Zhi-Hao Yao*, Ya-Ting Ruan, Jian-Xin Dong, Qiu-Ying Yu, Shi-Qing Zhang and Xi Chen

# Study on Gamma Prime and Carbides of Alloy A286 by Traditional Thermodynamic Calculation

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**Abstract:** Equilibrium phases in alloy A286 and the influence of element contents on gamma prime (γ′) and carbides were studied by Thermo-Calc calculation. The phase equilibria, solidification behavior, and precipitation behavior of equilibrium phases were investigated. In the results, Al is considered as the critical element for γ′ phase control, and C is the vital element for the regulation of MC and $M_{23}C_6$ phases. The influence extents of different elements on the transition temperature and the maximum content of γ′ phase, MC phases, and $M_{23}C_6$ phases are determined in order as Al>Ti>Cr>Mo, C>Ti>Ni>Cr>Mo, and C>Ni>Cr>Mo, respectively.

**Keywords:** iron-based superalloy A286, precipitates, thermodynamic calculation, change of contents

## Introduction

Due to the good thermal resistance, superior mechanical properties, and simple fabrication, iron-based superalloy A286 (SUH660) is widely used in gas turbine industry at 550 ~ 650 °C as the transition piece material, connecting gas turbine to power turbine inlet [1-4]. Besides, because of the excellent hydrogen embrittlement resistance, alloy A286 also can be used as an equipment material candidate, exposing to high pressure hydrogen, such as in a pressure accumulator. The demand of alloy A286 is incremental with the development of hydrogen economy. The alloy performance is mainly dependent on its composition and microstructure. Sometimes the stability and ultimate performance of the alloy are greatly affected by the tiny variation of chemical composition within a certain standard range [5–9]. As shown in the previous work [10, 11], it was the lattice parameter mismatch could be changed by the composition modification, affecting the formation of second phases. Therefore, the element control is critical to the microstructure and properties of the alloy during a certain process. To control the microstructure and properties precisely, it is necessary to study the influence of different elements on the potential phases and the precipitation behavior in alloy A286.

However, too much attention was paid to the hot working behavior of alloy A286 [12–16]. The mechanisms of deformation and recrystallization have been widely studied, while the related literatures of composition influence on precipitation behavior by calculation are very limited [17], let alone the systematic reports. Therefore, it is necessary to investigate the element influence on the precipitation behavior of alloy A286.

Alloy A286 is mainly strengthened by the precipitation of the ordered fcc gamma prime (γ′) $Ni_3(Al,Ti)$ phase, which is coherent with the matrix. After solution and aging heat treatments, the main phases of alloy A286 include γ, γ′, η($Ni_3Ti$), σ$(FeNi)_x(CrMo)_y$, $M_3B_2$, MC, and G ($Ni_{16}Nb_6Si_7$) phases. However, in many cases, the formations of these precipitation phases are very complicated, it is hard to find out the exact composition. Equilibrium phases are important information sources for materials development. In this paper, the influence of composition on potential phases, such as γ′ phase and carbides, was investigated, and their contents in alloy A286 were studied by using thermodynamic software Thermo-Calc [18]. The results may be helpful for the optimization of composition, thermal processing, and heat treatment, which may be an important significance for guiding the actual production process.

## Calculation method

The commercial CALPHAD software (Thermo Calc) and the corresponding Fe-Ni-based superalloy database were used during thermodynamic calculations, which is the general and flexible software system for calculations of thermodynamic properties, equilibrium and partial-

***Corresponding author: Zhi-Hao Yao,** Department of Materials Science, School of Materials Science and Engineering, University of Science and Technology Beijing, Beijing 100083, China, E-mail: zhihaoyao@ustb.edu.cn
**Ya-Ting Ruan, Jian-Xin Dong, Qiu-Ying Yu,** School of Materials Science and Engineering, University of Science and Technology Beijing, Beijing 100083, China
**Shi-Qing Zhang,** Chongqing Materials Research Institute, Chongqing 400707, China
**Xi Chen,** School of Engineering, Columbia University in the city of New York, New York, 10027, USA

equilibrium quantities, chemical driving forces, various types of stable/meta-stable phase diagrams, and property diagrams of multi-component system for materials [19, 20]. All thermodynamic information, including phase diagrams and thermodynamic databases, can be obtained through the thermodynamic relationship system function, linking the system to calculate the potential equilibrium phase. Various parameters of temperatures and elements were input into Thermo Calc software. The possible phases and their equilibrium composition were calculated mainly by adjusting the contents of elements, such as C, Al, Ti, and Cr. The nominal composition of alloy A286 is shown in Table 1, and the main calculated composition range of alloy A286 is defined as C (0.02 %-0.08 %), Cr (13.5 %-16 %), Mo (1 %-1.5 %), Ni (24 %-27 %), Ti (1.8 %-2.4 %), and Al (0.15 %-0.4 %).

The specimens were prepared by standard metallographical techniques before being etched via waterless Kalling's reagent (100 mL ethanol, 100 mL HCl, and 5 g $CuCl_2$), and then characterized by SEM (scanning electron microscope). The typical microstructure of alloy A286 after heat treatment of 960 °C /1 h /WC (water cooling) + 730 °C /16 h /AC (air cooling) is shown in Figure 1. It can be seen that, $M_{23}C_6$ precipitates are presented at grain boundary, and the fine γ′ precipitates marked as black arrows are dispersed in γ austenitic matrix.

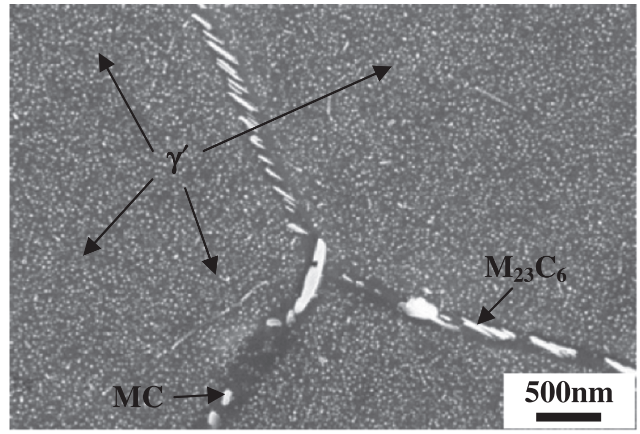

Figure 1: Microstructure of alloy A286 after heat treatment.

## Calculation results

### Thermodynamic equilibrium phases of alloy A286

According to Table 1, the average contents of A286 alloy are C 0.04 %, Si 0.17 %, Mn 0.17 %, Ni 26.2 %, Cr 14.7 %, Mo 1.25 %, Ti 2.1 %, Al 0.2 %, V 0.24 %, Fe of balance 54.0 % (in mass fraction). The relationship among the contents, phases, and temperatures of A286 alloy was obtained by thermodynamic equilibrium calculation, the results is shown in Figure 2. The main equilibrium phases of alloy A286 consist of γ, η, σ, γ′, $M_{23}C_6$, and MC phases. The initial and final melting temperatures are 1294 and 1409 °C, respectively, and the solidification range is calculated to be 115 °C. The initial precipitation temperatures of MC, γ′, and $M_{23}C_6$ are 1313, 630 and 596 °C, respectively. It is generally known that the γ′ phase makes the matrix strengthen, and the MC and $M_{23}C_6$ phases have the significant influence on the properties. To illustrate the influence trend of alloying elements on equilibrium phases in this study, the "positive" influence was defined as that the content/temperature of equilibrium phase increased with the increase of element content, while the "negative" influence showed the opposite. The compositions of each equilibrium phase at 550 °C are shown Table 2. The different influences of elements on equilibrium phases occurred will be discussed in detail below.

