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Verification of a commercial CALPHAD database for Re and Ru containing nickel-base superalloys

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Abstract. The addition of rhenium and ruthenium to single crystal nickel-base superalloys improves the high-temperature properties of the alloys. In this work the applicability of the database TTNi7 (ThermoTech Ltd, UK) for developing 4th generation single crystal superalloys containing rhenium (Re) and ruthenium (Ru) was investigated. We systematically compared experimentally determined alloy properties to the predictions of ThermoCalc with the database TTNi7. The investigated properties were liquidus, solidus and γ' solvus temperature as well as incipient melting point and segregation. Calculations were based on thermodynamic principles with the assumption of either equilibrium or Scheil-Gulliver conditions, i.e. no diffusion in the solid and complete diffusion in the liquid. Furthermore the composition of the γ and the γ' phase of a Re- and Ru-containing superalloy was measured and compared to calculations. Our results show that the database is capable of simulating general trends of 4th generation superalloys up to 6 weight percent (wt.-%) Re and 6 wt.-% Ru. The present work shows that Scheil-Gulliver calculations can only be used as a first approximation for nickel-base superalloys.

Introduction

Single crystal nickel-base superalloys are important high-temperature load bearing materials used in particular for turbine blades in industrial gas turbines and aero engines [1,2,3]. These materials show excellent mechanical properties up to high homologous temperatures due to their γ / γ' microstructure with the ordered intermetallic γ' phase [4,5]. The aim of the current development of gas turbines is to reduce carbon dioxide emissions and fuel consumption and therefore to increase efficiency [6]. To achieve that, the firing temperature has to be increased and materials have to be found that are capable of enduring those higher temperatures. Prospective candidates are single crystal superalloys with additions of rhenium (Re) and ruthenium (Ru) [1,7,8]. The addition of rhenium to superalloys is beneficial as rhenium is a solid solution strengthener. Nevertheless, rhenium strongly promotes the precipitation of topologically close-packed (TCP) phases during service, which may embrittle the material under certain conditions [9]. Several papers show that the addition of ruthenium can strongly reduce the TCP-phase formation [10,11]. Therefore, the combined addition of rhenium and ruthenium improves the mechanical properties of superalloys at high temperatures, especially the creep strength while the precipitation of brittle TCP-phases can be

suppressed. These so-called 4th generation superalloys typically contain about 6 wt.-% rhenium and 3 wt.-% ruthenium.

During a conventional development process for metallic alloys many samples have to be cast and analyzed. This is time-consuming and expensive. In the last decades new software solutions have been developed, which allow the calculation of phase diagrams and thermal properties of materials, the so-called CALPHAD method (Computer Calculation of Phase Diagrams). It is possible to save time by performing a first screening of the interesting alloy compositions on the computer and only investigating the most prospective alloys experimentally. Several commercial software packages are available - one of them is ThermoCalc [12]. A suitable database is needed for the calculations and there exist now a lot of databases for many material classes. For superalloys there is beside others the database TTNi7 [13]. While there is validation work existing for Re-containing alloys [14][15], little is known about the quality of simulations of Ru-containing alloys.

Methods

Thermodynamic equilibrium simulations. We applied the software ThermoCalc version R (ThermoCalc, Stockholm, Sweden) for the thermodynamic calculations together with the thermodynamic database TTNi7 (ThermoTech Ltd, Surrey, UK), which is containing the elements and phases stated in Table 1 [13].

Included information in the database TTNi7

Included elements	Ni, Al, Co, Cr, Cu, Fe, Hf, Mn, Mo, Nb, Ru, Re, Si, Ta, Ti, V, W, Zr, B, C, N, O
Included phases (only selected)	liquid, γ , γ' , Laves, σ , μ , R, P, π

Table 1: All included elements and selected included phases relevant for 4th generation superalloys in the database TTNi7 (ThermoTech Ltd.).

