Numerical simulation of equiaxed grain formation in weld solidification

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Abstract

Numerical simulation is developed on grain structure development during weld solidification of steel. Monte Carlo (MC) method is applied to the simulation of nucleation and growth of solid, being combined with finite difference calculation of heat conduction and solute diffusion. Based on the experimental result that titanium nitride (TiN) works as a nucleating agent of equiaxed grain formation, given number density of TiN is allocated to MC cells randomly and instantaneous nucleation is assumed to occur when the melt undercooling of the cell exceeds a given critical level. It is found that the simulation can reproduce the weld solidification by reflecting the effect of TiN as a nucleating agent and the effect of soluble titanium that increases melt undercooling. Those effects have been recognized only as combined effects in previous experimental studies, but through the present simulation, they are first investigated in a separate manner. The simulation results indicate that equiaxed grain formation is promoted not only by a nucleating agent, TiN, but also by melt undercooling increased by soluble titanium and that both are requisite to bring about the columnar-to-equiaxed transition (CET). The results are discussed in connection with theoretical models on CET and confirm the rationality of the models.

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1. Introduction

Equiaxed grain formation is essential to the grain refinement of castings and welds, but it is not so easily achieved in welds [1] since their solidification proceeds under high $G/R$ condition, where $G$ is thermal gradient and $R$ is solidification rate. Columnar grain growth is almost always favored under the condition, and there are little chances of equiaxed grain formation, which thereby results in coarse, low-ductility columnar grain structure in welds. In castings, the equiaxed grain formation is enhanced through grain multiplication caused by the break-off or remelting of secondary dendrite arms in mushy zone [2], which is unlikely in welds with steep temperature gradient and thereby very narrow mushy zone. Nucleation of new solid at melt surface and mold surface is also believed to be a source of equiaxed grains in castings [3], but it is again highly unlikely in welds because the melt surface is the highest temperature region under welding arc and the mold of weld pool is the ‘matching’ mold that encourages the epitaxial, continuous growth of columnar grains. Therefore, in most of welding conditions, columnar coarse grain structure is predominant, and equiaxed grain formation would not be achieved without strong nucleating agents to induce the columnar-to-equiaxed transition (CET) in welds [4].

Low-carbon ferritic stainless steel is one of the typical steel grades whose welds exhibit very coarse columnar grain structure. The steel grade is fully ferritic for all the temperature range from solidification down to room temperature without any solid-state transformation at intermediate temperatures. Thus its welds retain coarse columnar grains developed during the solidification. The modification of the weld grain structure has been investigated, and Villafuerte and Kerr [5] demonstrated that the addition of titanium increased equiaxed grains in those welds. Titanium nitride (TiN), which has a good lattice coherency with $\delta$-iron [6], was supposed to be
primarily responsible for the equiaxed grain formation, acting as a strong nucleating agent. This beneficial effect of TiN on equiaxed grain formation was also confirmed by some of the present authors [7] in laboratory-melted ferritic stainless steel welds. It was found that equiaxed solidification selectively occurs in welds containing such titanium and nitrogen contents that produce TiN in the melt in advance of solidification. In fact, equiaxed grains were found to nucleate on TiN in the melt ahead of solidification front in the weld pool quenched by liquid tin during the welding. However, while increase in titanium makes TiN precipitation feasible in the melt, it increases melt undercooling ahead of the solid–liquid interface as well. The undercooling is essential for the embryos nucleated on TiN to survive and grow as equiaxed grains. Therefore, the equiaxed grain formation should be due to both effects of TiN precipitation and increased undercooling. In the experiments mentioned above, the effect of TiN as a nucleating agent and the effect of soluble titanium on melt undercooling are recognized only as combined effects, and the contribution of each factor is not separately identified.

In the present study, grain structure development in welds is simulated using Monte Carlo (MC) method coupled with finite difference (FD) calculation of thermal and solute diffusions. This makes it possible to examine the contribution of each effect separately. Based on the results, discussions are made on quantitative contribution of each effect in comparison with the theoretical CET models.

