Simulation of the Weld Heat Affected Zone of a 0.5Cr-Mo-V Steel

B. Radhakrishnan and T. Zacharia
Metals and Ceramics Division
Oak Ridge, TN 37831-6140

RECEIVED
DEC 08 1995
OSTI

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

MASTER
DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

Abstract

By using a Monte Carlo grain growth algorithm and a methodology for obtaining a one-to-one correlation between Monte Carlo and real parameters of grain size and time, the grain structure in the weld heat affected zone of a 0.5 Mo-Cr-V steel has been simulated. The simulations clearly show that the kinetics of grain growth can be retarded by the presence of steep temperature gradients in the weld heat affected zone. Additional pinning, due to the formation of grain boundary liquid near the solidus temperature, has also been simulated. It is shown that in order to accurately predict the observed grain size in the weld heat affected zone of the 0.5Cr-Mo-V steel, the retardation in growth kinetics due to temperature gradients as well as liquid pinning should be considered.

THE MICROSTRUCTURE OF THE WELD HEAT AFFECTED ZONE (HAZ) of single-phase materials can be described in terms of the average grain size and the grain size distribution. These quantities are influenced by the peak temperature, the heating rate, and the cooling rate in the HAZ, all of which decrease with distance from the heat source. The gradients in the above parameters give rise to a gradient in the HAZ grain size, with the coarsest grains typically forming near the fusion line. In alloy systems where there is a solid-state transformation from a high-temperature to a low-temperature phase, the kinetics of formation and the morphology of the low temperature phase are determined, to a large extent, by the parent-phase grain size. A common example is found in steels where the kinetics of austenite transformation on cooling are sensitive to the prior austenite grain size (1).

Several studies are available in the literature that deal with the estimation of grain size in the HAZ (2-4). These

studies are generally based upon the use of the well-known equations describing curvature-driven grain growth given by

$$D^{\frac{1}{n}} - D_0^{\frac{1}{n}} = kt \quad (1)$$

where D is the average grain size at time t , D_0 is the average initial grain size, n is the grain growth exponent and k is a temperature-dependent boundary mobility given by

$$k = k_0 \exp \left(\frac{-Q}{RT} \right) \quad (2)$$

where k_0 is a constant, Q is the activation energy for grain growth, T is the absolute temperature and R is the universal gas constant. Non-isothermal grain growth is modeled by using the differential form of equation 1 or 2 and then integrating it over the thermal cycle.

However, it has been recognized (4) that the use of equation 1 for calculating the HAZ grain size is not strictly correct because it assumes an average thermal cycle for an HAZ width equal to the grain size. Often, the temperature gradient in the weld HAZ can be so steep that the temperature can vary across a single grain. This is especially true near the fusion line where the grains are the coarsest and the temperature gradient is the steepest. Under such conditions, the quantity k in equation 2 varies across a grain, and hence the grain growth rate can be significantly different than the estimates obtained using equation 1. The above phenomenon, termed "thermal pinning" was first reported in the weld HAZ of a 0.5Cr-Mo-V steel by Alberly et al (2). Although the effect of thermal pinning on the HAZ grain size has been recognized for quite some time, the phenomenon has not been quantitatively modeled.

B. Radhakrishnan and
T. Zacharia

Monte Carlo Simulation of Grain Growth: The Monte Carlo (MC) technique has been used to simulate grain growth in single-phase and two-phase materials under isothermal conditions (5-18). As a first step, the technique involves the mapping of a grain structure on to a discrete lattice. Each grain is then represented by a collection of lattice sites which have a unique orientation number. Curvature-driven grain growth is simulated by calculating the net energy change at each of the grain boundary sites as the orientation changes from that of the existing grain to the orientation of a neighboring grain. The orientation change is allowed only if the net energy change is zero or negative, which corresponds to a reduction in the local curvature of the grain boundary. A detailed description of the MC grain growth algorithm is available in the literature (5-18) and will not be repeated here. A major advantage of using the MC simulation over other analytical techniques for studying curvature-driven grain growth is that the MC simulation presents both microstructural and kinetic information, while the analytical models provide only kinetic information. MC simulation is particularly attractive for studying grain growth in a temperature gradient because the spatial variation of grain boundary mobility can be easily incorporated into the algorithm.