The calculation of thermodynamic properties is based on the minimization of free energy. A thermodynamic database includes the descriptions of all relevant phases in the alloy system and for each phase the parameters of the free energy of that phase are stored in a composition and temperature dependent way. For example for the substitutional solution of the γ matrix (fcc) of Ni-base superalloys a two-sublattice description can be used where the substitutional elements are considered in one sublattice and interstitial atoms can be included in the second sublattice. In general, for all solution phases the Gibbs free energy G is given by the following equation [16]

$$G = G^0 + G_{mix}^{ideal} + G_{mix}^{xs}, \quad (1)$$

where G^0 is the contribution of the pure elements of the phase to the Gibbs energy, G_{mix}^{ideal} is the contribution of ideal mixing of the components and G_{mix}^{xs} is the contribution to the Gibbs energy by non-ideal mixing of the components which is the Gibbs excess energy of mixing. Considering the free energy of the fcc-phase G^{fcc} [16] we get the following from eq. 1.

$$G^{fcc} = \sum_i x_i G_i^0 + RT \sum_i (x_i \ln x_i) + G^{xs}, \quad (2)$$

where we have

$$G^{xs} = \sum_i \sum_{j>i} x_i x_j \sum_k L_{ij}^k (x_i - x_j)^k, \quad (3)$$

with x_i as the mole fraction of component i on the substitutional sublattice. The reference energy of the element i is G_i^0 . R is the gas constant and T is the temperature. The excess energy is G^{xs} and L_{ij}^k is the corresponding interaction parameter of the order k . The free energy term in eq. 2 is dependent on temperature and composition. One should note, that similar terms exist for the free energy of

other more complex phases such as the γ' phase of Ni-base superalloys which is an ordered phase [17]. It is possible to obtain the set of phases with the minimal free energy which will be stable in equilibrium by a mathematical minimization process.

Scheil-Gulliver simulations. Scheil simulations take full diffusion in the liquid and no diffusion in the solid phase into account, which is in contrast to equilibrium (lever rule) simulations where full diffusion is assumed. A more general approach which is also applicable to multicomponent alloys is the Scheil-Gulliver model. It is identical to the Scheil model in case of binary systems [18,19]. While this model cannot be described by analytical solutions, this is possible for the binary Scheil model. Eq. 4 gives the segregation profile for equilibrium solidification (lever rule) and eq. 5 the profile for Scheil solidification of a binary alloy A-B,

$$c_s^{lever} = c_0, \quad (4)$$

$$c_s^{Scheil} = k \cdot c_0 \cdot (1 - f_s)^{k-1}, \quad (5)$$

where k is the partitioning coefficient ($k = c_s/c_l$) for the element B with the liquid and solid phase concentrations c_l and c_s . The concentration of element B in the initial melt is c_0 , f_s is the fraction of solid phase, which is a quantity associated with the position in the dendrite, an example is given in Figure 1.

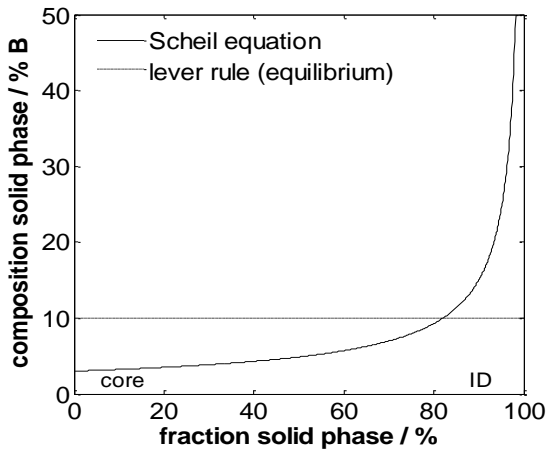


Figure 1: Composition profile for a dendrite of the binary alloy A-B calculated with lever rule and Scheil equation. An alloy composition of 90 % A and 10 % B-atoms is assumed, the partitioning coefficient is $k = 0.3$. Fraction solid is a quantity associated with the location inside the dendrite. The value 0 is equivalent to the dendrite core and 1 to the interdendritic region (ID). The strongest possible segregation of element B is represented by the Scheil equation, whereas no segregation will occur under equilibrium conditions. The real degree of segregation will be somewhere in between the two curves.