2. Review of experimental observation [7]

Low-carbon, 17 mass%Cr and 19 mass%Cr–2 mass%Mo ferritic stainless steel sheets containing different amounts of titanium and nitrogen were made in laboratory and full penetration autogenous gas tungsten arc welding was performed on the sheets. In titanium-free welds, the grain structure is fully columnar, as seen in Fig. 1(a), where coarse columnar grains grow epitaxially from the both sides of fusion zone until impinged at the center. In titanium-added welds, the effect of titanium and nitrogen on weld solidification is summarized in Fig. 2(a) for 17 mass%Cr welds and Fig. 2(b) for 19 mass%Cr–2 mass%Mo welds, along with calculated TiN solubility limit at liquidus temperature for each alloy system which is calculated using Thermo Calc [8]. Equiaxed grain formation is promoted with increasing titanium and nitrogen contents, and the comparison of the result with the solubility limit line indicates that the equiaxed grain formation is closely associated with TiN precipitation in the melt. In other words, precipitation of TiN in the melt prior to

![Fig. 1. Cross-section of ferritic stainless steel weld containing (a) 17 mass%Cr, 0.007 mass%Ti and 0.0097 mass%nitrogen, and (b) 17 mass%Cr, 0.3 mass%Ti and 0.0092 mass%nitrogen.](image)
the solidification seems to be a prerequisite to CET in both 17 mass%Cr welds and 19 mass%Cr–2 mass%Mo welds.

Effect of TiN is directly identified in the welds quenched by liquid tin during the welding. In titanium-free welds, grain growth is fully columnar toward the weld pool, as the solidification front quenched is shown in Fig. 3(a); no crystal seems to exist within the melt ahead of the columnar grains prior to quenching. In titanium-added welds, on the other hand, a number of solid grains are found to exist in the melt, as shown in Fig. 3(b). These grains are clearly differentiated from the surrounding microstructure formed by quenching from the melt, in terms of grain size and morphology. Thus, the grains in the weld pool are concluded as equiaxed grains that have been formed before quenching. The equiaxed grains floating in the melt are often seen having a four-fold morphology, typical cross-section of octahedron, and exhibits a cubic-like nucleant at the center as seen in Fig. 4. EDS and AES analyses of the nucleants indicate that they are primarily TiN. As typically seen in Fig. 3(b), equiaxed grain formation is confined within 200–300 μm from the solidification front. This implies that the nucleation and subsequent growth of equiaxed grains occur in the undercooled region that extends for hundreds microns ahead of the solidification front. TiN should precipitate apriori in the outer higher-temperature melt and be supplied to this undercooled region; otherwise, the equiaxed grain formation is difficult or limited in such narrow undercooled region within such short time. This is consistent with the results shown in Fig. 2. In summary, based on the experimental results mentioned above, the process of equiaxed grain formation on TiN is schematically given in Fig. 5.

3. Simulation of weld solidification

A numerical simulation was attempted to simulate the equiaxed grain formation in welding and to discuss factors affecting the solidification behavior. In the simulation, MC method is employed for nucleation and growth of solid, and is combined with FD method to take into account heat conduction and solute diffusion. The combination of MD method and FD method is primarily based on the technique developed by Zhu and Smith [9].

Two-dimensional simulation is conducted for the weld solidification of 1 mm-thick plate, assuming that the weld solidification proceeds on a plane perpendicular to welding direction, i.e. on a cross-section as shown in Fig. 1(a) and (b). On the plane, an area of 1 mm (thickness) × 5 mm (length in horizontal direction) is taken from the weld center as the calculation area so that the area contains a half of the fusion zone at one end due to symmetry. The area is divided into cells in two different ways; rectangular cells are used for FD calculation and triangular cells for MC calculation. Fig. 6 shows a flow of the calculation within one time step. Heat conduction and solute diffusion are calculated by using FD cells and nucleation and growth (i.e. movement of liquid–solid interface and solid grain boundary) are by using MC cells.