In MC simulations, the grain size is expressed as a dimensionless number which, in 2-D simulations, is either the square-root of the number of sites within a grain, or $1/N_L$, where N_L is the number of grain intersections per unit length of a test-line. The unit of simulation time is the Monte Carlo Step (MCS), which corresponds to one re-orientation attempt per lattice site, for all the sites in the simulation domain. MCS is also a dimensionless number. In order to apply the simulation to quantitatively predict the grain growth kinetics, the real space-time coordinates should be correlated with MC space-time coordinates. For this purpose, a methodology previously developed by the authors (19) is used. The objective of the present study is to simulate the evolution of grain structure in the weld HAZ of the Cr-Mo-V steel used by Alberly et al (2). The extent of thermal pinning is determined by comparing the grain size at a given location in the HAZ of a weld with the grain size obtained by subjecting the entire workpiece to a thermal cycle identical to the one experienced by the HAZ location (similar to Gleeble simulation).

Methodology

The methodology used for obtaining one-to-one correspondence between MC and real parameters of grain size and time involves the determination of scaling constants between MC space and real space, K_1 , and between MCS and real time, K_2 . The inputs to the methodology include experimental isothermal grain growth data for the given material at different temperatures, and a simulated grain growth curve which has the same grain growth exponent, n , as the material under consideration. K_1 is given by

$$K_1 = \frac{D_R}{D_M} \quad (3)$$

where D_R is the real grain size and D_M is the MC grain size. K_2 is defined by

$$K_2 = \frac{MCS}{t} \quad (4)$$

The temperature dependence of K_2 is given by

$$K_2 = K_2^0 \exp\left(\frac{-Q}{RT}\right) \quad (5)$$

where K_2^0 is an empirical "frequency factor" for a MC lattice site. The constant K_1 can be assumed such that it matches the scale of the microstructure. For example, if the average grain size is of the order of several microns, the value of K_1 can also be chosen in the micron range so that there will be a finite number of points per grain. On the other hand, if the initial grain size is in the submicron range, the value of K_1 can be appropriately chosen such that the number of points within an average grain is still finite. It can be shown that (19),

$$\frac{dD_R}{dt} = K_1 K_2 \left(\frac{dD_M}{dMCS}\right) \quad (6)$$

In equation 6, dD_R/dt is known from experimental results, $dD_M/dMCS$ is known from simulations, and hence, K_2 can be calculated for an assumed value of K_1 . Using equation 4, an equivalent MCS value can be calculated for an isothermal hold at any given temperature. Also, a real thermal cycle can be converted into an effective MCS value, by breaking it down into a number of isothermal steps and summing the MCS value for each step.

Simulation Procedure

Two-dimensional (2-D) MC simulations were carried out using a 300 x 300 lattice in which the lattice points were arranged in a square geometry. The total number of initial orientations was 300². A neighborhood of 8 lattice points consisting of the first and second-nearest neighbors was used for local interaction energy calculations. The details of the MC algorithm used for the simulations are described elsewhere (18). The MC algorithm predicts a grain growth exponent of 0.5 for an ideal material in which anisotropy in grain boundary energy, preferred orientation, and solute-drag are absent. However, the Cr-Mo-V steel under consideration showed an experimental grain growth

exponent of 0.368 (2). The lower grain growth exponent was attributed to solute drag, the presence of a texture, and a non-equiaxed grain structure in the initial microstructure (2). It has been shown (10) that a lower grain growth exponent can be obtained in MC simulations through the introduction of an anisotropy parameter. In the present simulations, the anisotropy parameter was treated as an adjustable quantity. It was found that an anisotropy parameter of 0.45π resulted in a grain growth exponent of 0.368, which was the same as the experimental value. The effect of solute drag is to enhance the orientation dependence of grain boundary energy and mobility, and thereby influence the magnitude of the grain growth exponent. Hence, although solute-drag has not been modeled directly, the overall effect of solute drag on the grain growth exponent is built into the algorithm through the anisotropy term.