Experimental methods. A set of 12 3rd and 4th generation alloys was chosen for the experiments (see Table 2). All alloys are based on one master melt, produced by Doncasters Precision Castings Bochum GmbH, Germany. From this master melt different alloy compositions were created by alloying with Re and Ru in an electric arc furnace with a copper chill plate. Afterwards the alloys were directionally solidified in a Bridgman induction furnace with a withdrawal speed of 9 mm/min. A high degree of macroscopic homogeneity was obtained and assured by SEM-analysis of several samples taken from different parts of the cast specimens. All measurements were done in the as cast state of the alloys, except for the measurements of the composition of γ and γ' phase for the experimental 4th generation alloy 12 (see Table 2). For determining the chemical composition of the γ and γ' phase of this alloy at elevated temperatures, specimens were annealed at different temperatures for 1 hour and quenched in water afterwards; the sample at 850 °C was annealed for 24 hours without quenching.

All physical alloy properties have been obtained via differential scanning calorimeter (DSC) measurements on a Netzsch STA 409 DC. The DSC samples had a weight of approximately 300 mg and were throughout prepared in the same manner for best comparability. The heating and cooling curves were acquired with a rate of 5 K/min while the unit was flushed with argon. Since the heating curve neither provided peaks for γ' -dissolution nor for the incipient melting point of the alloys, only the measured cooling data was evaluated. Hence the extracted temperature values describe γ' -precipitation, eutectic phase formation, as well as liquidus and solidus temperatures including a small degree of undercooling due to the solidification process.

For measuring the composition of γ and γ' phase, transmission electron microscopy (Philips CM200T) with an attached energy dispersive x-ray spectroscopy analyzer (TEM-EDS) was used. The samples were prepared by electrolytic thinning using an agent of perchloric and acetic acid in mixture of 1:10. The measurements were performed in the scanning mode with a nominal spot size diameter of 27.5 nm except for the samples annealed at 1200 °C, 1250 °C and 1275 °C where secondary γ' precipitation occurred during quenching. Therefore for these temperatures sampling over a larger area was inevitable as secondary γ' precipitates were not existing during annealing but were precipitated from the matrix later on and must therefore be included in the measurements. A standardless routine applicable to measurements in thin samples was used, which is provided by the EDAX DX-4 analysis package belonging to the EDS system. There is no foil thickness correction for absorption in this routine which is justified for thin film TEM-samples. The measurements were carried out on the γ and the γ' -phase; for each alloy ten measurements were done to obtain sufficient statistics.

Composition of examined superalloys (in wt.-%)

Alloy	Al	Co	Cr	Mo	Re	Ru	Ta	Ti	W	Ni
1	6.13	8.92	5.25	0.97	0.00	0.00	6.70	0.00	6.19	rest
2	6.00	8.73	5.14	0.95	3.07	0.00	6.56	0.00	6.06	rest
3	6.08	8.86	5.21	0.96	0.00	1.69	6.65	0.00	6.14	rest
4	5.88	8.56	5.03	0.93	6.01	0.00	6.42	0.00	5.93	rest
5	6.04	8.80	5.17	0.95	0.00	3.35	6.60	0.00	6.10	rest
6	5.96	8.67	5.10	0.94	3.05	1.65	6.51	0.00	6.01	rest
7	5.80	8.44	4.96	0.92	5.93	3.22	6.34	0.00	5.85	rest
8	5.92	8.61	5.07	0.94	3.02	3.28	6.47	0.00	5.97	rest
9	5.88	8.56	5.03	0.93	3.00	4.89	6.42	0.00	5.93	rest
10	5.84	8.50	5.00	0.92	2.98	6.48	6.38	0.00	5.89	rest
11	5.76	8.38	4.93	0.91	5.89	4.79	6.29	0.00	5.81	rest
12	4.90	4.10	8.20	2.50	3.00	3.00	1.60	3.90	0.00	rest

Table 2: Nominal chemical composition of the examined superalloys in wt.-%. The alloy compositions were designed for the following alloy composition in at.-% except for alloy 12: 13.5 % Al – 9.00 % Co – 6.00 % Cr – 0.60 % Mo – 2.20 % Ta – 2.00 % W – x % Re – y % Ru with x = 0.00, 1.00, 2.00 and y = 0.00, 1.00, 2.00. For convenient comparison with other alloys they were converted to wt.-%.

The microstructure of the as cast alloys was analysed by a microprobe JEOL JXA 8100 using an acceleration voltage of 20 kV. Mappings were taken with a beam diameter of 5 μm , a step size of 2.5 μm and a measurement period of 200 ms per point. Dendritic and interdendritic compositions were quantified using mean values of multiple 9-point measurements.