3.1. Heat conduction and solute diffusion

Heat conduction and solute diffusion are calculated in two-dimension coordinate (x, y) with rectangular FD cells. A change in the temperature of a FD cell, T(x, y, t), within
a time step $\Delta t$ is given by the following equation

$$T(x_i, y_i, t + \Delta t) = T(x_i, y_i, t) + \frac{\Delta t q_t}{C_p \rho} + \left[\lambda_1 (T(x_i + \Delta x, y_i, t) - T(x_i, y_i, t)) \right]$$

$$+ \lambda_2 (T(x_i - \Delta x, y_i, t) - T(x_i, y_i, t)) \Delta x^2 + \left[\lambda_3 (T(x_i, y_i + \Delta y, t) - T(x_i, y_i, t)) \right]$$

$$+ \lambda_4 (T(x_i, y_i - \Delta y, t) - T(x_i, y_i, t)) \Delta y^2] \Delta t / (C_p \rho)$$

(1)

where $C_p$ is specific heat and $\rho$ is density, assuming that both are constant and not changed by the phase transition from liquid to solid. $q_t$ is a latent heat of crystallization. When there is an increase in fraction solid as a result of MC calculation, then the latent heat for the increase of solid is included. $\lambda_k (k = 1, 4)$ is thermal conductivity. When one of the neighboring FD cells of interest or both, are the mixture of liquid and solid, the conductivity is obtained by using a weighted average of the fraction of liquid. For example, $\lambda$ between FD cell 1 and FD cell 2 is defined as

$$\lambda = [(f_{l1} + f_{l2})/2] \lambda_l + [1 - (f_{l1} + f_{l2})/2] \lambda_s$$

(2)

where $\lambda_l$ and $\lambda_s$ are thermal conductivity of liquid and solid, respectively, and $f_{l1}$ and $f_{l2}$ are the fraction liquid in FD cell 1 and FD cell 2, respectively. If both of the neighboring cells of interest are with the same single phase, then simply either $\lambda_l$ or $\lambda_s$ is applied to $\lambda_k$ depending on the phase.

Solute diffusion is given by a similar equation to heat conduction, but the diffusion in liquid and that in solid are treated separately and connected at the liquid/solid interface.
by equilibrium partitioning coefficient. A change in concentration of a solute, \(C(x, y, t)\), within a time step \(\Delta t\) is given by

\[
C(x_i, y_i, t + \Delta t) = C(x_i, y_i, t) + \Delta t q_c + \left\{ \begin{array}{l}
D_1 (C(x_i + \Delta x, y_i, t) - C(x_i, y_i, t)) \\
- \frac{\Delta x^2}{2} \left[ D_2 (C(x_i, y_i + \Delta y, t) - C(x_i, y_i, t)) + D_3 (C(x_i, y_i - \Delta y, t) - C(x_i, y_i, t)) \right]
\end{array} \right\}
\]

(3)

where \(q_c\) is a change in concentration due to partitioning caused by the advance of solid. The above equation is used for both liquid and solid. \(D_k\) (\(k = 1, 4\)) is a diffusivity of the solute element of interest, and when one of the neighboring FD cells of interest or both are the mixture of liquid and solid, the diffusivity is obtained by using a weighted average of the fraction of liquid. For example, diffusivity \(D\) between FD cell 1 and FD cell 2 is defined for liquid part as

\[
D = \frac{f_{l1} + f_{l2}}{2} D_l
\]

(4)

and for solid part as

\[
D = \frac{1 - (f_{l1} + f_{l2})/2} D_s
\]

(5)

where \(D_l\) and \(D_s\) are diffusivity of the solute element of interest in liquid and solid, respectively, and \(f_{l1}\) and \(f_{l2}\) are the fraction liquid in FD cell 1 and FD cell 2, respectively.

In terms of boundary conditions, one vertical end of the calculation area (\(x = x_0\) or \(x = 0\) mm) is treated as a mirror because of symmetry at the center of fusion zone, and the other vertical end (\(x = x_e\) or \(x = 5\) mm) is assumed to have the same gradient as the nearest neighbor cell at \(x_{e-1}\) (or \(x = 5\) mm \(- \Delta x\)) in terms of both temperature and solute concentration. Both horizontal ends (\(y = y_0\) and \(y_e\), or \(y = 0\) and \(y = y_{e}\)) are treated as free boundary conditions.
and 1 mm) are assumed to be adiabatic in terms of both heat and solute.

