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A Study on Cooling Rate Modelling of Dentrite between the Temperature and Composition

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Abstract

According to composition at solid and liquid interface in solidification the line model of temperature and composition in dentrite has been established. The equation is gained as T=-1000C+2273。Meantime the cooling rate and time has been discussed. In the intersection the cooling rate of solid and liquid ΔT is gained. According to dentrite therefore the composition can determine temperature. Y changes from pure X to pure Y ie. 0 to 100%Y the temperature will change from maximum to minimum at Al composition in materials like TiAl. The period one of cooling rate is from 0.5K/s to 11 K/s in speed of 360mm/hr. The gap is bigger between 720mm/h with drawing speed v than that of 360mm/h. For engineering use the speed is better when the speed is higher like 720mm/h when the cooling rate attains from 2K/s to 22K/s with the composition difference increasing with maximum value. When cooling rate is 1160mm/hr the biggest one in these three conditions will happen with 35K/s. When DS is 2J/ (mol•K) the DG changes from1500J to -500J with the temperature increases same in TiAl. It means that when DS becomes big the DG will decrease. From diagram the concentration of Al is measured to be 1.6at% in 46Al at%. The calculation value is thought to be phase forming element due to the minus. That has been the low concentration with and solid solution in TiAl.

Keywords: Modelling; Dentrite; Analysis; Temperature; Cooling rate; Composition; Interface; Gibbs free energy

Introduction

The change of temperature in the solid and liquid in solidification transformation can deduce the their related formula. The curve expresses its trend better. From this relation their composition will change when the transformation happens. It is known that the temperature in solidification can solve their relationship. In this study in terms of these equations the deduction and analysis is done and the error analysis to them is done. Here the solid and liquid equation is explored within line and find the simple formula which make us to calculate the cooling rate rapidly [1,2]. Therefore in this study the model of temperature and composition has been established to observe the trend and intrinsic relationship between them. Then the error is checked with variance to both of constant. On the other side the relationship with cooling rate and energy difference & temperature has been investigated according to varied speed and ΔS respectively for the application. According to the solidified crystalline and phase diagram the application will be known. In addition relationship between cooling rate and energy difference & temperature are drawn for further research in this study. To calculate the cooling rate is our destination in the end in terms of the composition in TiAl alloys. Therefore the establishment equation between temperature and cooing rate in terms of the equilibrium diagram.

Calculation

The relationship between composition and temperature (Figure 1)

Figure 1 shows that the two lines with liquid and solid phase meet in one point. The cooling rate ΔT is known. It shows two phases decrease below the liquidus phase line. It shows these two line relations in constitutional super cool. We choose the certain value to proceed experiment.Here C is the Al composition, Cl and Cs is the liquid and solid composition of Al.

Let T=aC+b (1)

We have

$T_l=aC_l+b$ (2)

$T_s=aC_s+b$ (3)

According to Ti-Al state equilibrium state we have supposed

$C_l=0.44$, $T_l=1833K$ and

$C_s= 0.46$, $T_s=1813K$

Substitute above constant to (2) and (3), so

a=-1000, b=2273. The formula (1) is

T=-1000C+2273 (4)

This is the equation to calculate temperature in terms of composition (Figure 2).

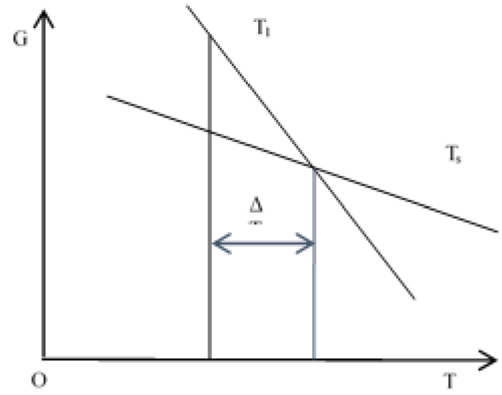


Figure 1: *The relations of dentrite and equilibrium state.*

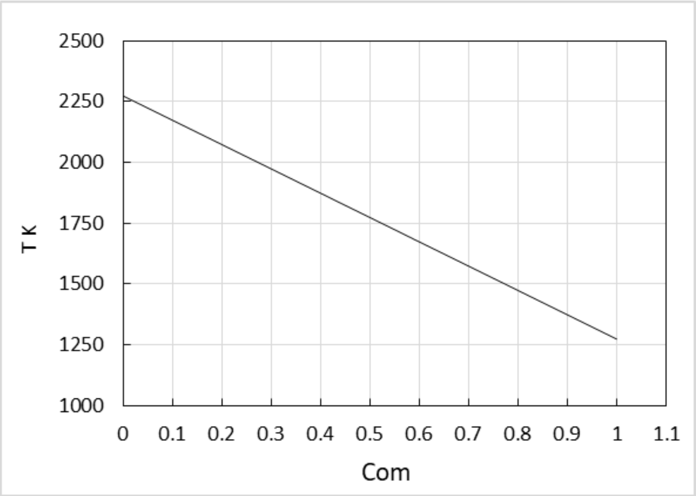
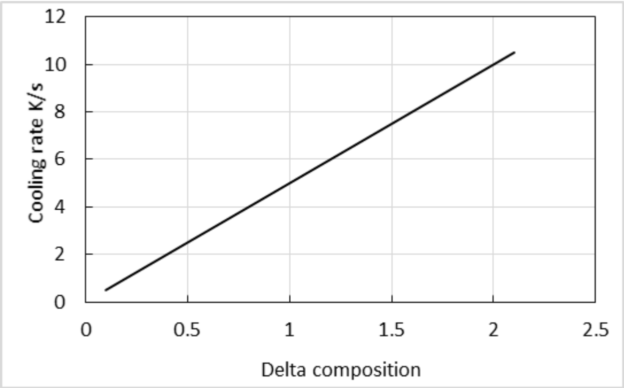
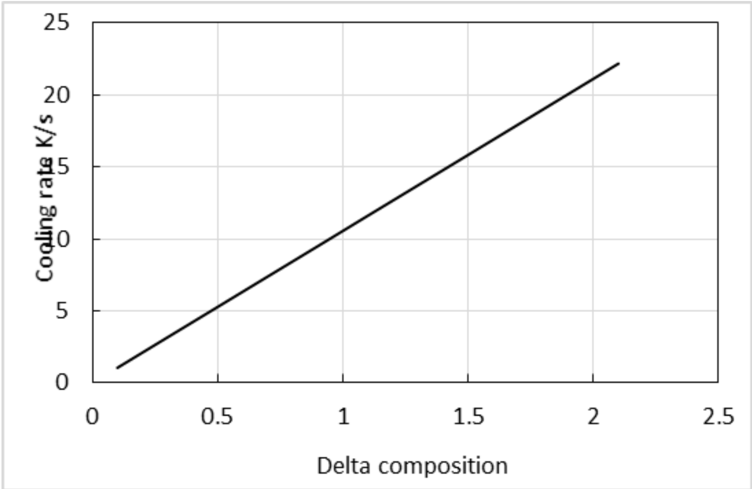


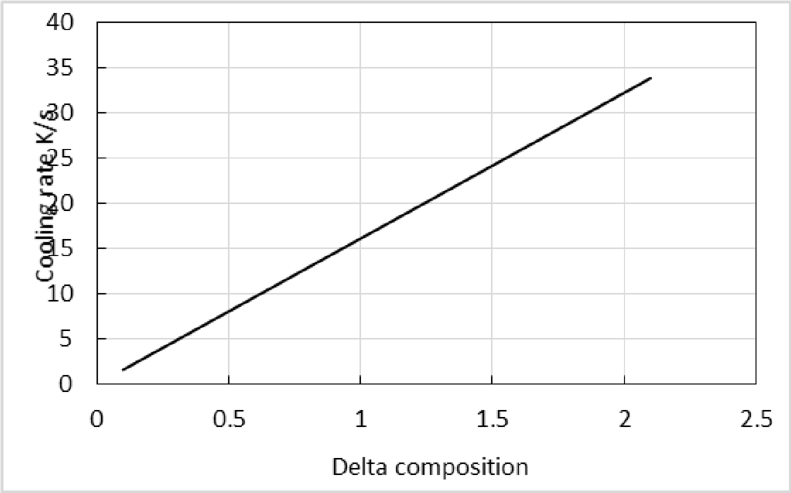
Figure 2: *The relationship between temperature ad compositions in dentrite.*



(a) 360mm/hr.

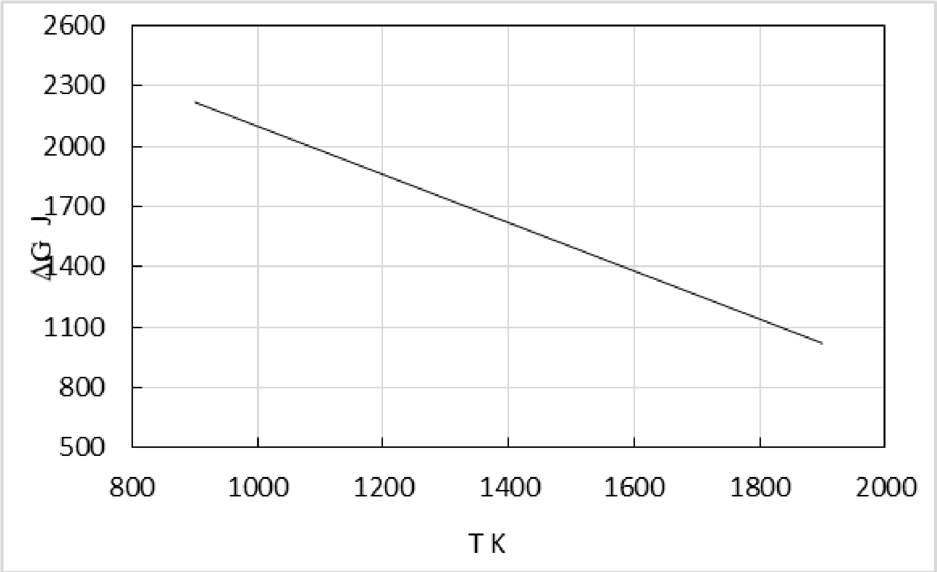


(b) 760mm/hr.

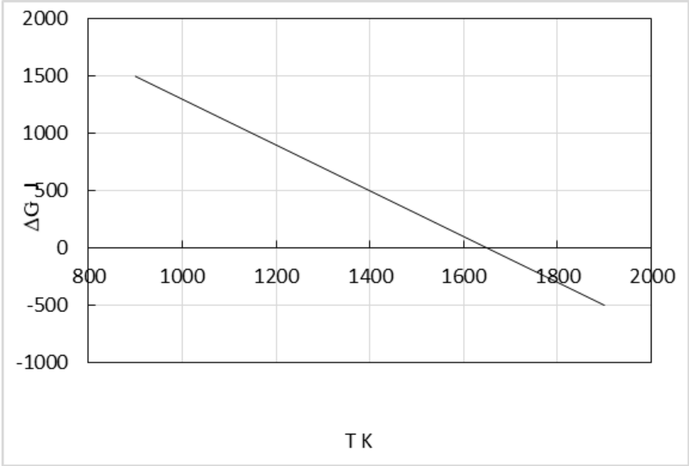


(c) 1160mm/hr.

Figure 3: *The relation between cooling rate and Δ composition under different speed in directional solidification.*



(a) DS=1.2J/(mol•K)



(b) DS=2J/ (mol•K).

Figure 4: *The relations between DG and temperature in solidified state.*

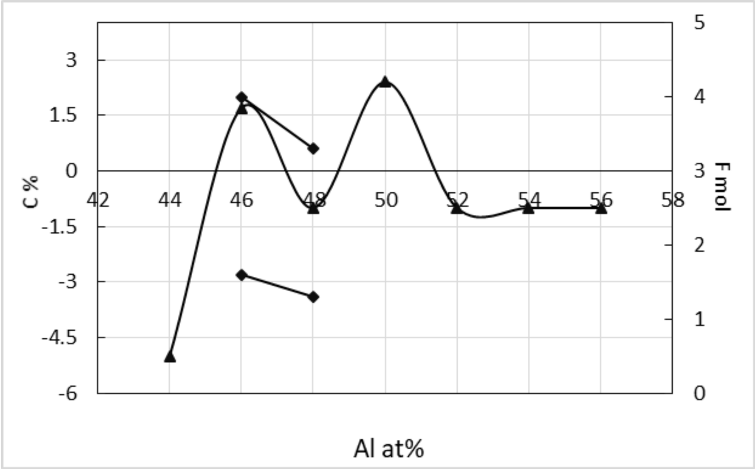


Figure 5: *Trend F_{mol} and C_{Al} with Al content in γ TiAl，β and α is formed and L is remained.*