The initial step was to determine K_2 at various temperatures using the isothermal grain growth data of Alberry et al (2), and determine the activation energy Q , and the frequency factor K_2^0 for various assumed values of K_1 . As a check, the isothermal simulations were repeated using the computed values of MCS for various temperatures, and the grain growth kinetics were compared with the experimental results. In order to generate the thermal cycle for each HAZ location, the welding parameters and material properties used by Alberry et al (2), were chosen. Thermal cycles were calculated using the same form of the Rosenthal equation used by Alberry et al (2). MCS value corresponding to each thermal cycle was calculated by breaking down the thermal cycle at a given location into a number of isothermal steps using a time step of 0.01 second. For all weld simulations, K_1 was assumed to be 25 microns, and the appropriate value of K_2 was chosen for each temperature. The initial grain size in the simulations was assumed to be 25 microns, which is approximately the same as that in the steel samples used by Alberry et al (2). Hence, the initial microstructure consisted of one lattice point per grain.

Since the thermal cycle in the weld HAZ is a function of the distance from the fusion line there is a corresponding gradient in the MCS. The gradient in MCS was incorporated into the simulations by carrying out the simulations for the maximum value of MCS, MCS_{max} , and visiting each MC site with a probability $p(x)$ given by

$$p(x) = \frac{MCS(x)}{MCS_{max}} \quad (7)$$

where $MCS(x)$ is the MCS at a distance x from the fusion line. The mean grain size at various distances from the fusion line was measured using linear intercept counts on test lines placed parallel to the fusion line. In MC simulations, periodic boundary conditions are normally used so that the grains at the top of the domain wrap around those at the bottom, and those at the left end wrap around those at the right end of the domain. Although such a scheme can be

applied to isothermal grain growth, in the case of grain growth under a temperature gradient, the peak temperature must be located at the center of the domain, so that the grains that wrap around are at the same temperature. Hence, in the simulations the center of the domain corresponds to the region adjacent to the fusion line, and the ends correspond to the locations which are roughly 3.75 mm from the fusion line (for $K_1 = 25$ microns).

Alberry et al (2) described the thermal pinning by computing the grain size in a bulk sample subjected to a thermal cycle corresponding to a HAZ location ≈ 120 microns from the fusion line by integrating the differential form of equation 1, and comparing it with the grain size obtained in an actual weld HAZ at an identical location. Hence, in order to calculate thermal pinning, the simulations were repeated by applying to the entire domain the MCS corresponding to the thermal cycle at a distance of 120 microns from the fusion line (hereafter referred to as "bulk heating"). All simulations were repeated using five different starting seed values for the random number generator, and the results shown in each case is an average of 5 runs.

Results and Discussion

Figure 1 shows an Arrhenius plot of $\ln(K_2)$ versus $1/T$, the K_2 values having been obtained using the methodology described earlier. An activation energy of 470 KJ/mole is

Figure 1. Plot of $\ln(K_2)$ versus $1/T$. Activation of 470 KJ/mole is obtained.

obtained, which is the same as that obtained using K_2 values from the isothermal grain growth data of Alberry et al(2), as shown in figure 1. The unit of K_2 obtained using the methodology described above is sec^{-1} , while the experimentally determined K_2 values have the unit of $\text{mm}^{2.73}\text{sec}^{-1}$, as shown in figure 1. The isothermal grain growth data of Alberry et al (2) were for a holding period of 100 seconds, at temperatures ranging from 1391K to 1576K. Assuming a K_1 value of 25 microns, the MCS for

Figure 2. Grain Growth data of Alberly et al (2) (symbols), on which the simulation results (lines) are superimposed.

a 100 second hold at 1391K was 102. However, for the same value of K_1 , the MCS value corresponding to a 100 second hold at 1576K was 148000. Since a much larger computer time is required to carry out the simulation for an MCS of 148000, a higher K_1 value was assumed for the 1576K heat treatment. For K_1 equal to 141 microns, the MCS for a 100 second hold at 1576K was 100. As described earlier, the advantage of the above methodology for relating MCS and real time is that the constant K_1 can be chosen such that it matches the scale of the microstructural evolution. Consequently, K_2 , and hence, MCS can be kept reasonably small and the computational time can be kept reasonably constant for a large grain growth range. Figure 1 shows the Arrhenius plots for the various assumed values of K_1 used in the isothermal simulations. Figure 2 shows the raw grain growth data of Alberly et al (2), on which the grain growth kinetics obtained by simulation are superimposed. There is excellent agreement between simulation and experiments.