The area of 1 mm × 1 mm at one end of the calculation area is instantaneously heated up to a temperature \( T_0 \) above the melting point and melted;

\[
T(x, y, 0) = \begin{cases} T_0 & 0 \leq x \leq 1 \text{ mm}, \text{ all } y \\ 298 \text{ K} & 1 < x \leq 5 \text{ mm}, \text{ all } y \end{cases}
\]

(6)

Then as the heat diffuses, melting is spread towards the other end of the area to form fusion zone of welding. The initial heat input is equivalent to welding heat input giving a fusion zone area similar to that in actual weld. Solute partitioning at the liquid/solid interface is ignored during the melting but considered during the solidification. Grain growth in the heat-affected zone adjacent to the liquid/solid interface (i.e. fusion boundary) is always calculated. At a certain point, the melting no longer proceeds and then solidification starts from the fusion boundary in the reverse direction to the melting. Solid grows epitaxially from existing, coarsened grains at the fusion boundary unless there is new solid formation in the melt ahead of the fusion boundary.

### 3.2. Nucleation and growth

In terms of the nucleation of solid in the melt, which is the origin of equiaxed grains, we consider only the heterogeneous nucleation on TiN in the melt, because there is no other potential nucleation mechanisms that can prevail over it. TiN is distributed randomly throughout the calculation area apriori with a given number density. A MC cell is allocated to each TiN. TiN is assumed to work as the nucleation site of solid when the melt undercooling, \( \Delta T \), exceeds a given critical value, \( \Delta T_N \), in the FD cell in which TiN of interest is contained. It is noted that \( \Delta T \) is defined for each FD cell as a difference between actual temperature of the FD cell and the melting point determined by composition of the FD cell. The probability of nucleation of solid, \( P_n \), is given by

\[
P_n = \begin{cases} 1 & \text{at } \Delta T \geq \Delta T_N \\ 0 & \text{at } \Delta T < \Delta T_N \end{cases}
\]

(7)

Such instantaneous nucleation assumption appears to be most reasonable for nucleation event on a strong agent that works effectively with a small undercooling.

The probability model of growth into the liquid is basically the same as described by Zhu and Smith [9]. Total free energy change of a MC cell, \( \Delta F_g(x, y, t) \), is obtained considering bulk free energy change and interfacial free energy change. In the case of triangular MC cell, it is given by:

\[
\Delta F_g(x, y, t) = -1.5\sqrt{3}r^2 \delta \Delta H_l \Delta T(x, y, t)T_m(x, y, t) + (n_s \sigma_{ls} + n_m \sigma_{ms}) \delta r
\]

(8)

The first term of the right-hand side is the bulk free energy change and the second the interfacial free energy change. In the equation, \( r \) is the MC cell length, \( \delta \) cell height, \( \Delta H_l \) the latent heat of crystallization, \( n_s \) an increase in the number of liquid/solid interface for the MC cell of interest, \( n_m \), the number of solid/solid cell interfaces with different orientations. By differentiating the \( \Delta F_g \) with respect to cell length \( r \) and putting the derivative equal to zero, then a critical energy barrier \( \Delta F_g^c \) for the growth of the MC cell of interest is obtained:

\[
\Delta F_g^c = (n_s \sigma_{ls} + n_m \sigma_{ms})/6\sqrt{3}\Delta H_l \Delta T(x, y, t)T_m(x, y, t)
\]

Thus, the probability of the growth, \( P_g \), is given by

\[
P_g = \begin{cases} 0 & \text{if } \Delta T \leq 0 \\ \exp(-\Delta F_g/kT) & \text{if } \Delta T > 0 \end{cases}
\]

(10)

where \( k \) is Boltzmann constant. When the temperature of FD cell is higher than the melting point, no solid will grow into the liquid, and the growth probability is increased with increasing undercooling. In terms of grain growth in fully solid state, we modify the growth probability as:

\[
P_g = \exp(-\Delta F_g/kT)A \exp(B/T/T_m)
\]