From Figure 2 we know the distribution of temperature and composition in directional solidification. When composition difference increases temperature decreased somewhat in term of content in dentrite. When composition difference is from 0 to 1 the temperature changes from 230K to 1300K respectively. It means Y changes from pure X to pure Y ie. 0 to 100%Y the temperature will change from maximum to minimum at Al composition in materials like TiAl.

Calculation of cooling rate (Figure 3)

As Figure 3 when composition deference increases cooling rates rate increases properly at 20mm solidified length. Drawing speed increases so that cooling rate increases a certain. The period one of cooling rate is from 0.5K/s to 11 K/s in speed of 360mm/hr. The gap is bigger between 720mm/h with drawing speed v than that of 360mm/h. For engineering use the speed is better when the speed is higher like 720mm/h. When the cooling rate attains from 2K/s to 22K/s with the composition difference increasing with maximum value. When cooling rate is 1160mm/hr the biggest one in these three conditions will happen with 35K/s. This is the result of concentration of liquid and solid in terms of composition.

DT=T1-T2=-1000(C1-C2) =-150K (5)

t=L/v=20*3600/360=200s

So C= (T1-T2)/t (6)

Here C and DT is cooling rate and temperature difference respectively (Figure 4).

From Figure 4 DG decreases with temperature increasing. It decreases with enthalpy DS increasing from 1, 2 to 2J/mol/K. It's decreasing means cooling rate increases along the dendrite. When speed increases it decreases like 1160mm/h. Here DS is entropy. This is the result of concentration of liquid and solid in terms of composition. When DS is 1.2J/ (mol•K) the DG changes from 2200J to 1000J with the temperature increases from 850K to 1900K respectively. When DS is 2J/ (mol•K) the DG changes from1500J to -500J with the temperature increases same. It means that in TiAl when DS becomes big the DG will decrease. G is Gibbs free energy [3].

DG=DH-TDS (7)

In Ti-Al DH and DS are to be

DH=3.3KJ/mol，DS=1.2 J/mol/K at 1492℃ [4] (Figure 5).

The concentration of Al under the reaction will be known in Figure 5. The interface stability is highly expected because of the constitutional super cooling. Well-developed dendrites are found at relatively high solidification rate with 25~100μm/s. From diagram the concentration of Al is measured to be 1.6at% in 46Al at%. The calculation value is thought to be phase forming element due to the minus. That has been the low concentration with and solid solution in TiAl. Maybe good result will be obtained use the inferior solution model. They agreed with each other well. So they are approximate value calculated with the method.

Conclusion

- According to composition at solid and liquid interface in solidification the line model of temperature and composition in dentrite has been established. The equation is gained as T=-1000C+2273。Meantime the cooling rate and time has been discussed. In the intersection the cooling rate of solid and liquid ΔT is gained. Composition difference has been deduced and analysed according to dentrite therefore the composition can determine temperature. When composition difference is from 0.4 to 0.6 the temperature changes from 1880K to 1680K. Y changes from pure X to pure Y ie. 0 to 100%Y the temperature will change from maximum to minimum at Al composition in materials like TiAl.
- The period one of cooling rate is from 0.5K/s to 11 K/s in speed of 360mm/hr. The gap is bigger between 720mm/h with drawing speed v than that of 360mm/h. For engineering use the speed is better when the speed is higher like 720mm/h when the cooling rate attains from 2K/s to 22K/s with the composition difference increasing with maximum value. When cooling rate is 1160mm/hr the biggest one in these three conditions will happen with 35K/s.
- When DS is 2J/ (mol•K) the DG changes from1500J to -500J with the temperature increases same. It means that in TiAl alloys when DS becomes big the DG will decrease. From diagram the concentration of Al is measured to be 1.6at% in 46Al at%. The calculation value is thought to be phase forming element due to the minus. That has been the low concentration with and solid solution in TiAl.

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