Figure 3 shows the effective MCS as a function of distance from the fusion line for a specific heat input of 730 J/mm. The effective MCS at a given HAZ location is computed by first calculating the thermal cycle at the location, breaking it down into a number of isothermal steps with a corresponding time step of 0.01 second, and then using equation 4 to calculate the MCS for each time step. Figure 4 shows the kinetics of grain growth at the 120 micron HAZ location and the kinetics of grain growth for bulk heating using an identical thermal cycle. It can be clearly seen that the kinetics of grain growth in the HAZ location is lower than that for bulk heating for an identical thermal cycle, thus indicating grain boundary pinning exists in the HAZ due to the temperature gradient.

Using bulk heating, the simulations predict an average grain size of 393 microns at a location of 120 microns from the fusion line, which compares favorably with the grain size

Figure 3. Cumulative MCS for each thermal cycle as a function of distance from the fusion line.

320 microns computed by Alberly et al(2) by integrating the differential form of equation 1 over an identical thermal cycle. However, for the actual HAZ where thermal pinning is present, the simulations yield an average grain size of about 275 microns, which is significantly higher than the

Figure 4. Grain growth kinetics at the 120 micron location in the HAZ and for bulk heating using corresponding thermal cycle.

experimentally measured value of 100 microns. Hence, while the simulations capture the thermal pinning effect, the magnitude of the pinning predicted by the simulations is significantly lower than in the actual weld HAZ. This is because of the additional pinning due to the formation of the grain boundary liquid in HAZ locations where the peak temperature exceeds the liquation temperature, and its retention to subsolidus temperatures on rapid cooling.

Figure 5. Cumulative MCS for the weld thermal cycles for various assumed liquation temperatures.

In figure 3, it is assumed that there is no intergranular liquid in the HAZ above the solidus temperature. However, it is known that grain boundary liquation can occur in the HAZ above the solidus temperature and that the presence of liquid on grain boundaries can effectively stop grain growth in the HAZ (20). The temperature range in which the boundaries are pinned depends upon the on-heating liquation temperature and the on-cooling solidification temperature. The on-heating liquation temperature depends upon several microstructural and kinetic parameters. The presence of soluble second phase particles can cause subsolidus liquation (21, 22). The liquid from the fusion zone can wet the HAZ

Figure 6. Simulated grain structures for various assumed liquation temperatures. Fusion line is at the left. Arrow indicates the 120 micron location.

grain boundaries and spread along the boundaries to locations where the temperature is lower than the equilibrium solidus. The extent of spreading depends upon the solute backdiffusion kinetics and grain boundary diffusion kinetics. The on-cooling solidification kinetics also depend upon the

backdiffusion kinetics of solute into the matrix. The liquation and solidification temperatures under rapid heating and cooling conditions are not known for the 0.5Cr-Mo-V steel. The equilibrium solidus computed using Thermocalc™ (23) is 1743K. DTA experiments using steels of similar carbon content have shown that undercoolings of the order of 100K are possible for a cooling rate of 10K/min (24). Hence, in the case of the weld HAZ where the cooling rates are much higher, the undercooling is expected to be much higher.

Since the liquation and solidification temperatures under rapid thermal cycling are not known, the simulations were

Figure 7. Final grain size at the 120 micron location in the HAZ as a function of the liquation temperature, and the grain size for bulk heating using the same thermal cycle.

carried out for various assumed values to predict the effect of pinning due to grain boundary liquid. Figure 5 shows the MCS as a function of distance from the fusion line for various assumed liquation temperatures. In these calculations, it was assumed that the on-heating liquation temperature was equal to the on-cooling solidification temperature. Since grain boundary liquid effectively pins the grain boundaries in the temperature range in which the liquid exists, the corresponding portion of the thermal cycle was not considered in the calculation of MCS. Notice that the MCS values closer to the fusion line decrease as the liquation temperature decreases. Figure 6 shows the HAZ grain structure for the cases shown in Figure 5, and also the grain structure under bulk heating conditions using the 120 micron location thermal cycle. The grain size at the 120 micron location (indicated by arrow) is lower than the grain size under bulk heating conditions for all assumed liquation temperatures. Figure 7 shows the grain size at the 120 micron location as a function of the liquation temperature. The grain size decreases with decreasing liquation temperature. Figure 7 also shows that undercoolings greater than 100K must be assumed in order to match the simulated grain size with the experimentally observed grain size.