(11)

The multiplication by a factor of \( A \exp(B/T/T_m) \) is necessary to take into account the effect of temperature gradient [10,11]. This temperature-dependent factor corresponds to the mobility of grain boundary in a physical sense. Temperature gradient is steep in heat-affected zone, and the coarsening of grains is affected by the maximum temperature that is changed from place to place by heat conduction from the fusion boundary. If the multiplication by the above-mentioned factor is not introduced, grain coarsening will not be changed by place and similar coarsening behavior may be obtained throughout the heat-affected zone regardless of the maximum temperature reached. In Eq. (11), \( A \) and \( B \) are fitting parameters which should be experimentally determined.

### 3.3. Application

As described already, the calculation is conducted in the area of 1 mm (x-direction) × 5 mm (y-direction). The initial temperature at one vertical end, i.e. \( T_0 \) in Eq. (6), is determined as 5000 K to obtain a fusion zone area similar to actual welds as shown in Fig. 1. This temperature is also close to the temperature under welding arc. This initial heat input extends the area of melt until the solidification starts.

Iron–17 mass%chromium–titanium ternary alloys are considered in the calculation. The reason of the alloy system employed is to examine the effect of soluble titanium apart from the effect of TiN precipitation. In other words, in this calculation, the number of TiN particles is given apriori, independent of titanium concentration, so that the effects of
TiN and soluble titanium can be discussed in a separate manner. The melting point of an alloy is given as a function of chromium and titanium mass concentration by the following regression form:

\[ T_m (K) = 1818 - 3.798w_{Cr} + 0.1181w_{Cr}^2 - 18.84w_{Ti} \]  

(12)

Equilibrium partitioning coefficient at the liquid/solid interface is also given by the following regression forms:

\[ k_{Cr} = 0.8857 + 6.552 \times 10^{-3}w_{Cr} + 2.573 \times 10^{-5}w_{Cr}^2 + 3.038 \times 10^{-2}w_{Ti} \]  

(13)

\[ k_{Ti} = 0.2724 + 6.841 \times 10^{-3}w_{Cr} - 8.546 \times 10^{-5}w_{Cr}^2 + 2.462 \times 10^{-2}w_{Ti} \]  

(14)

Both the melting point and partitioning coefficients are determined by calculations using Thermo Calc [8] with database SSOL.

In practice of the calculation, FD cells have a rectangular shape of $2 \times 10^{-3}$ m in x-direction $\times \sqrt[3]{10^{-3}}$ m in y-direction, and MC cells have a triangular shape with $5 \times 10^{-6}$ m edge length. Physical properties used in the calculation are listed in Table 1. Critical undercooling necessary for the heterogeneous nucleation on TiN, i.e. $\Delta T_N$ in Eq. (7), is determined as 1.8 K based on the measurement of undercooling by Bramfill [6]. In terms of grain growth, fitting parameters $A$ and $B$ in Eq. (11) are determined to be 500 and $-10.5$, respectively, by trial and error in comparison with grain sizes in heat-affected zone in actual welds.

In the coupling of FD calculation and MC calculation, time step for the two different calculations is a major issue, since MC time generally has no correspondence with the real time. In the present work, FD calculation is conducted using explicit formulation, and a time step, $\Delta t$, is determined to be $1.25 \times 10^{-5}$ s so as to satisfy the stable criterion of explicit method. This time step is directly applied to MC time step. The assumption is applicable in solidification, because increase in the fraction solid is not only determined by the frequency of MC calculations but also by heat conduction. If the increase of solid is too large by MC calculation within one time step, then it will be restricted in next time steps until the latent heat of crystallization diffuses out of the FD cell, and if it is too small, then the driving force of solidification is thermally increased in next steps. Therefore, the frequency of MC calculations within one FD time step is not a strong function for the growth of solid during the solidification. Although the issue may be significant for the grain growth in solid state because the restriction by heat conduction is not expected, our primary interest in the present work is grain formation and growth during the solidification and in this context the present simulation should be sound.

### 4. Results

Fig. 7 shows different stages of grain development during weld solidification, calculated for the alloy of Fe–17 mass%Cr–0.4 mass%Ti with the number density of TiN of 1000/mm$^2$. Melting is from the left side of the figures, and in Fig. 7(a), the melting stops and solidification is just about to start toward the left side of the figure. Note that grains in heat-affected zone near the fusion boundary are already coarsened, from which epitaxial growth of columnar grains is about to start out. The columnar growth continues in Fig. 7(b) and (c), and the transition from columnar to equiaxed solidification is seen in Fig. 7(d). This transition is caused by changes in temperature gradient as the solidification proceeds, along with high density of TiN in the melt. The final microstructure in Fig. 7(e) consists of columnar grains at the initial stages of solidification and equiaxed grains around the center of the weld, i.e. at the latter stages of solidification. Typical examples of comparison of calculated

### Table 1  
Physical properties used in the present simulation

| Symbol | Value used | Reference |
|--------|------------|-----------|
| $D_{L}$ (Cr) | Diffusivity of Cr in liquid (m$^2$/s) | $2.67 \times 10^{-7}$ exp($-6.69 \times 10^{4}/RT$) | [15] |
| $D_{L}$ (Ti) | Diffusivity of Ti in liquid (m$^2$/s) | $1.81 \times 10^{-7}$ exp($-4.77 \times 10^{4}/RT$) | [15] |
| $D_{S}$ (Cr) | Diffusivity of Cr in ferrite (m$^2$/s) | $2.3 \times 10^{-6}$ exp($-2.39 \times 10^{4}/RT$) | [16] |
| $D_{S}$ (Ti) | Diffusivity of Ti in ferrite (m$^2$/s) | $6.8 \times 10^{-5}$ exp($-6.21 \times 10^{4}/RT$) | [16] |
| $C_{PL}$ | Specific heat of liquid (J/kg/K) | 821.6 | –$^{a}$ |
| $C_{PS}$ | Specific heat of solid (J/kg/K) | 821.6 | –$^{a}$ |
| $\lambda_{L}$ | Thermal conductivity of liquid (W/m/K) | 35 | [17] |
| $\lambda_{S}$ | Thermal conductivity of solid (W/m/K) | 30 | [17] |
| $\rho_{L}$ | Density of liquid (kg/m$^3$) | $7.25 \times 10^{3}$ | [16] |
| $\rho_{S}$ | Density of solid (kg/m$^3$) | $7.25 \times 10^{3}$ | –$^{a}$ |
| $\sigma_{SL}$ | Interfacial energy between liquid and solid (J/m$^2$) | 0.212 | [18] |
| $\sigma_{SS}$ | Interfacial energy between solid grains (J/m$^2$) | 0.468 | [18] |
| $\Delta H_f$ | Latent heat of fusion (J/kg) | $1.854 \times 10^{5}$ | –$^{a}$ |

$^{a}$ Calculated by using Thermo Calc [8].
microstructure with actual weld microstructure are exhibited in Fig. 8. The simulation produces fully columnar structure in titanium free weld and mixture of columnar and equiaxed grains in titanium bearing weld, which are consistent with actual weld microstructures. Grain size of columnar and equiaxed grains and fraction of equiaxed solidification are also in a reasonably good agreement between the simulation and experiments, and thereby, the effects of different factors are hereafter examined based on simulation results.