### Influence of composition on maximum content and complete solution temperature of γ′ phase

The complete solution temperature is vital to the determination of hot working window of alloy A286. The complete solution temperatures of γ′ phases with the contents of C, Cr, Mo, Ni, Ti, and Al were calculated, the results are shown in Figure 3. The solution temperatures of γ′ phases have the negative correlation with the increase of C and Ni contents, while their negative influences are relatively weak. Oppositely, the positive correlation occurs between

Table 1: Nominal composition of alloy A286 (mass fraction %).

| Fe | C | Si | Mn | Ni | Cr | Mo | Ti | Al | P | S | V |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Bal. | ≤ 0.08 | ≤ 0.35 | ≤ 0.35 | 24~27 | 13.5~16 | 1.0~1.5 | 1.8~2.4 | ≤ 0.4 | ≤ 0.015 | 0.002 | 0.1~0.5 |

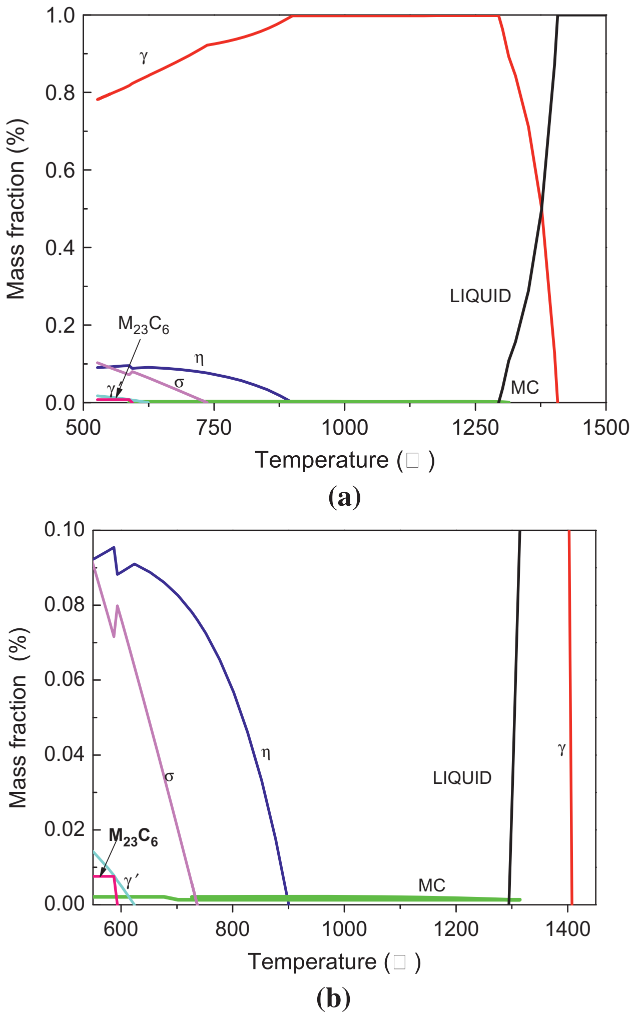


**Figure 2:** Variation of equilibrium phase content with temperature (a) and its partial enlarged detail (b).

the solution temperatures of γ′ phases and the contents of Cr, Mo, Ti, and Al. The effects of Cr, Mo, and Ti are slightly weak, while the variation of Al content has the most significant influence on the solution temperature of γ′ phases from 550 °C to 800 °C.

The influence of chemical composition in standard range on the maximum precipitation contents of γ′ phases is illustrated in Figure 4. The variation of C content has little influence on the maximum precipitation contents of γ′ phases, while the increases of Cr, Ti, and Al contents, in particular, Al content, could promote the formation of γ′ phases. In addition, the increases of Mo and Ni contents could lead to the decrease of the maximum contents of γ′ phases.

Based on the above results, it can be inferred that Al content has the most significant influence on the complete solution temperature and the maximum precipitation content of γ′ phase. However, the contents of C, Cr, Mo, Ni, and Ti have the little influence on complete solution temperature and the maximum contents of γ′ phase.

## Influence of composition on the maximum content and transition temperature of primary carbide MC

The influence of chemical composition on solution temperatures of MC phases was investigated, the solution temperature was calculated from 1300 °C to 1345 °C, the results are shown in Figure 5. The increases of C, Ni, and Al contents can lead to the positive correlation with the increase of solution temperatures of MC phases, while the increase of Cr, Mo, and Ti contents shows the negative correlation with solution temperatures of MC phases.

Figure 6 shows the influence of chemical composition on the maximum content and the corresponding precipitation temperature of MC phases when the maximum content is present. It can be seen that the variation of C content has the most significant influence on precipitation contents of MC phases, while Ti content has the most significant influence on the precipitation temperature where the maximum content occurs.

**Table 2:** Calculated compositions of equilibrium phases at 550 °C.

| Phases | Mass fraction | C | Al | Ti | Mo | Si | Ni | Cr | Fe |
|---|---|---|---|---|---|---|---|---|---|
| η | 9.24 | – | 0.02 | 21.04 | – | – | 76.67 | trace | 2.06 |
| σ | 8.99 | – | – | – | 8.78 | trace | 4.46 | 43.89 | 42.84 |
| γ′ | 1.39 | – | 4.92 | 13.41 | trace | trace | 76.45 | 0.19 | 5.01 |
| MC | 0.21 | 18.10 | – | 81.68 | 0.09 | – | trace | 0.13 | trace |
| $M_{23}C_6$ | 0.76 | 5.15 | – | trace | 19.78 | – | 0.77 | 70.30 | 4.01 |
| γ | 79.61 | trace | 0.10 | 0.01 | 0.48 | 0.21 | 24.22 | 13.08 | 61.89 |

