Introduction to High Temperature Materials

Problem Set 4

Cap Morales, Shannon Nazareth
N25MA13

October 8, 2025

1

1.1 Ni-Al system plotted using Thermo-Calc

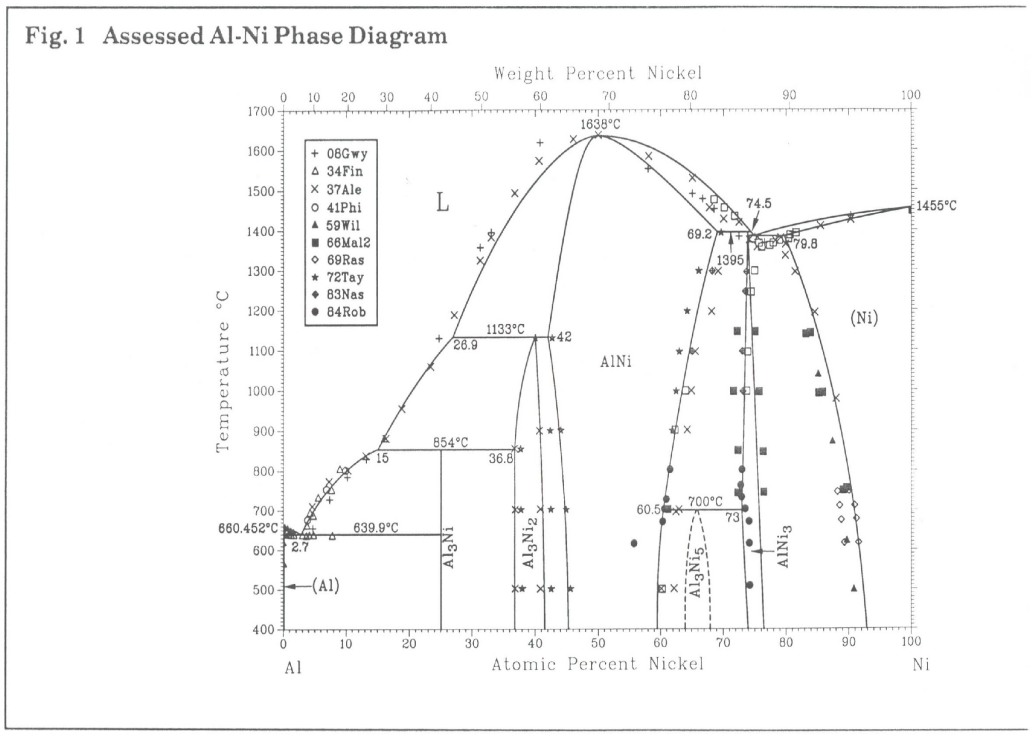
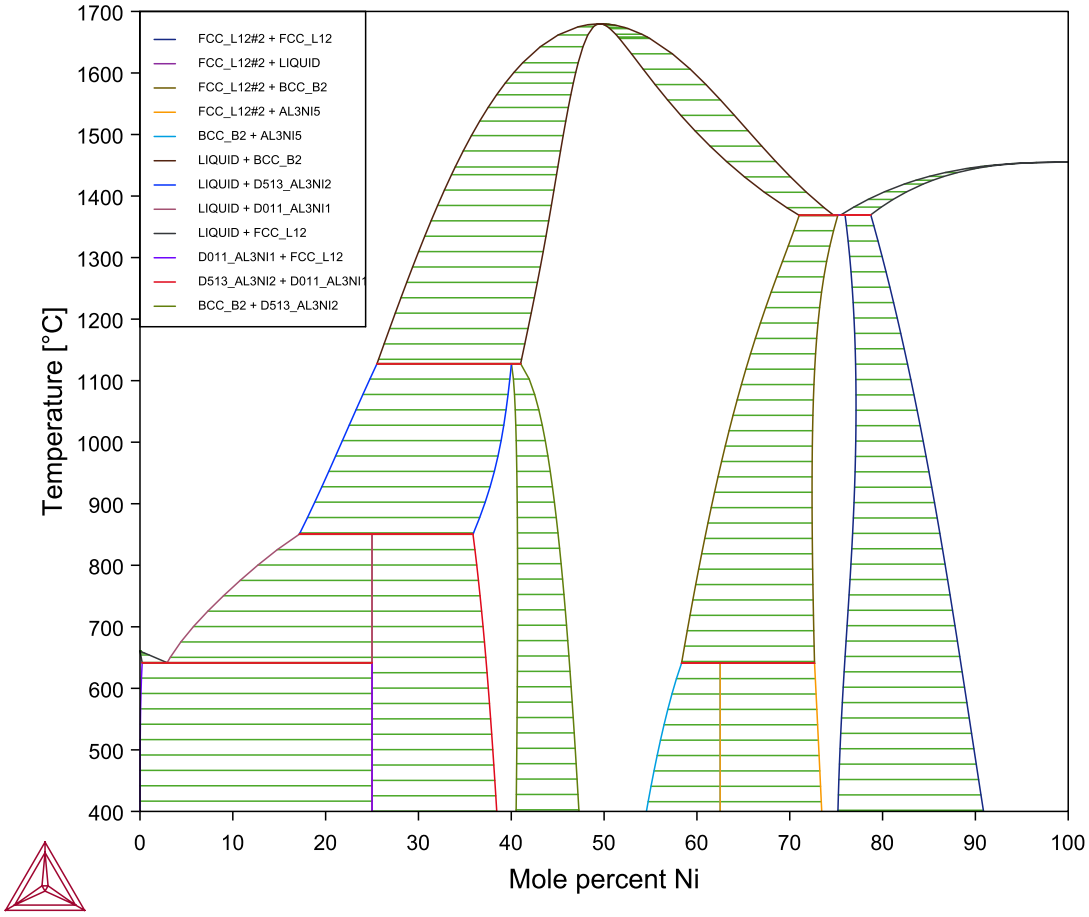