Fig. 9 shows the effect of the number density of TiN in Fe–17 mass%Cr–0.4 mass%Ti. Without TiN, no equiaxed grain is formed as in Fig. 9(a), and the equiaxed grain formation is increased with increase in the number density of TiN as seen in Fig. 9(b)–(d). Equiaxed grains become finer as the number density of TiN increases, which implies that the chance of nucleation of equiaxed grains increases. It is noted that we find that not all the TiN particles can work as a nucleation site or can survive as an equiaxed grain in the simulation. As shown in Fig. 10, the number density of equiaxed grains is low as compared with the number density of TiN, and in addition, it is not linearly increased with the number density of TiN. At the beginning of solidification, temperature gradient in the melt is relatively steep and columnar growth is favored under the thermal condition. In that case, TiN is likely to be entrapped by columnar grain growth before working as a nucleation agent, and even if it succeeds in working as a nucleation agent, the equiaxed grain is to be entrapped by columnar grains and to disappear by Ostwald-like ripening of the columnar grains. It is when the temperature gradient decreases to a certain level that TiN works as a nucleation agent and a solid grain nucleated.
Fig. 8. Comparison between actual weld grain structure and calculated grain structure.

Fig. 9. Calculation results showing the effect of the number density of TiN on the grain structure of welds containing 17 mass% Cr and 0.4 mass% Ti.
on TiN can have a margin for growth and survival against the growth of columnar grains. The transition from CET is encouraged with increasing the number density of TiN, as typically seen when the number density of TiN increases from 100 to 500/mm². It is obvious that the number density of TiN and thermal condition of the solidification are closely associated each other on equiaxed grain formation.

Fig. 11 shows the effect of titanium content that controls solutal undercooling ahead of the liquid/solid interface, assuming the fixed number density of TiN as 500/mm². Even though there is sufficient number of TiN in the melt, equiaxed grain formation is limited when titanium content is 0.1 mass%, and it is increased with increasing titanium content. This implies that the solutal undercooling due to titanium partitioning at the liquid/solid interface exerts a major influence to the nucleation and survival of equiaxed grains in the melt. This is also clear in Fig. 10; the number density of equiaxed grains is significantly increased with increase in titanium content from 0.1 to 0.4 mass%. In a number of previous experimental studies, primary attention has been paid to the beneficial effect of TiN and it is believed that the addition of titanium to steel composition is important because it produces TiN in the melt. Little attention has been paid to the effect of soluble titanium in the melt, but this simulation points out that the enhancement of solutal undercooling due to titanium addition is also essential to the equiaxed grain formation. This would not have been recognized without this kind of simulation.

5. Discussions

The simulation results illustrate the effect of TiN as a nucleating agent and the effect of soluble titanium in a separate manner, and it is found that both of them are indispensable to achieve CET in welds. According to the model proposed by Hunt [12], the criterion for CET to occur is given by

$$G < 0.617(N_0)^{1/3} \left(1 - \frac{(\Delta T_N)^3}{(\Delta T)^3}\right) \Delta T$$

(15)

Fig. 11. Calculation results showing the effect of titanium content on the grain structure of welds with the number density of TiN of 1000 mm².
where \( N_0 \) is the number of equiaxed grain formed, \( \Delta T_N \) the undercooling necessary for the nucleation of the grain formation and \( \Delta T \) the melt undercooling. In comparison with the present case, increase in the number density of TiN should lead to the increase of \( N_0 \) and increase in soluble titanium to the increase of \( \Delta T \). Thus the calculation results are consistent with the model. More recently, Gaumann and Kurz [1] derived an expression for the criterion of CET similar to the Hunt model by a simple dimensional analysis. The analysis is physically straightforward, assuming that interspacing between newly nucleated grains should be smaller than the length of undercooled region for the continuous grain formation, as schematically shown in Fig. 12. The interspacing between nucleated grains is expressed as \( N_0^{-1/3} \), and the length of undercooled region as \( (\Delta T - \Delta T_N)/G \). Therefore, the criterion becomes:

\[
G < a(N_0)^{1/3} \Delta T \left(1 - \frac{\Delta T_N}{\Delta T}\right)
\]

(16)

With regard to the maximum \( G \) that allows the CET to occur, it should be proportional to both \( N_0^{1/3} \) and \( \Delta T \) assuming that \( \Delta T_N \) is constant. The simulation results are examined in this respect in order to evaluate the effect of TiN and soluble titanium in some quantitative manner.