Results and Discussion

Equilibrium simulations. The measured liquidus and γ' solvus temperatures of the investigated Re- and Ru-containing superalloys are compared to equilibrium calculations in Figure 2. Figure 2a shows the comparison of the liquidus temperatures and it can clearly be seen that the examined alloys can be simulated in a good manner with only a small difference to the experiments. Our simulations of the γ' solvus temperature (Figure 2b) are matching the experiments with an offset of approximately 50 °C. This discrepancy is due to the fact, that the simulation can only characterize the starting temperature of precipitation, whereas the experimentally measured DSC values could only be extracted for the peak of maximal precipitation rate.

We included the data of experimental work from other authors on Re- and Ru-containing alloys in Figure 2 in order to have a broader range of compositions. The results show, that the simulation quality is quite good for alloys in a broad range of compositions. Nevertheless, the results from different authors are clearly divided into groups of different data sets, lying systematically above or below the diagonal line which is probably due to differences in the experimental technique rather than simulation quality.

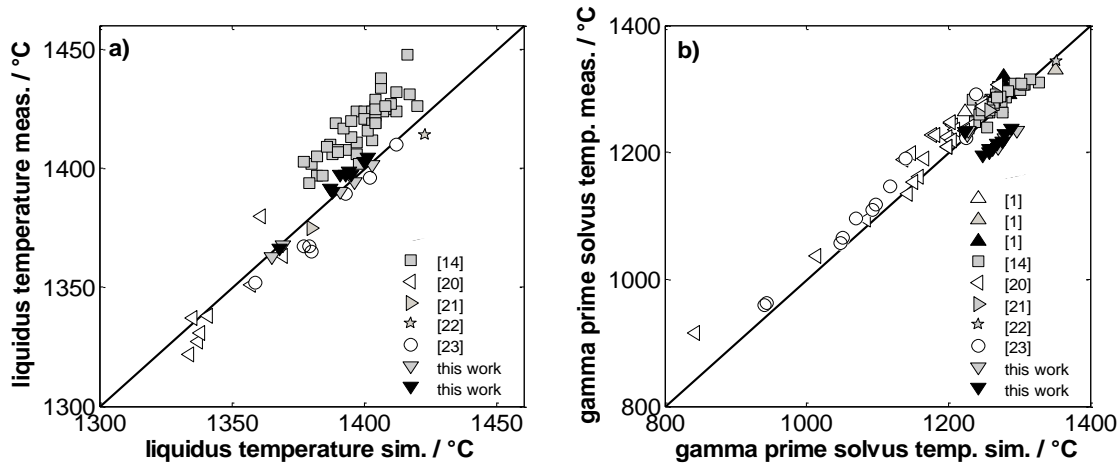


Figure 2: Comparison of simulated and measured liquidus temperatures (a) and γ' solvus temperatures (b) with one data point representing one alloy containing either Re and Ru (black), no Ru but Re (grey) or neither Re nor Ru (white). The experimental results are from this work as well as of other authors [1,14,20,21,22,23], whereas the simulations were performed by us using the database TTNi7.

The simulated and measured values of the equilibrium solidus temperatures of various alloys including Re- and Ru-containing alloys are presented in Figure 3.

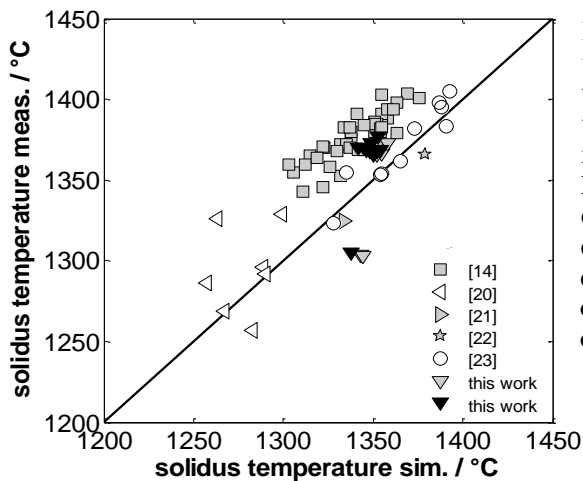


Figure 3: Comparison of simulated (TTNi7 + ThermoCalc version R) and experimental results of equilibrium solidus temperature. The experimental results are from this work as well as of other authors [14,20,21,22,23] with one data point representing one alloy containing either Re and Ru (black), no Ru but Re (grey) or neither Re nor Ru (white). The differences between experiments and simulations are strongly dependent on the experimental conditions, as near-equilibrium solidification with no segregation is difficult to obtain. Because of that, it is difficult to determine the quality of the equilibrium solidus temperature simulations.