Table 1 Special Points of the Assessed Al-Ni Phase Diagram

(a) Binary Ni-Al ASM Materials Handbook

Figure 1: Ni-Al binary phase diagram



(b) Ni-Al binary phase diagram.
Source: Diagram generated with ThermoCalc (Andersson et al., 2002)

Figure 1: Ni-Al binary phase diagram (continued)

Figure 1a presents the binary phase diagram from the ASM Materials Handbook; and figure 1b presents the Ni-Al binary diagram obtained using *ThermoCalc*, using the *binary calculator* tool.

1.2 Composition of Al in Ni-Al system for a γ' fraction is 75%. Target operating temperature 1000°C

The composition of the γ' phase was calculated using the *single point* tool in *Thermo-Calc*, from which the following results were obtained:

Property	Value
Moles	1
Mass (g)	51.9841
Temperature (K)	1273.15
Total Gibbs Energy (J)	-94721.9
Enthalpy (J)	-2475.10
Volume (m^3)	0

Component	Mole Fraction	Mass Fraction	Activity
Al	0.211490	0.109773	1.13944E-08
Ni	0.788510	0.890227	0.00159239

Table 1: Results obtained from the calculation of the composition of the Ni-Al system for a γ' phase at 75%
Source: Data calculated with ThermoCalc (Andersson et al., 2002)

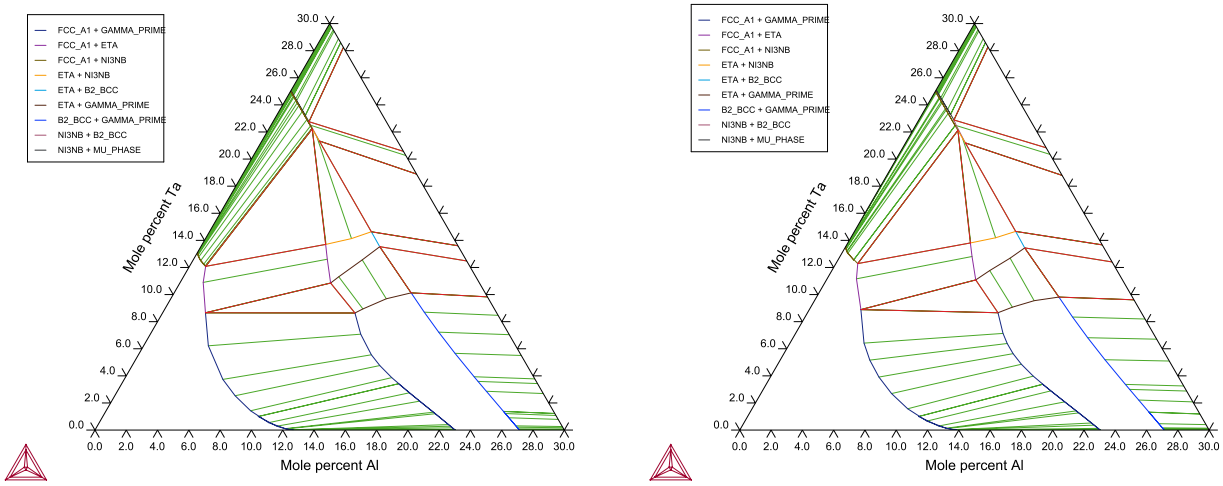
From the results presented in table 1 it can be seen that for the γ' wit a fraction of 75% at 1000°C the composition for Al is 0.2115 (21.15%) mole fraction which is equivalent to a 10.98 weight percent.