Conclusions

The grain structure in the weld HAZ can be simulated with reasonable accuracy using the MC technique and a methodology for converting the MC parameters of grain size and time to real parameters. The MC technique effectively captures the thermal pinning phenomenon that has been reported in the weld HAZ. However, the extent of thermal pinning reported in the literature for a Cr-Mo-V steel is significantly higher than the thermal pinning that can be obtained based on the temperature gradient alone. It is suggested that the formation of grain boundary liquid at HAZ locations where the peak temperatures on heating are above the liquation temperature, and the retention of the grain boundary liquid to lower temperatures on cooling because of incomplete backdiffusion of solute, can account for additional pinning at HAZ locations close to the fusion line. Incorporating the additional pinning due to grain boundary liquid has resulted in a closer match between simulated and experimentally measured grain sizes in the weld HAZ of a Cr-Mo-V steel.

Bibliography

1. Lange, W.F., M. E. Enomoto and H.I. Aaronson, *Metall. Trans. A.*, 20, 427-440 (1988).
2. Alberry, P.J., B. Chew and W. K. C. Jones, *Metals Technol.*, 4, 317-325 (1977).
3. Ashby, M.F., and K.E. Easterling, *Acta Metall.* 30, 1969-1978 (1982).
4. Reed, R., Ph.D. Thesis, University of Cambridge, U.K., September 1990.
5. Srolovitz, D.J., M. P. Anderson, G. S. Grest and P.S.Sahni, *Scripta Metall.*, 17, 241-246 (1983).
6. Sahni, P.S., D. J. Srolovitz, G. S. Grest, M. P. Anderson and S. A. Safran, *Physical Review B*, 28, 2705-2716 (1983).
7. Anderson, M.P., D. J. Srolovitz, G. S. Grest and P. S. Sahni, *Acta Metall.*, 32, 783-791 (1984).
8. Srolovitz, D.J., M. P. Anderson, P. S. Sahni and G. S. Grest, *Acta Metall.*, 32, 793-802 (1984).
9. Srolovitz, D.J., M. P. Anderson, G. S. Grest and P. S. Sahni, *Acta Metall.*, 32, 1429-1438 (1984).
10. Grest, G.S., D. J. Srolovitz and M. P. Anderson, *Acta Metall.*, 33, 509-520 (1985).
11. Srolovitz, D.J., G.S. Grest and M.P. Anderson, *Acta Metall.*, 33, 2233-2247 (1985).
12. Anderson, M.P., G.S. Grest and D.J. Srolovitz, *Scripta Metall.*, 19, 225-230 (1985).
13. Righetti, F., T. M. Liebling and A. Mocellin, *Acta Stereol.*, 8, 459-464 (1989).
14. Anderson, M.P., G.S. Grest, R.D. Doherty, K. Li and D.J. Srolovitz, *Scripta Metall.*, 23, 753-758 (1989).
15. Grest, G.S., M. P. Anderson and D. J. Srolovitz, *Physical Review B*, 38, 4752-4760 (1988).
16. Anderson, M.P., G. S. Grest and D. J. Srolovitz, *Phil. Mag. B.*, 59, 293-329 (1989).
17. Holm, E.A., D. J. Srolovitz and J. W. Cahn, *Acta Metall.*, 41, pp. 1119-1136 (1993).
18. Radhakrishnan, B., and T. Zacharia, *Metall. Trans. A.*, 26, 167-180 (1995).
19. Radhakrishnan, B., and T. Zacharia, *Proceedings of the International Conference on Modeling and Control of Joining Processes*, Orlando, FL, U.S.A., Dec. 1993.
20. Pepe, J.J., and W. F. Savage, *Welding Journal*, 49, 545-s-553-s (1970).
21. Pepe, J.J., and W. F. Savage, *Welding Journal*, 46, 411-s-422-s (1967).
22. Owczarski, W.A., D. S. Duvall and C. P. Sullivan, *Welding Journal*, 46, pp. 423-s-432-s (1967).
23. Sundman, B., B. Jansson and J. O. Andersson, *CALPHAD*, 9, 153-190 (1985).
24. Babu, S.S., S. A. David and J. M. Vitek, Oak Ridge National Laboratory, private communication.

Acknowledgement

The authors would like to acknowledge Dr. J.M. Vitek for reviewing the paper. The research was sponsored by the Division of Materials Sciences, U.S. Department of Energy, under contract no. DE-AC05-84OR21400 with Lockheed Martin Energy System, Inc.

"The submitted manuscript has been authored by a contractor of the U.S. Government under contract No. DE-AC05-84OR21400. Accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes."