

below the bainite start temperature. At this temperature the formation of pearlite and ferrite stops. If pearlite exists at the bainite start temperature then it is assumed that the austenite-pearlite interface continues to grow but now the formation of pearlite stops and instead bainite starts forming. At this lower transformation temperature the distance over which carbon atoms can diffuse is reduced and structures involving progressively shorter movements of atoms are formed. In this new structure carbide starts precipitating around or within the ferrite and it is in the shapes of needles or plates rather than equiaxed grains. This new structure is called bainite and is shown in Figure 7. As the temperature goes below the bainite start temperature, the amount of bainite formed increases. A rapid cooling rate favours bainite formation over pearlite. The structure of bainite can be divided into lower and upper bainite depending on the position of the carbide particles. In upper bainite, carbide precipitates around ferrite lath. In lower bainite, carbides form within the ferrite lathes and the carbide needles are oriented roughly at 60° to the axis of ferrite lath. Lower bainite forms just above the martensite start temperature and it is harder and tougher than the upper bainite which is formed at higher temperature. The needle like carbide acts as a pinning point to the mobile dislocations and hence increases the hardness of the HAZ. Lower bainite is harder, stronger and tougher than the fine pearlite of the same chemical composition. The main reason behind this is the size, shape and distortion of iron carbide. The ascending order of hardness is as follows: coarse pearlite, fine pearlite, upper bainite and lower bainite.

The ODE governing decomposition of austenite to bainite is taken from the work of Kirkaldy. This kinetic equation is similar to the kinetic equations proposed for the decomposition of austenite to ferrite and pearlite.

$$\frac{dX}{dt} = \frac{2^{\frac{(G-1)}{2}} (\Delta T)^2 \exp\left(-\frac{27500}{RT}\right)}{10^{-4}(2.34 + 10.1C + 3.8Cr + 19Mo)Z} X^{\frac{2(1-X)}{3}} (1-X)^{\frac{2X}{3}} \quad (2.24)$$

where

X - is the amount of bainite formed

ΔT - is the undercooling given as $(BS - T)$

Z is given by the following relation

$$Z = \exp[X^2(1.9C + 2.5Mn + 9Ni + 1.7Cr + 4Mo - 2.6)] \quad (2.25)$$

The value of Z is set to 1.0 if $(1.9C + 2.5Mn + 9Ni + 1.7Cr + 4Mo - 2.6) < 0$. The kinetic equation (2.24) is valid for both upper and lower bainite formation. Austenite decomposition to bainite stops as the temperature goes below martensite start temperature.

2.2.7 Austenite Decompositon to Martensite

If the cooling rate is very fast then the austenite transformation is depressed to lower temperatures and a new transformation product called martensite is formed. If temperature drops below the martensite start temperature and if austenite is available for decomposition then it starts decomposing to martensite. In this transformation the face centered crystal of austenite changes to a body centered crystal of martensite by means of a shear-type or displacive transformation. This transformation is different from the nucleation and growth process of pearlite or bainite. Because of the low transformation temperature the formation of cementite is not favoured and carbon atoms are trapped in the body centered lattice of martensite. The structure of martensite can be described as super saturated solution of carbon in ferrite. The hardness and brittleness of martensite increase with the carbon content. It is the hardest and most brittle amongst all the transformation products, therefore its formation must be avoided except in some special cases.

For this algorithm the kinetic equation for the martensitic transformation is taken from the work of Koistenen and Marburger [26].

$$X_M = 1 - \exp[-k_1(MS - T)] \quad (2.26)$$

where

X_M - is the volume fraction of martensite formed

T - is the instantaneous temperature

k_1 - is a constant and its value for most steel types is 0.011°C^{-1}

Martensite continues to form until the martensite finish temperature is reached. If even after reaching the martensite finish temperature, there is austenite available for decomposition then it remains as retained austenite in the final microstructure. I., some steels the martensite finish temperature is below room temperature. For steels used in this study it is assumed that the martensite finish temperature is equal to room temperature.

2.3 Hardness Calculation of the HAZ

The hardness of the HAZ is a very good indicator of its susceptibility to cracks and other problems. It has been observed that if the hardness of the HAZ is over 350 VPN in the case of a low alloy high tensile steel then it is susceptible to cracking. The hardness at any point in the HAZ can be calculated using the rule of mixtures. Once the volume fractions of ferrite, pearlite, bainite, martensite and austenite are known, then the rule of mixtures can be applied as follows to calculate the hardness [6]:

$$H = H_M X_M + H_B X_B + H_{AFP} X_{AFP} \quad (2.27)$$

where

H - is the total hardness in VPN

H_M - is the Vickers hardness of martensite

H_B - is the Vickers hardness of bainite

H_{AFP} - is the Vickers hardness of austenite-ferrite-pearlite mixture

X_M , X_B and X_{AFP} are the volume fraction of martensite, bainite and ferrite-pearlite-austenite mixture respectively. The relationship for hardness calculation of different phases are taken from the work of Maynier et al [27].

$$H_M = 127 + 949C + 27Si + 11Mn + 8Ni + 16Cr + 21(\log V_1) \quad (2.28)$$

$$H_B = -323 + 185C + 330Si + 153Mn + 65Ni + 144Cr + 191Mo \\ + [89 + 53C - 55Si - 22Mn - 10Ni - 20Cr - 33Mo]\log V_1 \quad (2.29)$$

$$H_{AFP} = 42 - 223C + 53Si + 30Mn + 12.6Ni + 7Cr + 19Mo \\ + [10 - 19Si + 4Ni + 8Cr + 130V]\log V_1 \quad (2.30)$$

All compositions are in wt % and V_1 is the cooling rate at 700°C ($^\circ\text{C}/\text{h}$). This can be obtained from cooling time from 800 to 500°C ($\tau_{8/5}$).

$$V_1 = \left(\frac{800 - 500}{\tau_{8/5}} \right) \left(\frac{1}{3600} \right) \quad (2.31)$$

The value of $\tau_{8/5}$ can be measured experimentally or computed from FEM or calculated from the Adams [28] relationship for thick plate as follows:

$$\tau_{8/5} = \frac{q/v}{2\pi\lambda} \left(\frac{1}{500 - T_o} - \frac{1}{800 - T_o} \right) \quad (2.32)$$

where

T_o - is the ambient or preheat temperature ($^\circ\text{C}$)

λ - is the thermal conductivity ($\text{J}/\text{m sec } ^\circ\text{C}$)

q/v - is the heat input (J/m)

Equation (2.26) to (2.28) are valid only for low carbon and low alloy steels [16]. Allowable limits for various elements are as follows: $0.1 < C < 0.5$ wt %, Si

$C < 1.0$ wt %, $Mn < 2.0$ wt %, $Ni < 4.0$ wt %, $Cr < 3.0$ wt %, $Mo < 1.0$ wt %, $V < 0.2$ wt %, $Cu < 0.5$ wt %, $(Mn + Ni + Mo) < 5.0$ wt % and $0.01 < Al < 0.05$ wt %. The effect of microalloying elements (Nb, Ti, Zr & B) is not taken into account. Using all these relations, the variation of hardness in the HAZ can be determined if its microstructure is known.

Chapter 3

Implementation of the Microstructure Algorithm

This Chapter provide details of computer implementation of the algorithm presented in Chapter 2. The details of the program presented in this chapter can be used to predict the transient and final microstructure in the HAZ of low alloy steel welds. As input it requires initial microstructure, material composition, details of the thermal cycle, and various reaction kinetics constants. As discussed before, this algorithm tracks the thermal cycle in the HAZ and according to different regions of thermal cycle, transient microstructure is calculated. The various regions into which the thermal cycle can be divided are shown in Figure 8. This chapter also shows that by using higher order adaptive ODE solvers higher efficiency and accuracy is obtained in integrating austenite decomposition equations for ferrite, pearlite and bainite. The starting problem involved in solving these equations is also discussed for both isothermal and non-isothermal conditions.

3.1 Determination of Start and Finish Time for Different Regions

In the present study, the temperature-time history of the weld is generated by finite element heat transfer model. It is assumed that thermal history of the weld is known. In a typical FEM analysis of a weld, the time step is 0.05 sec. or larger. This FEM time step can take two different situations as shown in Figure 9. In the first situation as shown in Figure 9a, the temperature change in a single time step is within a particular zone. In this case, the microstructure is calculated for that

Figure 8 - Schematic Representation of the Transformation Regions on the Thermal Cycle

particular zone according to temperature and time at the start and at the end of the time step. In the second case as shown in Figure 9b, the FEA time step spans two or more zones. In this case it becomes necessary to subdivide the FEM time step according to zone boundaries. It is assumed that within a FEA time step, the temperature varies linearly.

Figure 9 - Schematic representation of time step

The time at the region boundary can be obtained by following relation

$$t_B = t_1 + (t_3 - t_1) \left(\frac{T_B - T_1}{T_3 - T_1} \right) \quad (3.1)$$

where

t_1 & t_3 - are the time at the start and at the end of the FEA step

T_1 & T_3 - are the temperature at the start and at the end of the FEA step

t_B & T_B - are the time and temperature at the region boundary

The method which calculates these time and temperature steps in the program also specifies the name of the method to be executed within a specific region.

3.2 Initialization and Austenitization

Implementation of the algorithm in these two zones is straightforward. From room temperature to the lower critical temperature (A_1), the fraction of ferrite and pearlite is obtained by the equilibrium lever law given by equations (2.9) to (2.11). In the intercritical region, that is between A_1 and A_3 , fraction of ferrite and austenite is again obtained by the equilibrium lever law given by equations (2.12) to (2.15). In the recrystallized zone, between A_3 and the precipitate dissolution temperature, microstructure is all austenite and its new refined grains are formed. The grain size of refined grains is in the range of 5-10 μm . For the steel considered in the present analysis its value is set to 10 μm .

3.3 Austenite Grain Growth

During the heating part of the thermal cycle, above the precipitate dissolution temperature, the grain growth retarding precipitates become unstable and they dissolve. This allows the unstable austenite grains to grow as shown in Figure 6. The austenite grain growth kinetics follows Equation (2.16) and this equation can be written in incremental form as

$$\Delta g = \left[\frac{k}{2g} \exp \left(-\frac{Q}{RT} \right) \right] \Delta t \quad (3.2)$$

Q is the activation energy for the grain growth and it is calculated from the relationship suggested by Ashby [5].

$$\frac{Q}{RT_m} = k_Q \quad (3.3)$$

k_Q is a constant and it depends on the type of the grain growth retarding precipitate existing in the steel. The steel used in the present work is a Nb microalloyed and for this steel the value of k_Q is 19.0. T_m is the melting point of the steel. It is a function of carbon percentage of the steel and is given by the following equation

$$T_m = 1810 - 90C \quad (3.4)$$

In the grain growth equation, k is a grain growth constant and it is determined by comparing the experimental results with computed grain size. A value of $k = 1.26 \times 10^{12}$ is found suitable for accurate prediction of grain size.

To solve the differential equation (3.2), LSODE (the Lawrence Livermore National Laboratory solver for ordinary differential equation) routine is used. This does not require the programming consideration

$$\frac{\Delta g}{g} \leq 0.01 \quad (3.5)$$

required by Henwood [14]. Henwood used a simple Euler integration method to solve this equation, with small time steps for accuracy. Henwood concluded that for accuracy up to two decimal digits the maximum possible size of time step is 10^{-4} sec. In the present work the solver can be used with larger time steps because it automatically calculates the error at each step and accordingly sets the value for next time step. In the present work the size of time step used is equal to FEM time step, and various results with this are presented in Chapter 4.

3.4 Austenite Decomposition

Austenite starts decomposing into its daughter products as the temperature in heat-affected zone drops below A_3 line. The general reaction equation for ferrite, pearlite and bainite are similar as given by equation (2.17). To study the reaction kinetics and various parameters affecting it, austenite to ferrite decomposition

is discussed in detail and the same methodology apply for pearlite and bainite equations also.

3.4.1 Austenite Decomposition to Ferrite

The first daughter product formed on austenite decomposition is ferrite and it starts forming by nucleation and growth as temperature drops below A_3 as shown in Figure 8. The governing equation for this transformation can be written in incremental form as

$$\Delta X = \left[\frac{2^{\frac{(G-1)}{2}} (\Delta T)^3 \exp \left(-\frac{23500}{RT} \right)}{59.6\text{Mn} + 1.45\text{Ni} + 67.7\text{Cr} + 24.4\text{Mo}} X^{\frac{2(1-X)}{3}} (1-X)^{\frac{2X}{3}} \right] \Delta t \quad (3.6)$$

The variables are the same as in equation (2.18). The phantom phase fraction X is defined in equation (2.19). This reaction kinetics drives the amount of ferrite formed (X_F) towards the equilibrium amount of ferrite X_{FE} . G is the ASTM grain size index and it can be calculated from equation (2.20). In a time step equation (3.6) is integrated to get new value of X . The amount of ferrite formed is calculated as

$$X_{F\text{new}} = X_{\text{new}} \times X_{FE} \quad (3.7)$$

Equilibrium amount of ferrite changes in every time step and it is calculated using equilibrium lever law relationship given by equation (2.12). The value of X_{FE} at the end of the time step is taken as the starting value of X_{FE} for the next time step and it is assumed to be constant throughout the next step. The value of phantom fraction of ferrite for the next time step is upgraded as

$$X = \frac{X_{F\text{new}}}{X_{FE\text{new}}} \quad (3.8)$$

The equilibrium amount of ferrite increases continuously from upper critical to lower critical temperature. Its value is maximum at the A_1 line and as the temperature drops below this temperature its amount remains constant and is given

by equation (2.9). The amount of ferrite formed is always less than or equal to the equilibrium amount of ferrite and as soon as the amount of ferrite formed becomes equal to the equilibrium amount of ferrite this transformation stops.

3.4.1.1 Isothermal Decomposition of Austenite to Ferrite

In order to study the transformation kinetics in detail, first isothermal conditions are studied because this makes the undercooling and diffusion parameter constant. The different conditions are as follows

Table 3-1: Parameters for Isothermal Transformation

Temperature	650° C
ASTM Grain Size	8.54
Initial Fraction of Ferrite	1.0e-12
Composition of Steel (wt. %)	C 0.12
	Si 0.16
	Mn 0.91
	P 0.002
	S 0.005
	Al 0.04
	Nb 0.021
	N 0.011

In the previous work done on this algorithm Henwood used simple Euler integration. That method not only produces an error in the final answer but also requires very small time steps. To reduce this error Henwood used small time steps and that made this code CPU intensive and made real analysis of weld problems very expensive. The simple Euler method makes an error in each step due to the approximation of ordinary differential equation by the difference equation. This error can be measured as an amount by which the true solution to the ODE differs from the numerical solution. Schematically it is shown in Figure 10. Henwood tried to reduce this error by using smaller time steps.

In the present work, the author investigated two different ODE solvers to reduce the problem faced by Henwood. The first solver is taken from SLATEC

Figure 10 - Error in numerical solution of ODE

[29] mathematical library and the second solver is taken from LLNL [17]. Under isothermal conditions the austenite to ferrite decomposition equation is integrated using both the solvers. The output of these solvers is plotted for phantom fraction of ferrite (X) and time and is shown in Figure 11. The result of the two ODE solvers is almost the same as can be seen from the plot, but the SLATEC solver is unstable during starting of integration of the equation. For small values of X the output of the SLATEC oscillates and it goes negative also. The SLATEC solver also finds the tolerance to be very small and it increases its value automatically which leads to error in the final answer. But in the LLNL solver there is no such problem. Due to this advantage, the LLNL solver is selected for the integration of austenite decomposition equations. In the LSODE (LLNL ordinary differential equation solver) there are four parameters which should be decided for accurate

solution of the problem. These parameters are

- non-stiffness or stiffness of equation,
- tolerance for error calculations,
- time step and
- starting value of phase fraction.

All these austenite decomposition equations are found to be non-stiff. This is confirmed by Figure 12. This figure shows a family of curves with different initial values of phase fraction. These solutions remain separate over time which is a typical behaviour of non-stiff equations. In case of stiff equations these solution tend to merge quickly.

As discussed before in each step of integration there is an error due to approximation of a differential equation by a difference equation. The LLNL solver has built in error calculation routine and it keeps the error within the tolerance limits prescribed by the user. It varies the time step automatically in order to maintain the required accuracy. Plot of the phantom fraction formed versus time is shown in Figure 13 for different values of tolerance limits. Tolerance value is varied from 10^{-2} to 10^{-8} . The error involved in the solution of the equation reduces progressively as the tolerance is reduced. But at a tolerance value of 10^{-8} the solver stops the program because it can not handle such low values. Finally a tolerance value of 10^{-6} is selected to be the best because it gives accurate results and the program takes less CPU time.

Variation in time step of integration does not make a great difference in the answer as shown in Figure 14. Time step is varied from 10^{-1} to 10^{-4} . Normally the time step in FEM heat transfer analysis is 0.05 sec or larger, the time step involved in the ODE integration should be less than or equal to this value. In the present analysis time step is set equal to the FEM time step. The ODE solver automatically subdivide this time step into smaller time steps according to the

Figure 11 - Comparison of solution of austenite to ferrite decomposition using ODE integration routines from SLATEC and LLNL

Figure 12 - Isothermal decomposition of austenite to ferrite with different initial values of phase fraction

Figure 13 - Isothermal decomposition of austenite to ferrite with different tolerance values for ODE integration routine

Figure 14 - Isothermal decomposition of austenite to ferrite with different time steps

requirement of the tolerance. This reduces the CPU time considerably and solves the equation with required accuracy.