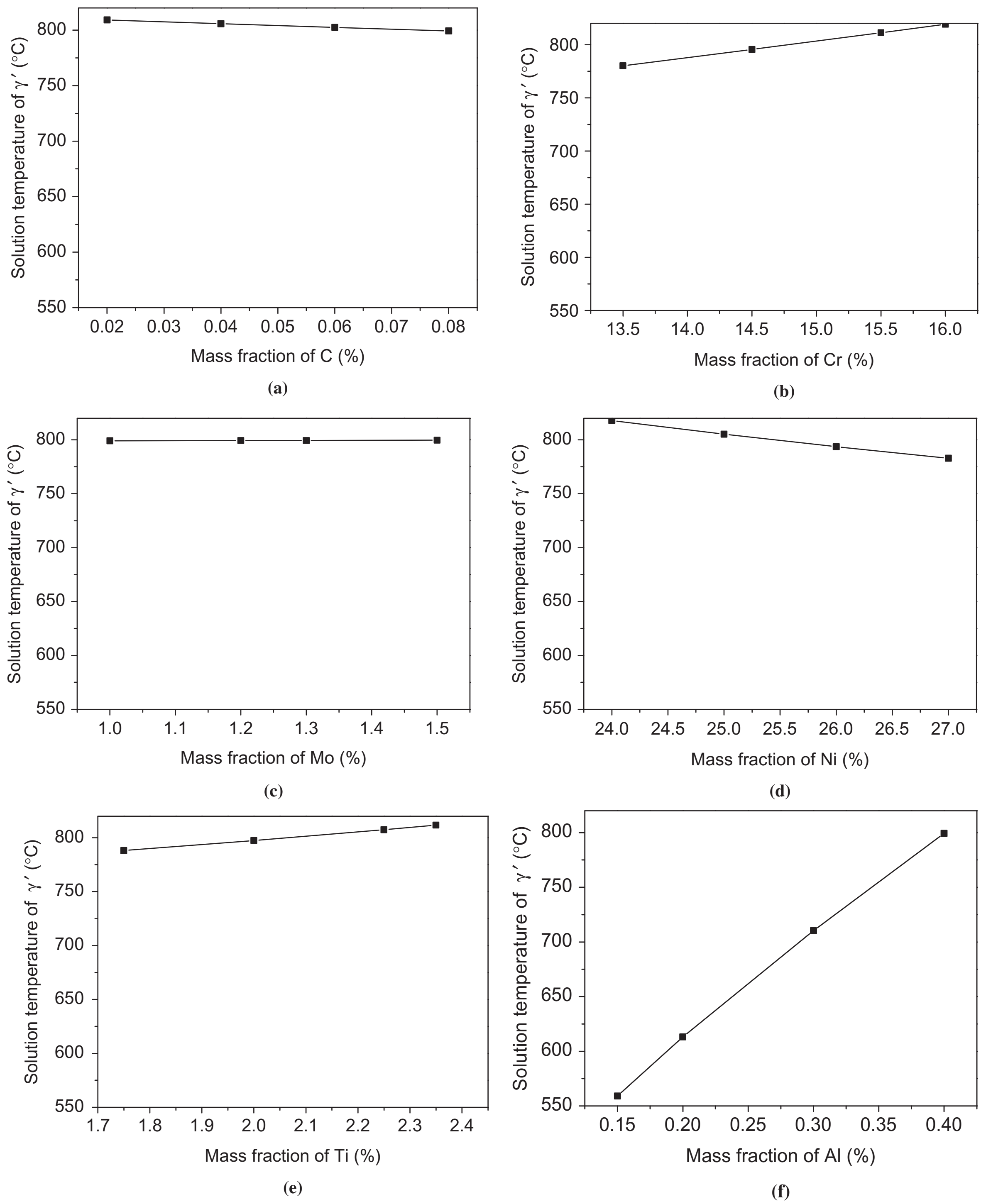


**Figure 3:** Variation of complete solution temperature of γ′ phase with the contents of (a) C; (b) Cr; (c) Mo; (d) Ni; (e) Ti; (f) Al.

In short, the content of C has a significant positive influence on the maximum content of MC phase, While the contents of Mo, Ti, Ni, and Al have the little influence on MC content. Ti content has the most significant influence on the precipitation temperature where the maximum content occurs.

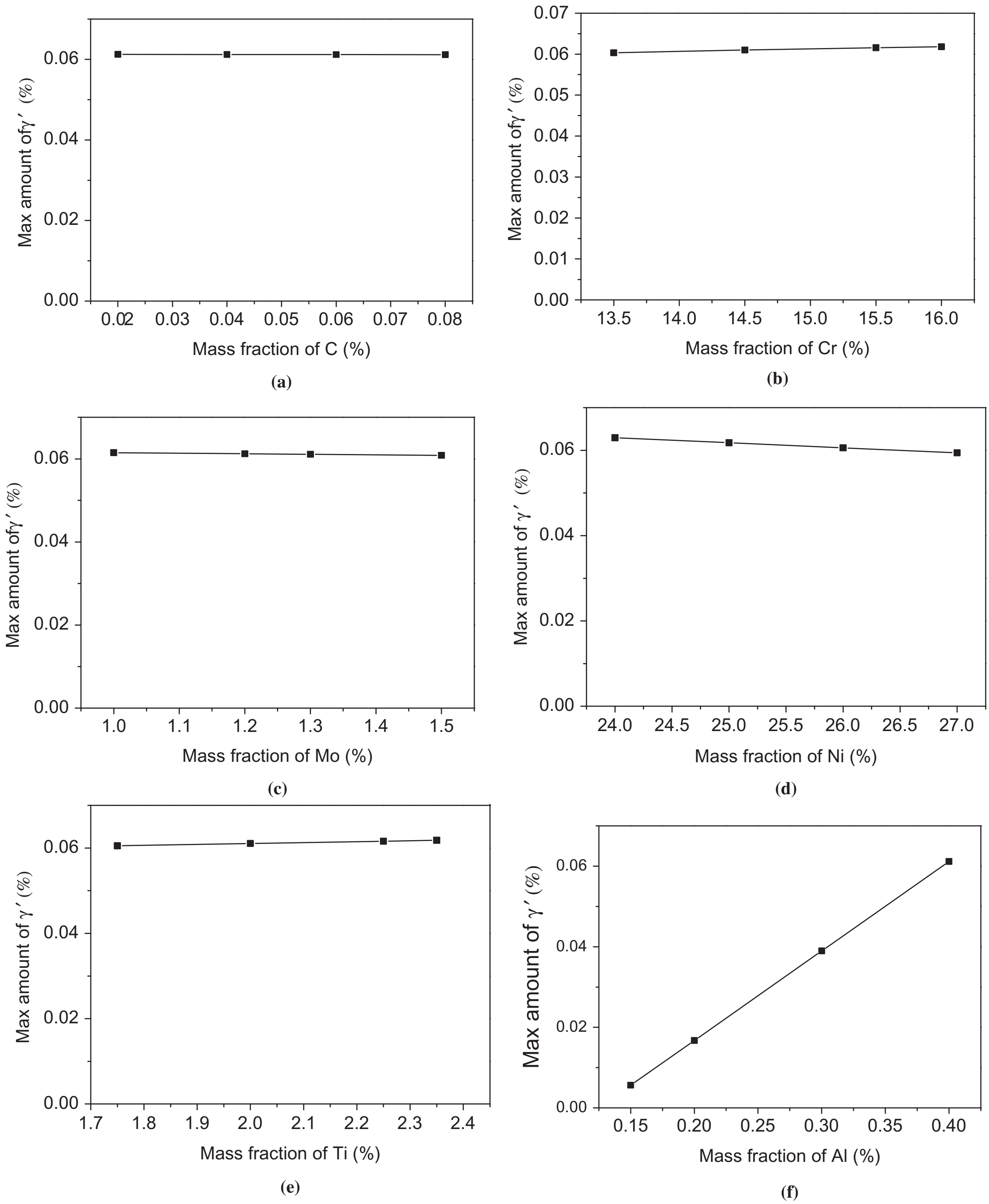


**Figure 4:** The variation of maximum precipitation amounts of γ′ phases with the contents of (a) C; (b) Cr; (c) Mo; (d) Ni; (e) Ti; (f) Al.