The simulations differ from the experimental results depending on the conditions used by the several authors. This is on the one hand due to unequal DSC heating or cooling rates. On the other hand there is also the fact, that DSC measurements in the as cast state or experimental data derived from cooling curves can not describe the equilibrium condition of the material, since this could only be achieved after exceeding heat treatment processes. Hence, a comparison of simulated equilibrium solidus temperatures with experimental results is difficult a priori. Nevertheless it can be seen from Figure 3, that it is possible to determine a tendency for the solidus temperature with ThermoCalc simulations. A distinct difference between the simulations for Ru- and non Ru-containing alloys is not evident.

Scheil-Gulliver simulations. In contrast to equilibrium simulations, Scheil-Gulliver calculations assume no diffusion in the solid, which leads to maximal segregation of the alloying elements. Assuming Scheil solidification, the solidus temperature is lower than in equilibrium. The real degree of segregation usually lies in between Scheil-Gulliver segregation and equilibrium and depends beside other factors on the cooling rate. Therefore Scheil-Gulliver simulations are of high relevance as they allow the calculation of the maximal possible segregation in the as cast microstructure.

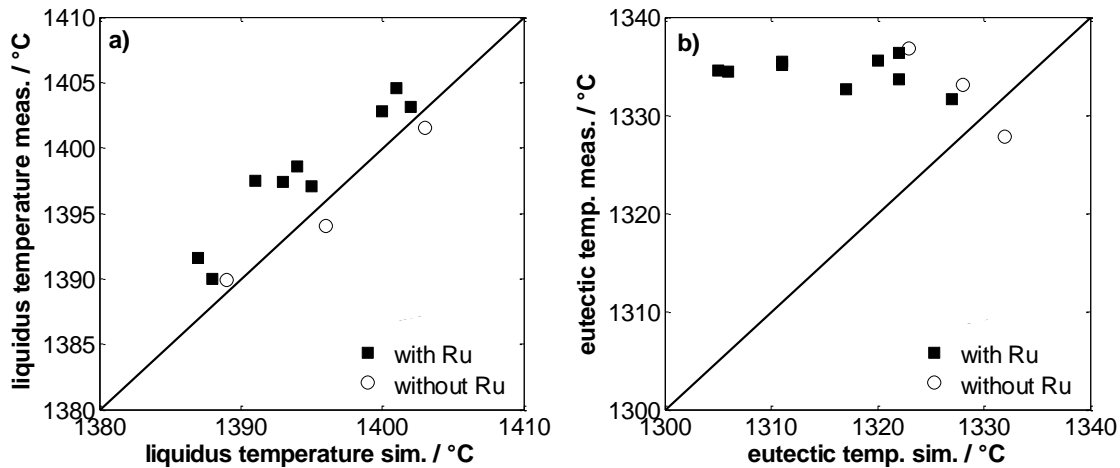


Figure 4: Comparison of Scheil-Gulliver simulations (TTNi7 + ThermoCalc version R) and experimental results of the liquidus temperature (a) and eutectic temperature (b) for Re and Ru-containing superalloys, where one alloy is represented by one data point.

The liquidus and eutectic temperatures calculated with Scheil-Gulliver simulations for the investigated alloys are shown in Figure 4. We can simulate the liquidus temperatures very well by applying Scheil-Gulliver simulations (see Figure 4a). In fact, the results of the Scheil-Gulliver simulations are not very different from the equilibrium calculations. For experimental liquidus temperatures no large effect of Ru could be found, although the simulations for Ru-containing alloys show some more deviation from the experiments than alloys without Ru.