The starting value of phase fraction does make a difference in the solution of equation as shown in Figure 12. As the initial value of the phase varies from 10^{-6} to 10^{-20} a family of curves is obtained. But as the initial value of the phase fraction is reduced curves become more spaced and unstable. On the other hand curves for 10^{-6} to 10^{-14} are closely spaced and follow a specific order. From these observations an initial value of 10^{-12} is selected as the optimum initial value for integration. By setting these four parameters the solution of austenite decomposition equation becomes stable and accurate answers are obtained.

Starting Condition for Integrating Austenite to Ferrite Equation

The initial fraction of ferrite has no effect on the number of evaluations but its value must be small enough to ensure accuracy. As discussed earlier, solution of equation (3.6) becomes unstable as the value of X is reduced below 10^{-14} . In order to avoid this problem a starting condition is required which can be used for calculation of the phase fraction of ferrite from its value of 0.0 to 10^{-12} and after that its value can be determined by the ODE solver. Bibby et al [30] suggested an analytical asymptotic approximation to equation (2.18). As $X \Rightarrow 0$ equation (2.18) can be written as

$$\frac{dX}{dt} = \frac{2^{\frac{(G-1)}{2}} (\Delta T)^3 \exp\left(-\frac{23500}{RT}\right)}{59.6\text{Mn} + 1.45\text{Ni} + 67.7\text{Cr} + 24.4\text{Mo}} X^{\frac{2}{3}} \quad (3.9)$$

or

$$\frac{dX}{dt} = A_F X^{\frac{2}{3}} \quad (3.9a)$$

where $A_F = \frac{2^{\frac{(G-1)}{2}} (\Delta T)^3 \exp\left(-\frac{23500}{RT}\right)}{59.6\text{Mn} + 1.45\text{Ni} + 67.7\text{Cr} + 24.4\text{Mo}}$, is a constant in

isothermal conditions. Solving equation (3.9a) analytically

$$X(t) = \left(\frac{A_F t + k_I}{3} \right)^3 \quad (3.10)$$

In equation (3.10) k_I is the integration constant and it is zero for the condition $X(0) = 0$. Thus the starting condition reduces to the following expression

$$X(t) = \left(\frac{A_F t^3}{27} \right) \quad (3.11)$$

Equations (3.6) & (3.11) are used together to compute the phase fraction of ferrite formed. Solution is started with equation (3.11) and as the phase fraction becomes sufficiently large (10^{-12}) it is switched to equation (3.6). Therefore with the starting condition initial phase fraction at $t = 0$ is zero and it grows according to the above prescribed equations.

3.4.1.2 Starting Condition for Integrating Austenite to Ferrite Equation for Non-Isothermal Transformation

In the real weld analysis there is continuous cooling. Austenite decomposition to ferrite starts and stops as the upper critical temperature and bainite start temperature are reached. In non-isothermal conditions the four parameters required by the ODE solver are unchanged. But it requires a new approach for the starting condition, because in this case the undercooling of austenite and the diffusion parameter ($\exp\left(-\frac{23500}{RT}\right)$) are not constant. The variation in value of diffusion parameter is very small as compared to the variation in undercooling from A_3 to BS temperature. Due to this fact, the diffusion parameter can be assumed to be constant. As $X \Rightarrow 0$, equation (2.18) can be written as

$$\frac{dX}{dt} = A_F (\Delta T)^3 X^{\frac{2}{3}} \quad (3.12)$$

where $A_F = \frac{2^{\frac{(G-1)}{2}} \exp\left(-\frac{23500}{RT}\right)}{59.6\text{Mn} + 1.45\text{Ni} + 67.7\text{Cr} + 24.4\text{Mo}}$, is a constant.

Undercooling is time dependent and can be written as

$$\Delta T_{(t)} = \dot{T}t \quad (3.13)$$

where

$\dot{T}$ - is the cooling rate and it is constant within a time step

t - is the time and it is zero when $T = A_3$

Substituting equation (3.13) into (3.12) the ODE equation reduces to

$$\frac{dX}{dt} = A_F(\dot{T}t)^3 X^2 \quad (3.14)$$

On solving equation (3.14) analytically, the starting condition is obtained

$$X(t) = \left(\frac{A_F \dot{T}^3 t^4 + k_I}{12} \right)^3 \quad (3.15)$$

k_I is the integration constant and it is equal to zero for the condition $X(0) = 0$.

Therefore finally equation (3.12) reduces to the following starting condition

$$X(t) = \left(\frac{A_F \dot{T}^3 t^4}{12} \right)^3 \quad (3.16)$$

The cooling rate within a time step can be assumed to be constant and can be found by the following relation

$$\dot{T} = \frac{T_3 - T_1}{t_3 - t_1} \quad (3.17)$$

In the case of non-isothermal conditions equation (3.6) and (3.16) are used together to compute the fraction of ferrite formed. The solution of the ODE equation is started with equation (3.16) and the amount of fraction of ferrite formed increases from zero to a value of 10^{-12} using this equation. As the fraction of ferrite becomes sufficiently large, the solution is switched to equation (3.6) which is solved by using LSODE.

3.4.2 Austenite Decomposition to Pearlite

In Region 6, as shown in Figure 8, as temperature drops below the lower critical temperature (A_1) the austenite starts decomposing to pearlite. Pearlite continues to form until the bainite start temperature (BS) or until the fraction of pearlite formed becomes equal to equilibrium amount of pearlite. The reaction kinetics for pearlite formation is governed by equation (2.21). In time incremental form this equation can be written as follows

$$\Delta X = \left[\frac{2^{\frac{(G-1)}{2}} (\Delta T)^3 D}{1.79 + 5.42(\text{Cr} + \text{Mo} + 4\text{MoNi})} X^{\frac{2(1-X)}{3}} (1-X)^{\frac{2X}{3}} \right] \Delta t \quad (3.18)$$

In the above equation D is a diffusion parameter and it is calculated by using equation (2.22). G is the ASTM grain size index and it is calculated by equation (2.20). The value of G is calculated after the grain growth stops and its value remains constant on further cooling. The undercooling (ΔT) is equal to ($A_1 - T$). To start the integration of equation (3.18) a starting condition similar to the ferrite transformation is required. In isothermal conditions as the phantom fraction of pearlite $X (\frac{X_P}{X_{PE}}) \Rightarrow 0$, equation (2.21) reduces to

$$\frac{dX}{dt} = A_P X^{\frac{2}{3}} \quad (3.19)$$

where $A_P = \frac{2^{\frac{(G-1)}{2}} (\Delta T)^3 D}{1.79 + 5.42(\text{Cr} + \text{Mo} + 4\text{MoNi})}$, is constant. After integrating and applying the condition that at time equal to zero the fraction of pearlite formed is also zero, equation (3.19) reduces to the following asymptotic solution

$$X(t) = \left(\frac{A_P^3 t^3}{27} \right) \quad (3.20)$$

In non-isothermal condition equation (2.21) reduces to

$$X(t) = \left(\frac{A_P \dot{T}^3 t^4}{12} \right)^3 \quad (3.21)$$

The reasoning used for the derivation of this non-isothermal starting condition is the same as that used for ferrite transformation. In this case at temperature equal to the A_1 time is equal to zero and fraction of pearlite formed is zero.

The starting condition for isothermal or non-isothermal transformation condition is used till the amount of pearlite formed increases from a value of zero to 10^{-12} . After this amount the prediction of pearlite transformation is switched to equation (3.18). Integration of this equation is done using LSODE and the various parameters required by the solver are same as required in the ferrite transformation equation. The amount of pearlite formed in a time step is given as

$$X_{P_{new}} = X_{new} \times X_{PE} \quad (3.22)$$

The value of X_{PE} is updated in each time step and for the next time step, the phantom fraction of pearlite is calculated as

$$X = \frac{X_{P_{new}}}{X_{PE_{new}}} \quad (3.23)$$

3.4.3 Austenite Decomposition to Bainite

As the temperature drops below the bainite start temperature (BS), austenite starts decomposing to bainite as shown in Figure 8 by Region 7. The formation of bainite stops as martensite start temperature is reached or if there is no austenite left for decomposition. Formation of bainite is governed by equation (2.24) and it can be written in incremental form as

$$\Delta X = \left[\frac{2^{\frac{(G-1)}{2}} (\Delta T)^2 \exp \left(-\frac{27500}{RT} \right)}{10^{-4} (2.34 + 10.1C + 3.8Cr + 19Mo) Z} X^{\frac{2(1-X)}{3}} (1-X)^{\frac{2X}{3}} \right] \Delta t \quad (3.24)$$

The variables in equation (3.24) are the same as defined in section (2.2.6). To start integration of equation (3.24), the initial value of bainite is set equal to the fraction of pearlite at the BS temperature. This equation does not require any starting condition because the initial value of X is sufficiently large ($\geq 10^{-12}$). In

the case of bainite there is no equilibrium bainite therefore whatever X is formed after each step of integration is the amount of bainite formed.

3.4.4 Austenite Decomposition to Martensite

In Region 8, from the martensite start temperature to room temperature the remaining austenite transforms to martensite. The formation of martensite is governed by a simple equation (2.26). This transformation is stopped if all the austenite has decomposed or if room temperature is reached. In the case of rapid cooling if austenite is still available at room temperature for decomposition, then it remains as retained austenite in the final microstructure.

3.5 Hardness Calculation of the HAZ

All the transformation reaction stops as the temperature in the HAZ drops to room temperature. At this point, the microstructure can be obtained anywhere in the HAZ. The phase fraction of ferrite, pearlite, bainite, austenite and martensite can be used to calculate the hardness of the HAZ at any point. These hardness calculations are done by implementing equations (2.27) to (2.32).

Chapter 4

Results

In this chapter weld microstructure predicted by the algorithm described in the previous two chapters is compared with the experimental results. In particular the available experimental data for austenite grain size, fraction of martensite and hardness is compared with the predicted results. The coupling of the microstructure model with the heat transfer model is illustrated with the transient microstructure at each time step. The main goal is to demonstrate the capability of the system for predicting the microstructure of the weld heat-affected zone. The computer generated results are compared to experimental data in order to illustrate the accuracy of the model.

4.1 Experimental Data

The experimental results for microstructure of the HAZ are obtained from the thesis work of Ion [21], performed at the University of Lulea, Sweden. In order to assess the validity of the present model a high strength low alloy structural steel is investigated. The composition of the steel is as follows:

Table 4-1: Composition of the Steel (wt. %)

C	Si	Mn	P	S	Al	Nb	N
0.12	0.16	0.91	0.002	0.005	0.04	0.021	0.011

It is a niobium microalloyed steel. In this steel niobium in combination with carbon forms a precipitate (NbC). This precipitate impedes the austenite grain growth in the recrystallization zone. As the precipitate dissolution temperature is

reached these precipitate particles dissolve and austenite grains begin to grow. Ion conducted a series of experiments of a bead-on-plate weld with different welding parameters. For this thesis work a weld with the following parameters is analysed.

Table 4-2: Welding Parameters of the Test Weld

Process	GMA
Efficiency	0.75
Welding Speed	6.7 mm/s
Current	71.0 Amps
Voltage	20.0 Volts
Bead Depth	1.0 mm
A ₁ Depth	1.74 mm
Plate Thickness	12.7 mm
Heat Input	0.2 kJ/mm

The bead depth is the fusion zone depth. The A₁ depth is the heat-affected zone depth.

4.2 Thermal Analysis

As discussed before, a three dimensional finite element heat transfer program is used to predict the thermal cycle in the heat-affected zone. In this analysis, the weld pool is simulated by a double ellipsoid model. At the centre of the ellipsoid, temperature is set to a peak value and temperature decays exponentially towards the boundary of the ellipsoid. In order to simulate the test weld peak temperature for ellipsoid is set to 2100 °C and dimensions of the ellipsoid are as follows:

Table 4-3: Dimensions of the Double Ellipsoid

a	b	c ₁	c ₂
2.0 mm	2.0 mm	2.0 mm	3.0 mm

These parameters give good simulation of bead depth and A_1 depth. A typical shape of ellipsoid is shown in Figure 15, it shows position of the ellipsoid after the end of eighth time step.

Eight node brick elements are used to represent the plate. The finite element mesh used to represent the plate is shown in Figure 15. Fusion welding is done from node A to node F. For this analysis the depth and width of the plate are assumed to be same, that is 3 mm, and the length is 12 mm. Each eight node brick has the same width, length and height and it is equal to 1 mm.

The thermal cycles computed by this analysis are plotted in Figure 16. These thermal cycles are plotted for nodes lying on plane BEIJ as shown in Figure 15. The computed time for cooling from 800 to 500 °C ($\tau_{8/5}$) is 0.8 sec, while the experimental value for $\tau_{8/5}$ is 1.0 sec. Thermal contours after the eighth time step are shown in Figure 17. The fusion zone spans from the centre of the weld to contour G and the heat-affected zone spans from contour G to C as shown in Figure 17. These computed values of the fusion zone and heat-affected zone depth match with the experimental values, not shown here. All the above observations lead to the conclusion that the FEA heat transfer program predicts the thermal history of the weld accurately.

4.3 Transient Microstructure

The microstructure code is coupled with the heat transfer code in the present work. This makes the system very effective in predicting the microstructure at each time step. At any give time step, the fraction of a specific phase and hardness can be determined anywhere in the heat-affected zone. This capability of the system is shown by Figures 18 and 19. These figures show the variation in different phases of the microstructure with time at nodes G and D respectively.

Figure 15 - Finite element mesh used for representation of plate

Figure 16 - Thermal cycles computed by the Finite Element Analysis
for nodes lying on plane BEIJ

TIME = 0.70000E+01
CONTOURS OF TEMPERATURE
MIN= 0.105E+03 AT NODE 46
MAX= 0.210E+04 AT NODE 188

Figure 17 - Temperature distribution contours after the eighth time step

Figure 18 - Transient microstructure at node D (peak temperature = 772.0 C)

Figure 19 - Transient microstructure at node G (peak temperature = 1273.0 C)

4.3.1 Distribution of Ferrite

The contours representing the fraction of ferrite in the plate are shown in Figure 20. In the vicinity of the solid-liquid transition zone the fraction of ferrite is of the order of 0.028 %. In this region microstructure is mostly martensitic. The amount ferrite increases gradually in the heat-affected zone as one moves towards the unaffected base metal. The fraction of ferrite is maximum at the outer edge of the heat-affected zone and its value is 0.8 %. In a region close to solid-liquid transition zone cooling rate is very high and it favours the formation of martensite and as a point moves towards the base metal slower cooling rate and higher ASTM grain index number favours the formation of ferrite.

4.3.2 Distribution of Pearlite

In the heat-affected zone the fraction of pearlite is negligible as can be seen from Figure 21. The amount of pearlite varies from 0.013 to 0.09 %. In the unaffected base metal the amount of pearlite varies from 0.104 to 0.117 %. The higher cooling rate does not favour the formation of pearlite and this is confirmed by the computed results.

4.3.3 Distribution of Austenite

On heating, the microstructure is partially or fully austenitized as temperature rises above A_1 and A_3 temperature. This can be seen clearly from the contours in Figure 22. The microstructure around the weld pool is fully austenitized. In the area behind the weld pool as temperature drops below A_3 , austenite becomes unstable and it decomposes into its daughter products. This leads to the reduction in fraction of austenite in this region. As temperature drops down to room temperature there is no austenite left or there is retained austenite in small quantities (0.008 %). This depends where the point is located in the heat-affected zone.

CONTOUR VALUES
 A= 8.83E-02
 B= 1.76E-01
 C= 2.65E-01
 D= 3.53E-01
 E= 4.41E-01
 F= 5.30E-01
 G= 6.18E-01
 H= 7.06E-01
 I= 7.94E-01

TIME = 0.70000E+01
 CONTOURS OF Ferrite
 MIN= 0.100E-09 AT NODE 196
 MAX= 0.883E+00 AT NODE 66

Figure 20 - Contours representing distribution of ferrite in the heat-affected zone

CONTOUR VALUES
 A= 1.30E-02
 B= 2.59E-02
 C= 3.89E-02
 D= 5.18E-02
 E= 6.48E-02
 F= 7.77E-02
 G= 9.07E-02
 H= 1.04E-01
 I= 1.17E-01

TIME = 0.200223+01
 CONTOURS OF Pearlite
 MIN= 0.100E-09 AT NODE 196
 MAX= 0.130E+00 AT NODE 162

Figure 21 - Contours representing distribution of pearlite in the
 heat-affected zone

CONTOUR VALUES
A= 1.00E-01
B= 2.00E-01
C= 3.00E-01
D= 4.00E-01
E= 5.00E-01
F= 6.00E-01
G= 7.00E-01
H= 8.00E-01
I= 9.00E-01

TIME = 0.70000E+01
CONTOURS OF Austenite
MIN= 0.000E+00 AT NODE 207
MAX= 0.100E+01 AT NODE 196

Figure 22 - Contours representing distribution of austenite in the
heat-affected zone

4.3.4 Distribution of Bainite

The contours of bainite distribution are shown in Figure 23. The fraction of bainite is negligible in most part of the HAZ. The maximum amount of bainite is found in a narrow band, where the peak temperature of the thermal cycle varies between 1200 to 1350 °C. In this range low cooling rate along with smaller grain size favours austenite decomposition to bainite. The HAZ region in which peak temperatures of the thermal cycle goes above 1350 °C, austenite decomposes to martensite on cooling. For the steel under consideration austenite decomposition to bainite starts at 605.0 °C and it stops at 474.0 °C. Figure 23 shows a transient microstructure, it is at the end of eighth time step. As shown in Figure 17, in this time step most of the plate behind the weld pool is in the range of 304.0 to 504.0 °C. This means that available austenite is decomposing to bainite in this step and the transformation is not complete yet. As the plate cools down to room temperature the final fraction of bainite varies from 0.11 to 0.18 in the HAZ.