Fig. 13 shows a change in temperature gradient \( (G) \) at the solidification front during fully columnar solidification calculated by the present simulation. Solidification starts approximately 1.6 mm away from the weld centerline (CL), which is also seen in Fig. 7(a), and progresses until it reaches the centerline. At the beginning, the temperature gradient is steep, close to the order of \( 10^6 \) K/m, and gradually decreases down to \( 10^3 - 10^4 \) K/m as the solidification comes to the end. The fluctuation of the calculated temperature gradient in the latter stages of solidification
results from not only multiple grain effect but also the fact that temperature gradient becomes more sensitive to the latent heat of crystallization as it decreases. On the basis of this trend, the maximum temperature gradient \( G_{\text{max}} \) that allows the CET can be evaluated for different calculation conditions. Fig. 14 plots \( G_{\text{max}} \) against the square root of the number density of TiN, which represents the average spacing of nucleation site in the two-dimensional simulation. Also Fig. 15 plots \( G_{\text{max}} \) against \( \Delta T \) owing to titanium. Normally, \( \Delta T \) is thought as the sum of contributions by all the solute elements contained, and is given by [13]

\[
\Delta T = \sum_i m_{L_i} C_0 i \left\{ 1 - \frac{1}{1 - (1 - k_i) I_i(P_c)} \right\}
\]

(17)

where \( i = \text{Cr and Ti} \) in the present case, \( m_{L_i} \) is the liquidus slope with respect to element \( i \), \( C_0 \) the initial concentration, \( k \) the equilibrium partitioning coefficient, \( I_i(P_c) \) the Ivantsov function [14] as a function of Peclet number, \( P_c \). However, since chromium content is kept constant as 17 mass\%, \( \Delta T \) owing to chromium is included as a constant as well as \( \Delta T_N \) when the relationship between \( G_{\text{max}} \) and \( (\Delta T \sim \Delta T_N) \) is examined, and then, linearity between \( G_{\text{max}} \) and \( \Delta T \) owing to titanium will be an issue of interest. \( \Delta T \) owing to titanium is calculated with \( m_{L} \) of \(-19 \text{ K/mass\%} \) and \( k \) of 0.36 and by assuming \( I_i(P_c) \) to be constant as 0.3.

Figs. 14 and 15 suggest that \( G_{\text{max}} \) is proportional to the spacing of nucleation sites and solutal undersooling owing to titanium. Fig. 16 plots \( G_{\text{max}} \) against the product of these two factors, which also suggests a linear relationship as a natural consequence of Figs. 14 and 15. These results imply that the present simulation verifies the CET criterion given originally by Hunt [12] and subsequently by Gaumann and Kurz [1], and at the same time, successfully confirms the roles of nucleating agent and melt undercooling on equiaxed grain formation in a quantitative manner.

Finally, although the potency of TiN has been kept constant so far based on Bramfitt’s result [6], its effect is examined. The results are shown in Fig. 17. \( \Delta T_N \) is changed from 1.3 to 2.3 K while the number density of TiN and
titanium content are fixed. As expected naturally, equiaxed grain formation is encouraged with decreasing $\Delta T_N$. This means that the potency of an inclusion as a nucleating agent is also a very important factor, and if we could find some other nucleating agents stronger than TiN, the equiaxed grain formation would be achieved with more ease.

6. Summary

Numerical simulation is developed on grain structure development during weld solidification of steel. MC method is applied to the simulation of nucleation and growth of solid, being combined with FD calculation of heat conduction and solute diffusion. Based on the experimental result that TiN works as a nucleating agent of equiaxed grain formation, given number density of TiN is allocated to MC cells randomly and instantaneous nucleation is assumed to occur when the melt undercooling of the cell exceeds a given critical level. It is found that the simulation can reproduce the weld solidification by reflecting the effect of TiN as a nucleating agent and the effect of soluble titanium that increases melt undercooling. Those effects have been recognized only as combined effects in previous experimental studies, but through the present simulation, they are first investigated in a separate manner. The simulation results indicate that equiaxed grain formation is promoted not only by a nucleating agent, TiN, but also by melt undercooling increased by soluble titanium and that both are requisite to bring about the CET. The results are discussed in connection with theoretical models on CET and confirm the rationality of the models.

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