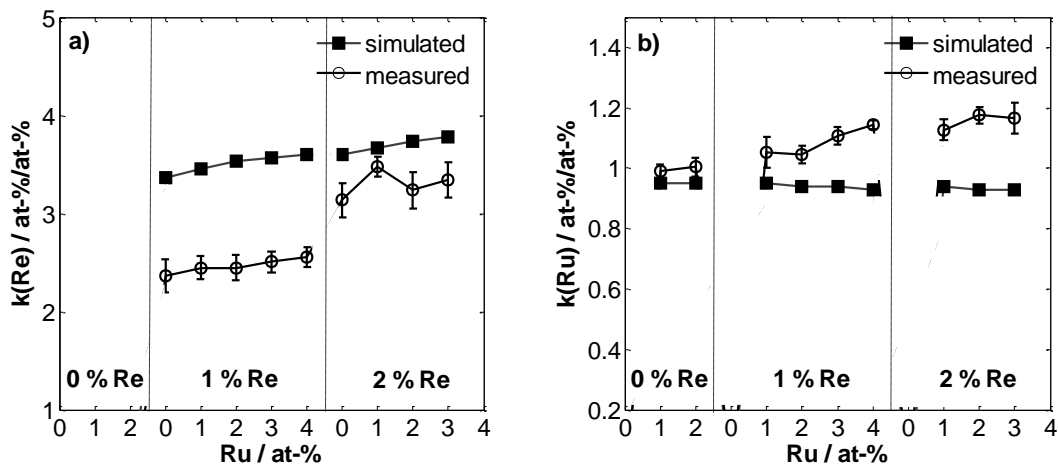


Figure 5: Comparison of Scheil-Gulliver simulations (TTNi7 + ThermoCalc R) and experimental results on the segregation coefficient ($k = \text{at-\% core} / \text{at-\% interdendritic region}$) of rhenium (a) and ruthenium (b) in the Re- and Ru-containing superalloys. The horizontal axis shows the alloys with their different Re/Ru-contents. Note the different scales of y-axis.

Figure 4b presents the results for the incipient melting point which is the eutectic temperature. In the simulations, the eutectic temperature is defined as the temperature where the precipitation of the $\gamma + \gamma'$ eutectic starts during cooling. It is a very important parameter for the heat treatment, as the eutectic melting is strongly deteriorating the mechanical properties of the alloys. Therefore proper heat treatment is very important to dissolve the eutectics, while the incipient melting point must not be exceeded during that process. It is obvious from Figure 4b, that the simulation of the eutectic temperature with a Scheil-Gulliver approach does not give reasonable results for most alloys. Furthermore Ru containing alloys appear to differ to a higher extend from the simulated values than alloys without Ru.

The segregation between the dendrite core and the interdendritic region is shown in Figure 5 for the two alloying elements Re (Figure 5a) and Ru (Figure 5b). The overall trend is reproduced by the simulations for both alloying elements. Nevertheless the difference between calculations based on Scheil-Gulliver simulations and the experimental results is large. Re shows very strong segregation,

whereas there is nearly no segregation for Ru. The error for the simulation of Re segregation is larger than for Ru. The simulated curves for Re are above the experimental and the reason is probably, that the real degree of segregation is somewhat less than predicted by Scheil-Gulliver because some diffusion does occur. But in case of Ru, the simulated values are in fact below the experimental values, although the differences are very small. Therefore we suppose that in case of very low segregation some database errors will dominate the Scheil solidification errors and no longer the neglect of diffusion. Our results show in general that Scheil-Gulliver simulations are only applicable as a first approach for cast superalloys. This is due to diffusion in the solid being in reality much more important than it is approximated by Scheil-Gulliver simulations.

Composition of γ and γ' phase. The partitioning of the alloying elements between the γ and the γ' phase strongly influences the alloy properties [24]. Figure 6 shows the temperature dependent composition of the γ and the γ' phase for an experimental 4th generation superalloy. In general, there is better agreement between the measurements and the (equilibrium) simulations in the γ phase (see Figure 6a,b). Nevertheless for many alloying elements rather good correlations between simulations and measurements can also be observed for the γ' -phase, especially for Al, Co, Cr and Ti (see Figure 6c). For other elements, there is less agreement in the γ' phase (see Figure 6d) which is especially the case for Mo, Re and Ru. This is a drawback, especially as Re and Ru are strongly influencing alloy properties [25]. But for those elements it is at least possible to simulate the qualitative temperature dependence rather correctly. This might be due to the physical basis of the governing terms describing the Gibbs energy terms of the γ' -phase. Therefore the temperature dependence can be simulated well, while there are larger errors for the concentration dependence.