## Influence of composition on the maximum contents and precipitation temperature of $M_{23}C_6$ phase

The variation of precipitation temperature of $M_{23}C_6$ phase with the contents of C, Cr, Mo, Ni, Ti, and Al is shown in Figure 7. The variation of C, Cr, Mo, and Ni contents have the positive correlation with precipitation temperature of $M_{23}C_6$ phase. However, the variation of Ti and Al contents has the negative influence on the precipitation temperature of $M_{23}C_6$ phase.

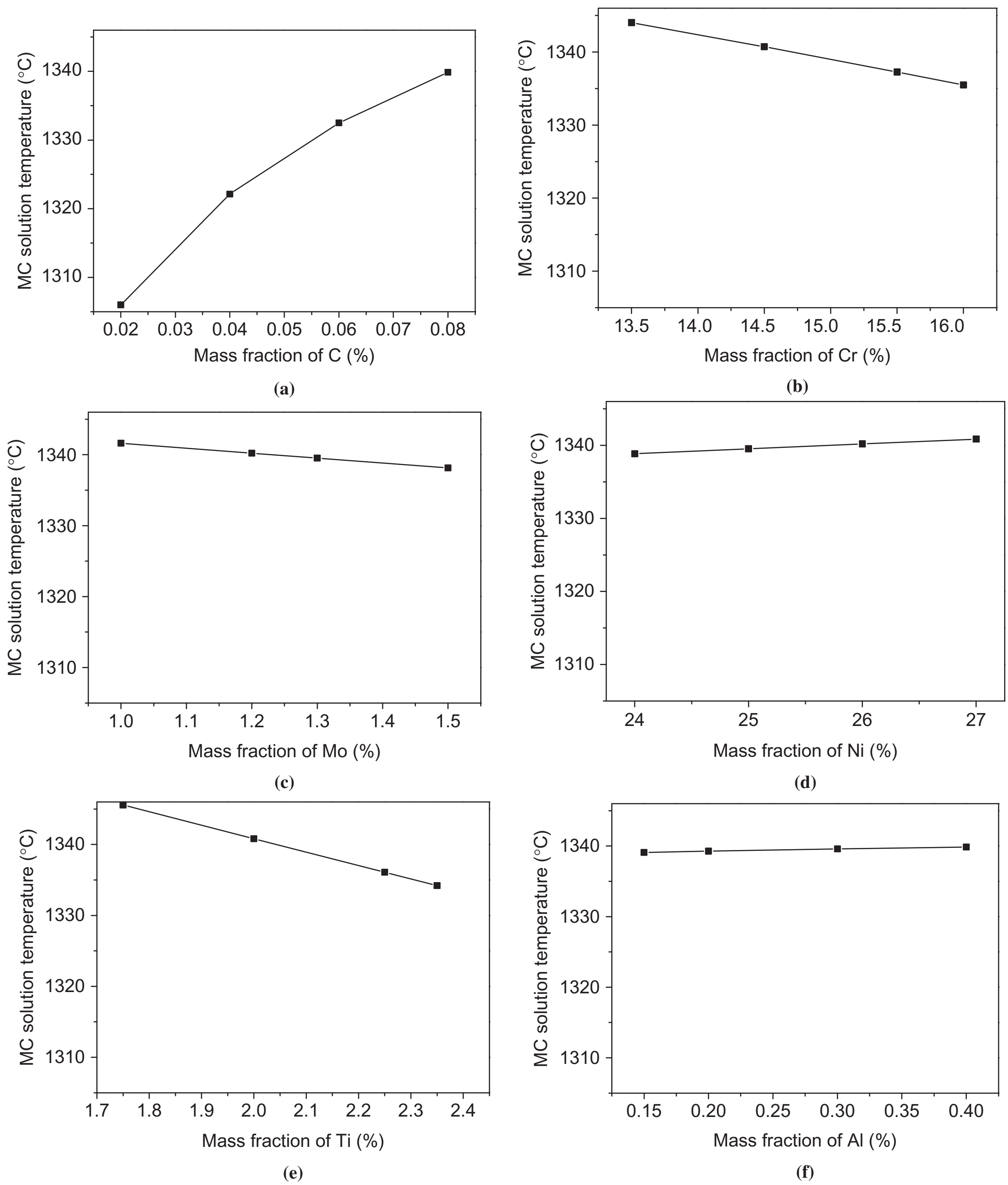


**Figure 5:** Variation of solution temperatures of MC phases with the contents of (a) C; (b) Cr; (c) Mo; (d) Ni; (e) Ti; (f) Al.

The influence of composition on the maximum content of $M_{23}C_6$ phase is illustrated in Figure 8. It can be found that the increase of C content can result in the increase of the maximum content of $M_{23}C_6$ phase, while the increase of Cr, Mo, Ni, Ti and Al contents has little influence on the maximum content of $M_{23}C_6$ phase. Therefore, element C has the most significant influence on the maximum precipitation content of $M_{23}C_6$ phase. When the content of C varies from 0.02 % to 0.08 %, the maximum content of $M_{23}C_6$ phase increases from 0.003 % to 0.015 %.

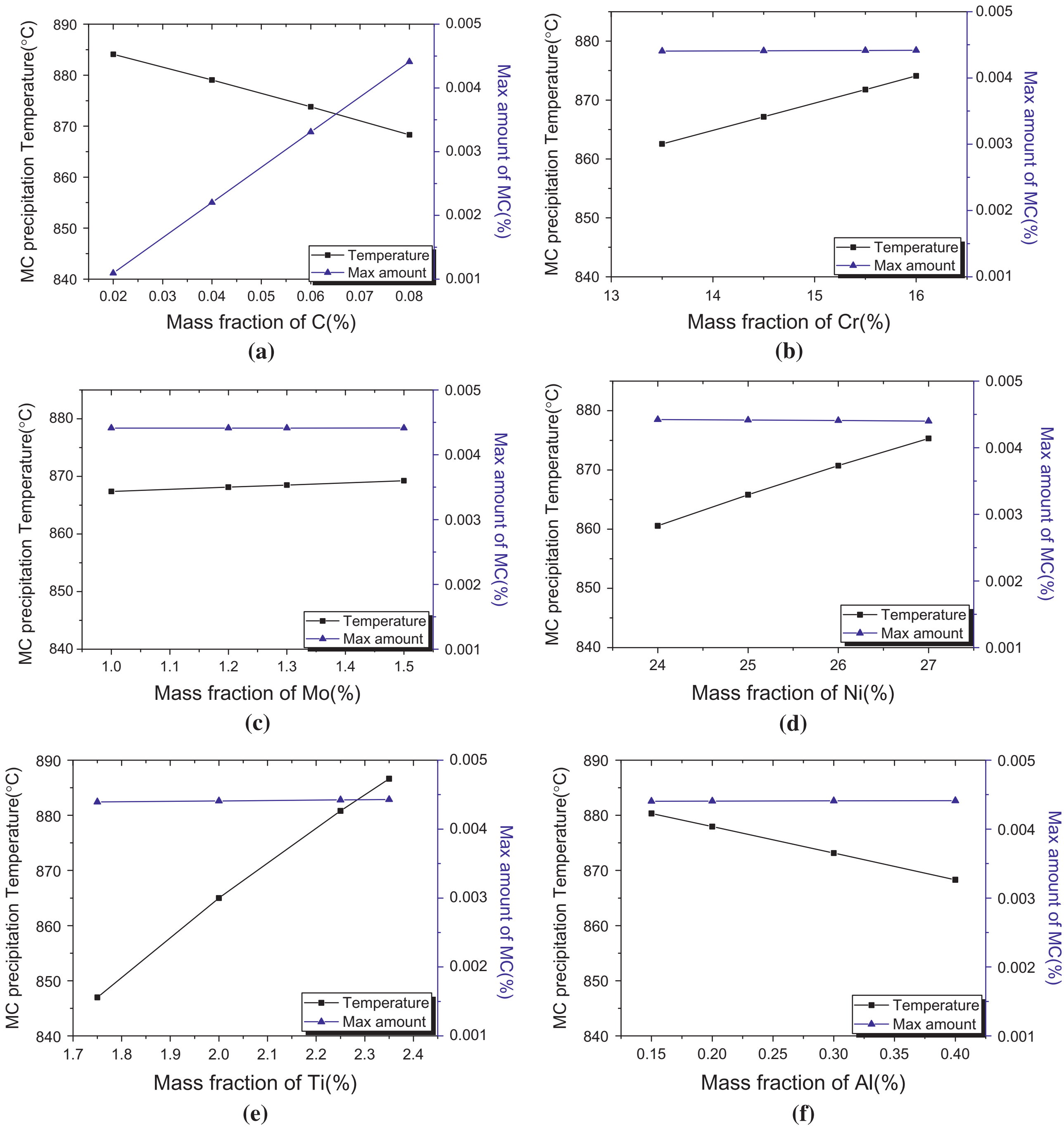


**Figure 6:** Variation of maximum amount and its corresponding precipitation temperature of MC phase with the contents of (a) C; (b) Cr; (c) Mo; (d) Ni; (e) Ti; (f) Al.

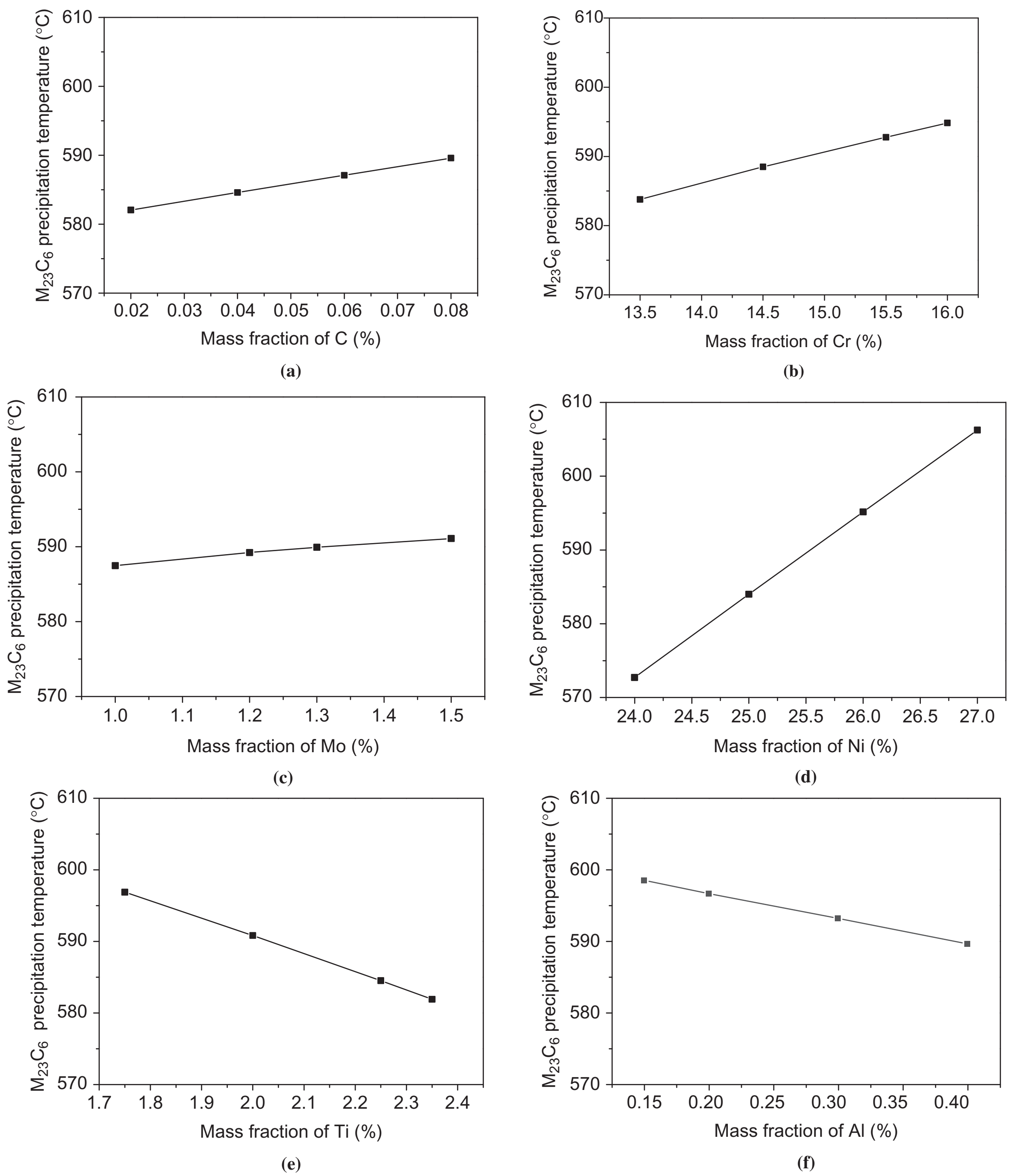


**Figure 7:** Variation of precipitation temperature of $M_{23}C_6$ phase with the contents of (a) C; (b) Cr; (c) Mo; (d) Ni; (e) Ti; (f) Al.

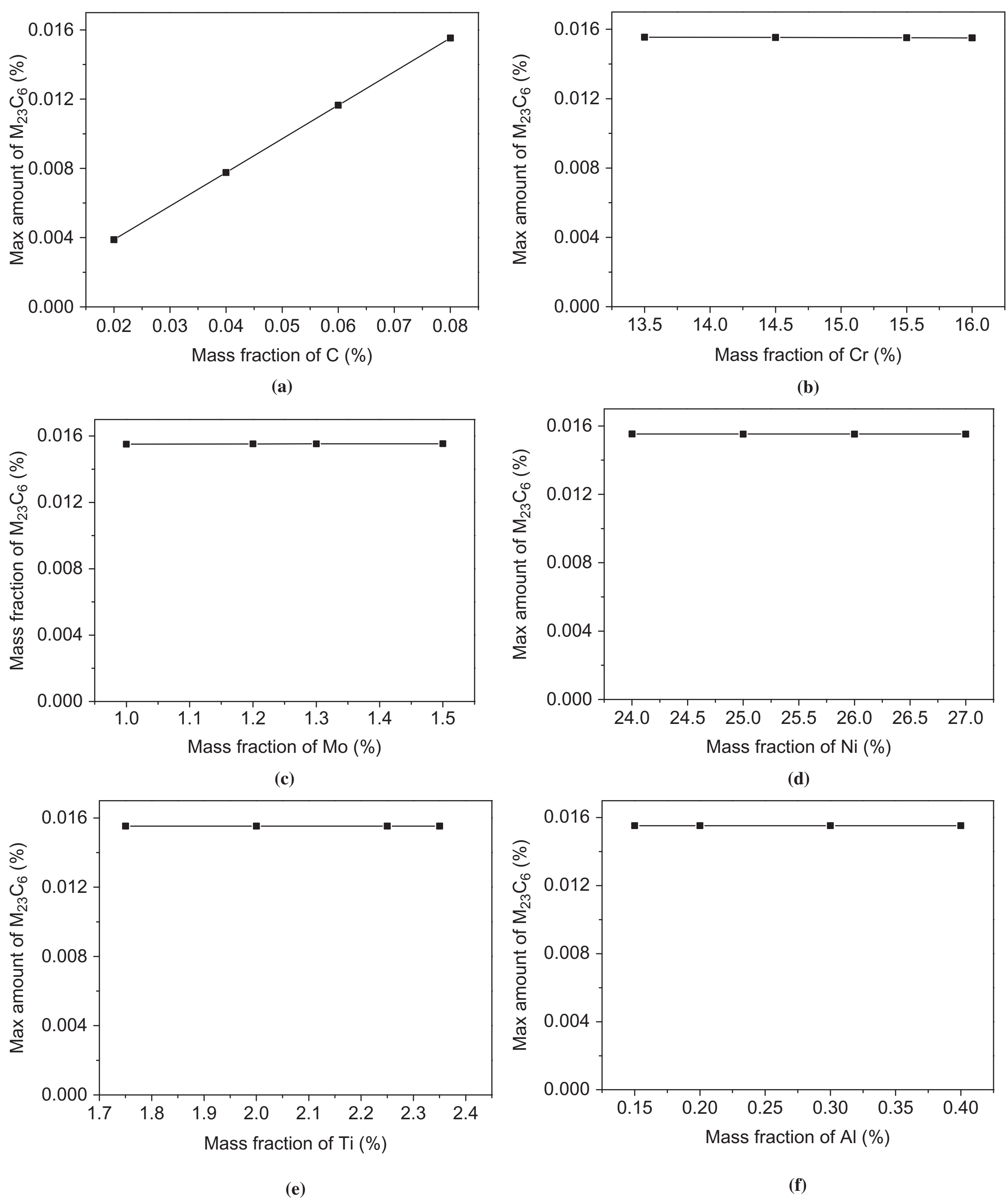


**Figure 8:** Variation of maximum precipitation amount of $M_{23}C_6$ phase with the contents of (a) C; (b) Cr; (c) Mo; (d) Ni; (e) Ti; (f) Al.

## Discussion

### Critical composition factors of solution temperature and precipitation content of γ′ phase

The influence of different elements on the solution temperature of γ′ phase is shown in Figure 9. Al content has a striking influence on solution temperature of γ′ phase, and the solution temperature of γ′ phase increases from 559 °C to 799 °C with the increase of Al content from 0.15 % to 0.4 %. The elements of Ti, Cr, and Mo are also found to have the positive effect on solution temperature of γ′ phase. And the influence extent of different elements in order is defined as Al> Ti >Cr >Mo. However, Ni content has the most obviously negative influence on the solution temperature of γ′ phase. Solution temperature of γ′ phase decreases from 817 °C to 782 °C when Ti content increases from 24 % to 27 %. C element is also the negative factor for solution temperature of γ′ phase. Through the comprehensive analysis, Al content is determined as the critical factor to control the solution temperature of γ′ phase in alloy A286.

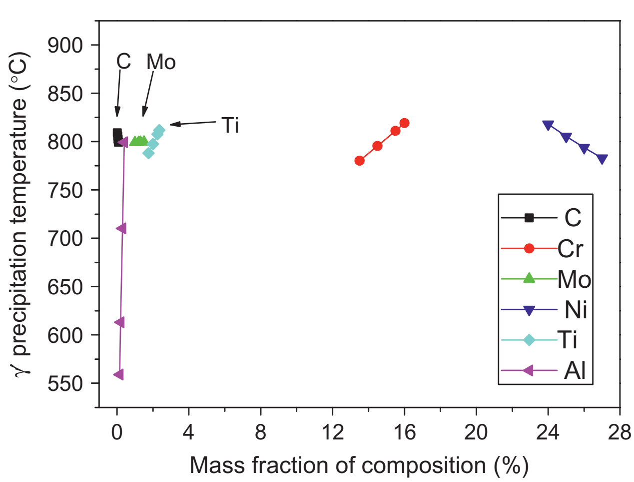


**Figure 9:** Influence of different elements on solution temperature of γ′ phase.

Figure 10 shows the influence of different elements on the maximum content of γ′ phase. It is clearly seen that the variation of Al content has the most influence on the maximum content of γ′ phase. The maximum content of γ ′ phase increases by 0.055 % from 0.005 % to 0.06 % with the increase of Al content from 0.15 % to 0.4 %. Compared with the results of Figures 9 and 10, the influence trend of Ti, Cr, Mo, Ni, and C contents on the

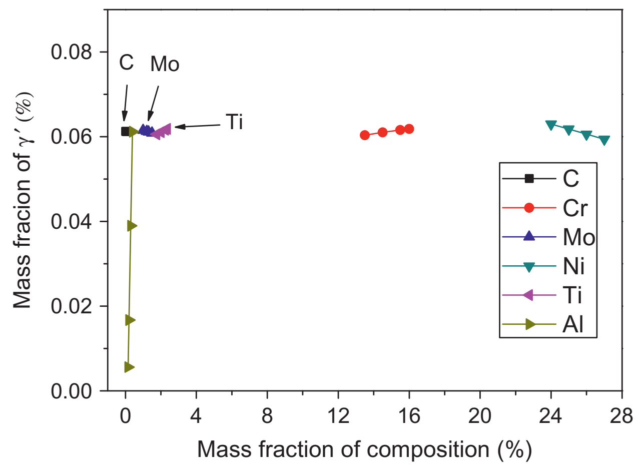


**Figure 10:** Influence of different elements on maximum amount of γ′ phase.

maximum content of γ′ phase is similar to that on the solution temperature of γ′ phase. Therefore, Al is also the critical element to control the maximum content of γ′ phase in alloy A286.

As the main constitutes of γ′ phase, the interactive influence of Al and Ti was studied. Figure 11 shows the influence of Al + Ti contents and Ti/Al ratio on the solution temperature of γ′ phase. Both of the increase in Al + Ti contents and Ti/Al ratio greatly contribute to the increase of solution temperature of γ′ phase. Figure 12 shows the influence of Al + Ti contents and Ti/Al ratio on the maximum content of γ′ phase. It is significantly illustrated that both Al + Ti contents and Ti/Al ratio have the most positive influence on the maximum content of γ′ phase.

In conclusion, it can be seen that Al is an critical factor to influence the maximum content and solution temperature of γ′ phase. Therefore, in actual production, more attention should be paid to Al element to control the solution temperature and the maximum content of γ′ phase in alloy A286.

### Critical composition factors of the content and transition temperature of primary MC carbides

Figure 13 shows the variation of solution temperature of MC carbide with the contents of different elements. It can be found that C content has the most obviously positive influence on solution temperature of MC carbides. And the solution temperature of MC carbide increases from 1306 °C to 1339 °C when C content increases from 0.02 %

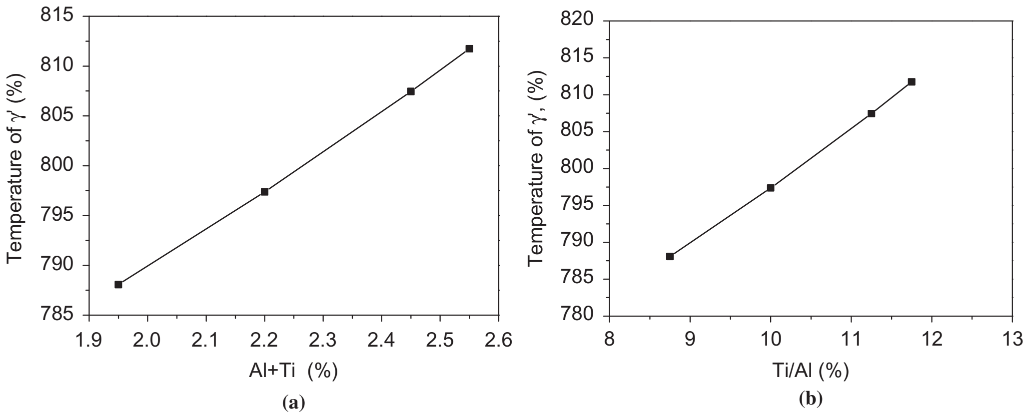


**Figure 11:** Influence of Al + Ti contents (a) and Ti/Al ratio (b) on solution temperature of γ′ phase.

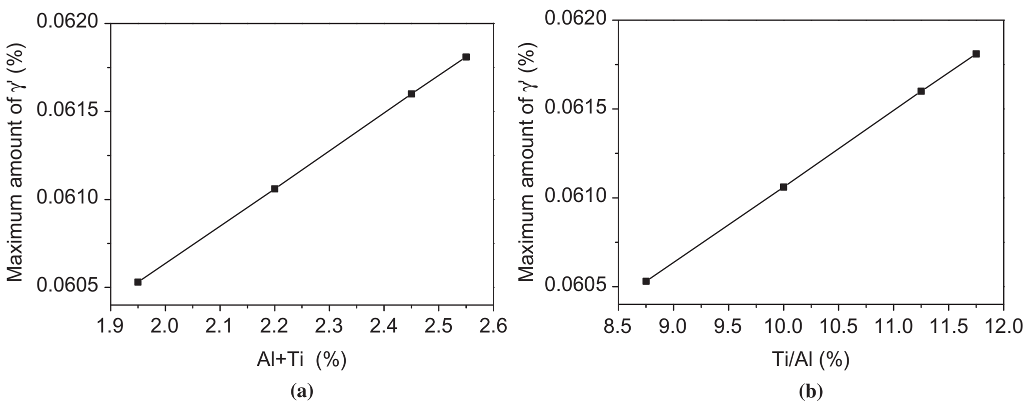


**Figure 12:** Influence of Al + Ti contents (a) and Ti/Al ratio (b) on maximum amount of γ′ phase.

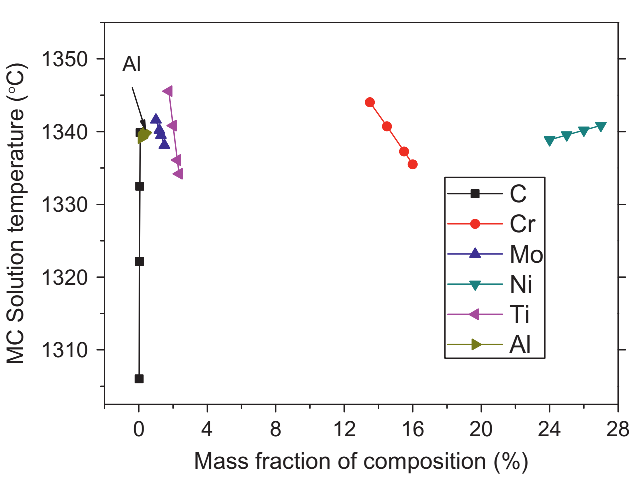


**Figure 13:** Influence of different elements on solution temperature of MC phase.

to 0.08 %. The elements of Al and Ni are also observed to improve the solution temperature of MC carbide. However, Ti content has the most obviously negative influence on the solution temperature of MC carbides. Solution temperature of MC carbide decreases from 1345 °C to 1331 °C when Ti content increases from 1.75 % to 2.35 %. Mo and Cr are also the negative factors for solution temperature of MC carbide in Alloy A286. In comparison, the influence extent of different elements on the solution temperature of MC carbide is C>Ti>Ni>Cr>Mo in order.

The variation of the maximum content of MC phase with the contents of different elements is shown in Figure 14. C element has the most obviously positive influence on the maximum content of MC, while Al, Mo, Ti, Cr, and Ni have the less influence. Besides, the increase of Ti/C ratio may increase the maximum content of MC carbide, as shown in Figure 15.

Figure 16 shows the influence of different elements on the precipitation temperature of MC phase when the maximum content occurs. Ti content has the most obviously positive influence on the precipitation temperature of MC phase. With the increase of Ti content