4.3.5 Distribution of Martensite

The contours of martensite distribution are plotted in Figure 24. It can be seen from the contours that the fraction of martensite decreases progressively from the solid-liquid transition zone to the unaffected base metal. In the region close to the fusion zone, the fraction of martensite is of the order of 0.75 (this value is at the end of eighth time step). This is because of the favourable conditions for austenite decomposition to martensite. Both the higher cooling rate and large grain size (100 μm) favour the formation of martensite. As the peak temperature drops below 1350 °C, austenite grain size reduces to a value of 15.0 μm . The smaller grain size along with lower cooling rate favours austenite decomposition to bainite and ferrite. In this region fraction of martensite reduces gradually and it drops to a value of 0.02 at 1045 °C. Figure 24 shows the transient values of martensite fraction. As the temperature of the plate drops to room temperature, the fraction

TIME = 0.70000E+01
CONTOURS OF Bainite
MIN= 0.000E+00 AT NODE 207
MAX= 0.199E+00 AT NODE 60

Figure 23 - Contours representing distribution of bainite in the heat-affected zone

TIME = 0.20000E+01
CONTOURS OF Martensite
MIN= 0.000E+00 AT NODE 207
MAX= 0.8332E+00 AT NODE 191

Figure 24 - Contours representing distribution of martensite in the heat-affected zone

of martensite in the the vicinity of solid-liquid transition zone increases to 0.90 %.

4.3.6 Austenite Grain Size

In this microalloyed steel, the austenite grains are pinned by the precipitate of niobium (NbC). As the temperature goes up in the HAZ, the precipitate particles become unstable and begin to dissolve. After the precipitate dissolution temperature the unstable austenite grains begin to grow. For the steel under consideration the precipitate dissolution temperature is 1044.0 °C [21]. The contours showing austenite grain size are plotted in Figure 25. In the vicinity of the solid-liquid transition zone, the austenite grains spend more time above the precipitate dissolution temperature, this makes the austenite grains very large (90.0-100.0 μm). Close to the recrystallization zone, austenite grains spend less time above the precipitate dissolution temperature. The austenite grain size close to the recrystallization zone is of the order of 12-15 μm and it increases to value of 100.0 μm near the solid-liquid transition zone.

4.3.7 Hardness Variation in the HAZ

The hardness at any point in the HAZ is calculated by the rule of mixtures. The contours of hardness are plotted in Figure 26. The contours of martensite fraction distribution and hardness variation are similar in shape because martensite is the hardest constituent of the steel microstructure. In the recrystallization zone the hardness is 150.0 VPN because the fraction of martensite is negligible. As the fraction of martensite increases in the HAZ its hardness also increases proportionately. In the grain growth zone close to the solid-liquid transition zone fraction of martensite increases to a value of 0.90, this leads to a hardness of 356.0 VPN.

TIME = 0.20000E+01
 CONTOURS OF Austenite Grain Size
 MIN= 0.100E+02 AT NODE 207
 MAX= 0.419E+03 AT NODE 124

CONTOUR VALUES
 A= 5.09E+01
 B= 9.18E+01
 C= 1.33E+02
 D= 1.74E+02
 E= 2.14E+02
 F= 2.55E+02
 G= 2.96E+02
 H= 3.37E+02
 I= 3.78E+02

Figure 25 - Contours representing distribution of austenite grain size in the heat-affected zone

CONTOUR VALUES
A= 1.58E+02
B= 1.76E+02
C= 1.95E+02
D= 2.13E+02
E= 2.32E+02
F= 2.50E+02
G= 2.68E+02
H= 2.87E+02
I= 3.05E+02

TIME = 0.70000E+01
CONTOURS OF Hardness
MIN= 0.140E+03 AT NODE 207
MAX= 0.324E+03 AT NODE 191

Figure 26 - Contours representing distribution of hardness in the heat-affected zone

4.4 Comparison of Computed Results with Experimental Values

The experimental data of the weld HAZ is taken from the thesis work of Ion [21]. Ion investigated different welding processes under different welding parameters. In a bead-on-plate weld Ion measured the martensite volume fraction, grain size and hardness at different locations in the HAZ. Comparison of the computed results and measured values are plotted in Figures 27-29. Results obtained by Henwood are also plotted in these figures.

Computed values of austenite grain size match with the measured values throughout the HAZ as shown in Figure 27. This confirms the fact that the present system can predict the value of austenite grain size accurately for the microalloyed steels. If this system is used for a different steel, then the grain growth constant needs to be calculated again.

The computed values of martensite volume fraction are compared with the measured values in Figure 28. The computed values of the fraction of martensite matches with the experimental values throughout the heat-affected zone excellently. The difference between the results from the present work and the results obtained by Henwood clearly shows the advantage of using ODE solvers to accurately predict weld microstructure.

The hardness in the HAZ is computed by the rule of mixtures. The computed values of hardness are compared with the measured values in Figure 29. The maximum hardness is at the inner edge of the HAZ, that is close to the solid-liquid transition zone. The maximum value of hardness is of real interest because it is a good measure of reliability of the joint. As can be seen from Figure 29, this model predicts hardness accurately close to the solid-liquid transition zone. But below 1250 °C computed values drop to 150.0 VPN gradually, while the measured values are in the range of 220.0-250.0 VPN. The drop in the computed value of

Figure 27 - Comparison of computed and measured results for the austenite grain size

Chapter 6

Conclusions

- Adaptive routines for solving the ordinary differential equations (austenite grain growth and austenite decomposition equations) with automatic error checking are implemented. These routines have made the microstructural computations fast and accurate. This advantage has brought the analysis of big problems within a reasonable reach.
- The microstructure code is coupled with the heat transfer code. This coupling allows the prediction of transient and final microstructure in the HAZ accurately.
- A kinetic equation for austenite to martensite transformation is implemented. This captures the austenite to martensite transformation accurately and it also predicts the retained austenite if it is there.
- The computed results have been successfully tested against the experimental measurements of austenite grain size, martensite volume fraction and the HAZ hardness. The agreement between the computed and measured values is found to be excellent.
- The three dimensional finite element analysis heat transfer program computes the weld thermal cycle accurately. It is verified by the accurate values predicted for fusion zone depth, A_1 depth and $\tau_{8/5}$.
- All these contributions have made the prediction of microstructural changes in the HAZ accurate and efficient. This code can also be used for microstructural analysis of castings.

Figure 29 - Comparison of computed and measured results for the hardness

the hardness corresponds to the drop in the fraction of martensite. Below 1250 °C the smaller grain size and lower cooling rates should prefer austenite decomposition to bainite and ferrite. This leads to smaller amount of martensite and reduced hardness. This is exactly what is observed from the computed results.

Chapter 5

General Discussion and Suggestions for Future Work

In the last three chapters, the theory of the microstructure algorithm, its computer implementation and various results are presented. It is demonstrated that the system can predict the transient and final microstructure accurately. This chapter presents general discussion about the research done and suggestions for future work.

5.1 Modelling of Microstructural Changes

5.1.1 Integration of the ODEs

The algorithm implemented in this thesis has been developed by Watt et al [15-16]. In this microstructure algorithm there are four ordinary differential equations which capture the physical phenomenon of austenite grain growth and austenite decomposition to its daughter products (ferrite, pearlite and bainite). In the previous work done on this algorithm the main drawback was the use of inefficient methods for integrating these ODEs. The use of Euler integration technique made this algorithm CPU intensive and results inaccurate. In the present work automatic error checking and adaptive ordinary differential equation integration routines are used. These routines have been developed after years of research at Lawrence Livermore National Laboratory [17]. These routines can be used with large time steps for solving the ODEs. In the present work the time step for integration is set equal to the maximum possible value, that is equal to the FEA heat transfer time step. These integration routines automatically check the error

in each time step. These routines subdivide the time step into smaller time steps if necessary, according to the acceptable limit of error. The use of these routines has made the microstructure code efficient and it predicts accurate results as shown in the previous chapter.

5.1.2 Austenite Decomposition to Martensite

In the previous work done [15-17] on this algorithm, it was assumed that as the HAZ temperature drops below the martensite start temperature, all the available austenite transforms to martensite. This assumption is incorrect because in experimentally measured values of microstructure some retained austenite is also observed. To simulate the transformation of austenite to martensite a kinetic relation developed by Koistinen and Marburger [26] is included in this algorithm. It is assumed that martensite transformation starts at martensite start temperature and stops at martensite finish temperature. Relationship for martensite finish temperature could not be located in the literature therefore its value is assumed equal to room temperature. For most of the low alloy steels martensite finish temperature is close to room temperature except in a few cases where its value is below room temperature. Using this new relation for austenite decomposition to martensite a small quantity (0.008 %) of retained austenite is obtained in the vicinity of solid-liquid transition zone.

5.1.3 Coupling of Microstructure Code with FEA Heat Transfer Code

Another progress made in the present work is the coupling of microstructure code with FEA heat transfer code. Using this coupled system, microstructure, grain size and hardness can be determined at any point in the HAZ. The microstructure is updated at each time step. In the previous work heat transfer analysis and microstructure computations were done separately. This coupled capability of the system is shown by results in the previous chapter. Effect of the

heat of transformation on thermal cycle can also be added into the system. This will help in more accurate prediction of heat flow and microstructure. This has been left for the future work in this area.

5.1.4 Prediction of the Thermal Cycle

A basic requirement for accurate prediction of the weld microstructure is the accurate prediction of the weld thermal cycle. A three dimensional finite element analysis program for heat transfer is used for the prediction of the weld thermal cycle. In this code the heat source for the weld is represented by a double ellipsoid model. Peak temperature of the thermal cycle is set at the centre of the ellipsoid. The temperature decreases exponentially towards the boundary of the ellipsoid. This method predicts the thermal cycle accurately as can be seen from the results. Fusion zone depth, A_1 depth and $\tau_{8/5}$ are predicted accurately by using FEA.

5.1.5 Microstructure in the Fusion Zone

Application of the present algorithm is limited to the HAZ. Implementation of algorithm for the prediction of fusion zone microstructure is left for future work. In the recent past a number of papers have been published on the prediction of fusion zone microstructure. Once the algorithm for the prediction of fusion and solid-liquid transition zone microstructure is developed then it can be easily added into the present code.

5.2 Application of the Present System

The present system requires the natural and essential boundary conditions for heat flow, weld parameters, composition of steel and initial microstructure as input. Using these parameters microstructure in the HAZ can be computed at any point. This kind of analysis can be used to predict the reliability of the joint and it can also help in optimizing the weld parameters to obtain the required weld

microstructure. Coupling of this system with a stress analysis code can be utilized for the prediction of residual stresses developed due to transformation plasticity and thermal strains. The whole of such a package can be used for simulating the welding process.

Chapter 6

Conclusions

- Adaptive routines for solving the ordinary differential equations (austenite grain growth and austenite decomposition equations) with automatic error checking are implemented. These routines have made the microstructural computations fast and accurate. This advantage has brought the analysis of big problems within a reasonable reach.
- The microstructure code is coupled with the heat transfer code. This coupling allows the prediction of transient and final microstructure in the HAZ accurately.
- A kinetic equation for austenite to martensite transformation is implemented. This captures the austenite to martensite transformation accurately and it also predicts the retained austenite if it is there.
- The computed results have been successfully tested against the experimental measurements of austenite grain size, martensite volume fraction and the HAZ hardness. The agreement between the computed and measured values is found to be excellent.
- The three dimensional finite element analysis heat transfer program computes the weld thermal cycle accurately. It is verified by the accurate values predicted for fusion zone depth, A_1 depth and $\tau_{8/5}$.
- All these contributions have made the prediction of microstructural changes in the HAZ accurate and efficient. This code can also be used for microstructural analysis of castings.

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