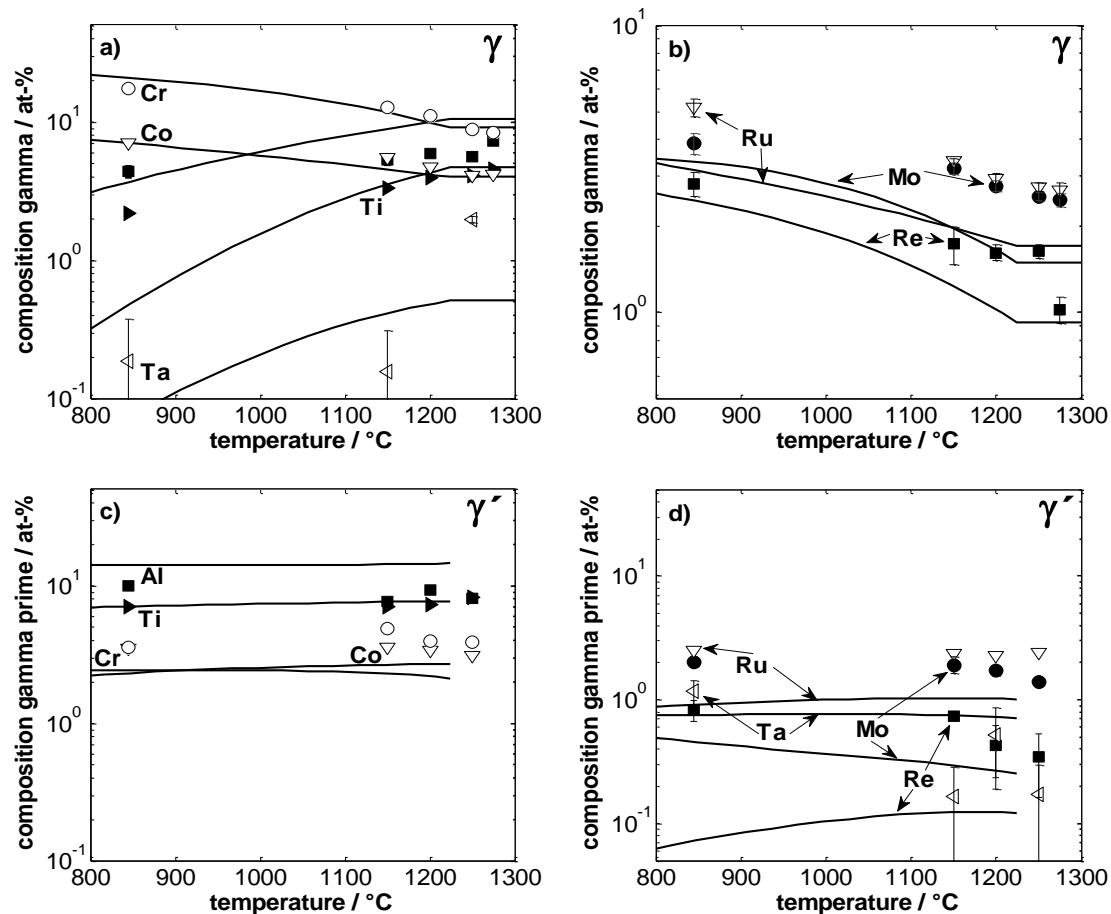


Figure 6: Comparison of simulations (TTNi7 + ThermoCalc version R) and experimental results for the composition of the γ (a,b) and the γ' (c,d) phase in the experimental 4th generation superalloy 12 (see Table 2). Error bars are shown for all elements if the error is at least of the size of the markers. The samples are largely homogenized. Only some Re-segregation occurs for most samples, but the sample at 850 °C is completely free of segregation. Segregation is not taken into account in the simulations.

Conclusions

In the present work we extend the verifications of the database TTNi7 to up to 6 wt.-% Re- and Ru-containing superalloys. The database is capable of simulating the equilibrium properties of the investigated superalloys. It is only possible to simulate the as cast properties of the examined superalloys in a qualitative way with Scheil-Gulliver simulations. The equilibrium composition of the γ and the γ' phase could be calculated in good agreement with measurements for the elements Al, Co, Cr and Ti. Large differences from the measurements could be found for Mo, Re and Ru, whereas the temperature dependence of the compositions can be simulated for all examined alloys.

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