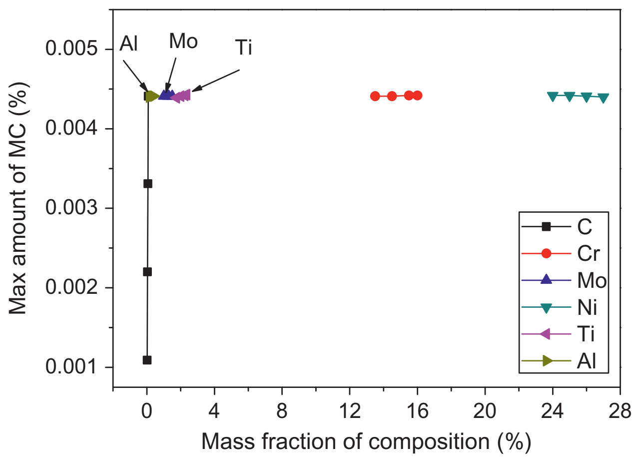


**Figure 14:** Influence of different elements on maximum amount of MC phase.

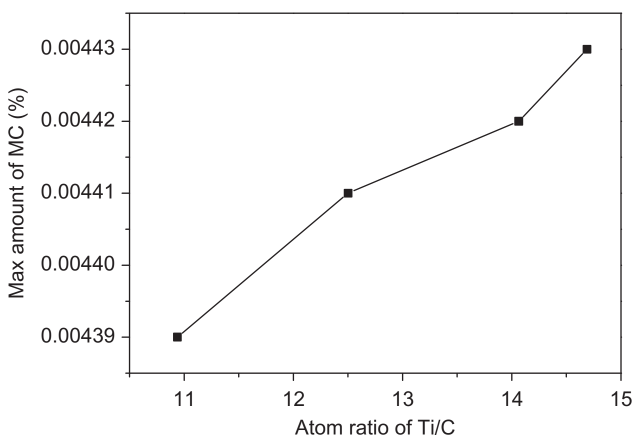


**Figure 15:** Influence of Ti/C on maximum amount of MC.

from 1.75 % to 2.35 %, the precipitation temperature of MC carbide increases from 846 °C to 886 °C. The elements of Cr, Mo, and Ni are also the positive factors for the precipitation temperature of MC phase. The positive influence extent of other different elements is Ti>Ni>Cr>Mo in order. However, C element has the most obviously negative influence on the precipitation temperature of MC phase. With the increase of C content from 0.02 % to 0.08 %, the precipitation temperature of MC phase decreases from 884 °C to 868 °C. The element of Al is also observed to decrease the precipitation temperature of MC phase to some extent. Therefore, the elements of C and Ti are the most critical to the precipitation temperature of MC phase in the maximum content, and the adjustment of C and Ti elements is preferred to control the precipitation of MC phase.

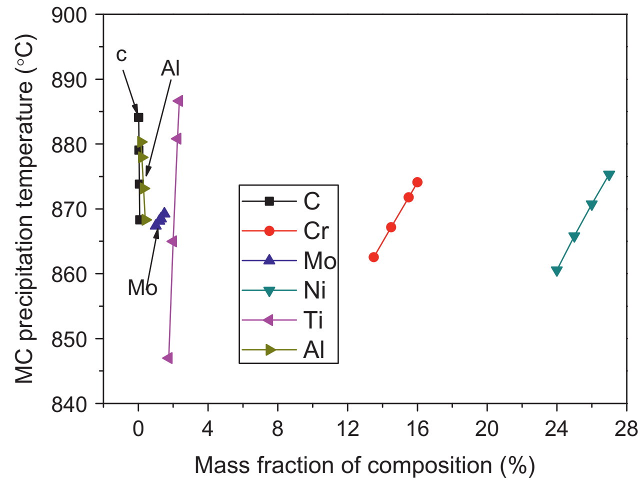


**Figure 16:** Influence of different elements on precipitation temperature of MC phase in maximum amount.

## Critical composition factors of the solution temperature and the maximum content of $M_{23}C_6$ carbides

Figure 17 shows the variation of solution temperature of $M_{23}C_6$ phase with the contents of different elements. C element has the most significantly positive influence on the solution temperature of $M_{23}C_6$ phase. With the increase of C content from 0.02 % to 0.08 %, the solution temperature of $M_{23}C_6$ phase increases from 582 °C to 590 °C. The elements of Ni, Mo, and Cr are also found to improve the solution temperature of $M_{23}C_6$ phase. The positive influence extent of different elements is C>Ni>Cr>Mo in order. However, Ti and Al contents have the negative influence on the solution temperature of MC carbides, and the

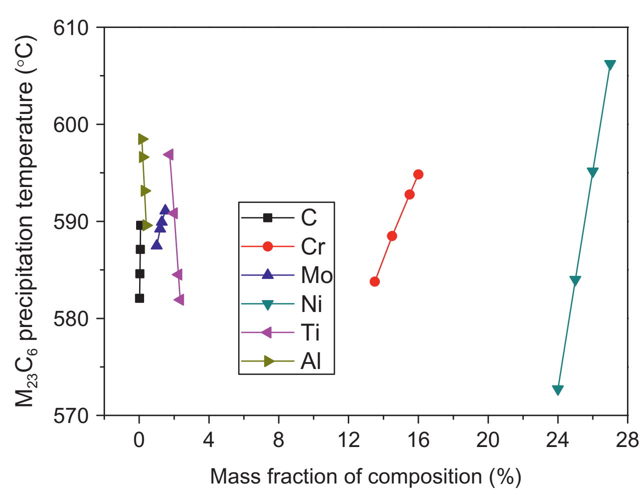


**Figure 17:** Influence of different elements on solution temperature of $M_{23}C_6$ phase.

influence extent is Ti>Al. Since Cr, C, and Mo are the main constitutes of $M_{23}C_6$ phase, the contents of Cr, C, and Mo should be reasonably adjusted for the better control of solution temperature of $M_{23}C_6$ phase.

Figure 18 shows the variation of the maximum content of $M_{23}C_6$ phase with the contents of different elements. It is clearly seen that C element is the critical factor to control the maximum content of $M_{23}C_6$ phase, while the other elements have the little influence. Therefore, more attention should be paid to C content for the control of the maximum content of $M_{23}C_6$.

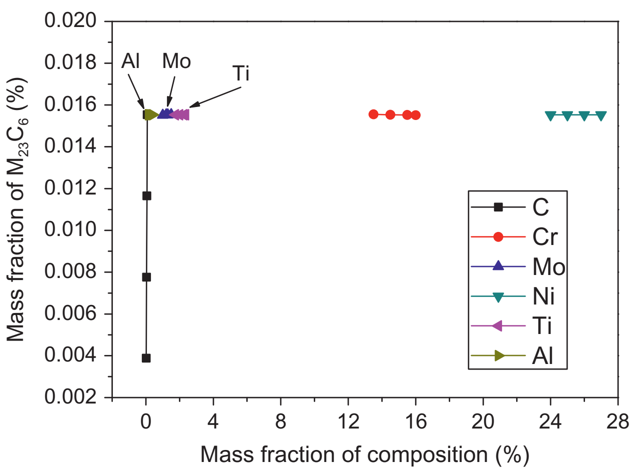


**Figure 18:** Influence of different elements on maximum amount of $M_{23}C_6$ phase.

## Conclusions

Equilibrium phases in alloy A286 and the influences of element contents were studied by Thermo-Calc calculation. The phase equilibria, solidification behavior, and precipitation behavior of equilibrium phases were calculated.

(1) The equilibrium phases of alloy A286 are determined to be γ, η, σ, γ′, $M_{23}C_6$, and MC. The solidification behavior and precipitation behavior of equilibrium phases with the average composition are calculated.

(2) Al is considered as the critical element to control the solution temperature and the maximum content of γ′ phase. The influence extent of different elements on the solution temperature and the maximum content of γ′ phase is Al>Ti>Cr>Mo in order.

(3) C is the crucial element for the control of MC carbide followed by Ti element. The influence extent of different elements on the solution temperature, maximum content, and precipitation temperature when the maximum content occurs is determined to be C>Ti>Ni>Cr>Mo in order.

(4) Compared to Cr and Mo as the main constitutes of $M_{23}C_6$ phase, C is the more vital element for the regulation of $M_{23}C_6$ phase. The influence extent of different elements on the solution temperature, maximum content of $M_{23}C_6$ phase is defined to be C>Ni>Cr>Mo in order.

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