2

2.1 Examine the Ni-Al-Ta ternary phase diagram, is there a strong temperature dependence?

To evaluate if there is a strong dependence on temperature, the Ni-Al-Ta ternary phase diagram was generated using the *phase diagram* tool at different temperatures, from 800°C to 1300°C, the resulting diagrams are shown in figure 2.

Figures 2a and 2b present the ternary phase diagram for the alloy at 800°C and 900°C respectively, from the diagrams it can be seen a small increase in the γ phase region. This can be noted in the γ boundary line that moves from a mole percent of 12% in figure 2a, to approximately 14% in the Al axis in figure 2b.

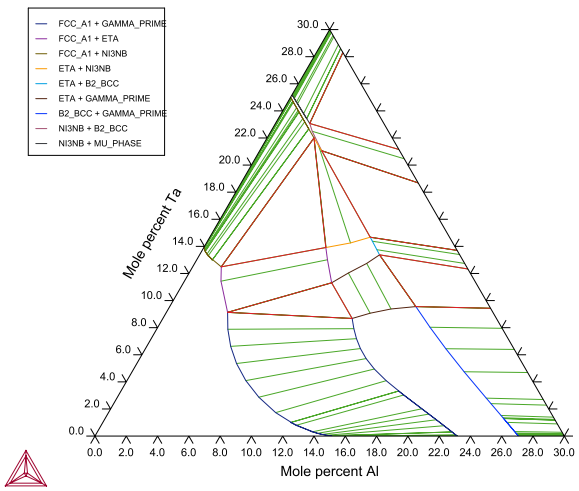


(a) 800°C

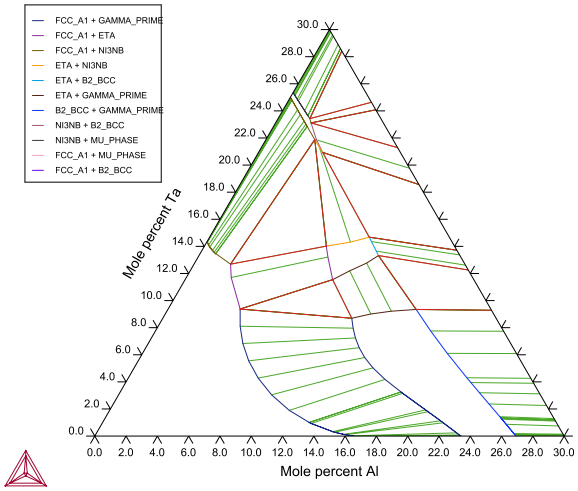
(b) 900°C

Figure 2: Ni-Al-Ta ternary diagram at different temperatures
Sourcce: diagrams generated with ThermoCalc (Andersson et al., 2002)

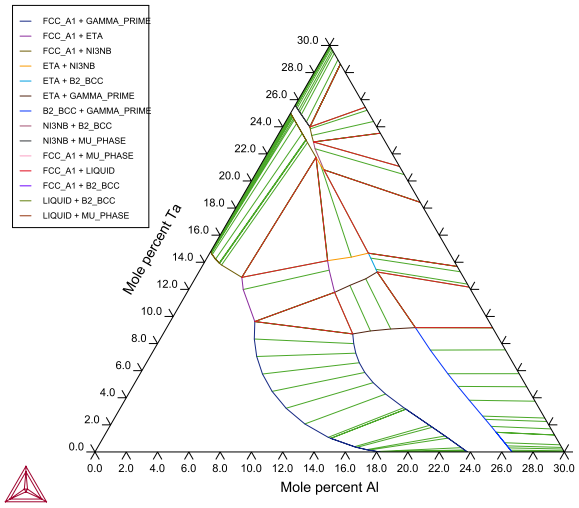
As temperature increases, the increase on the γ phase is more evident, where the bondary line of the γ phase moves from approximately 15% at 10000°C, in figure 2c, to 16% at 1100°C, in figure 2d. The change is more evident as the temperature increases to 1200°C and 1300°C, as it is shown in figures 2e and 2f; where at a temperature of 1200°C the boundary can be found at 18% and when the temperature is increased to 1300°C the boundary is at 20%.



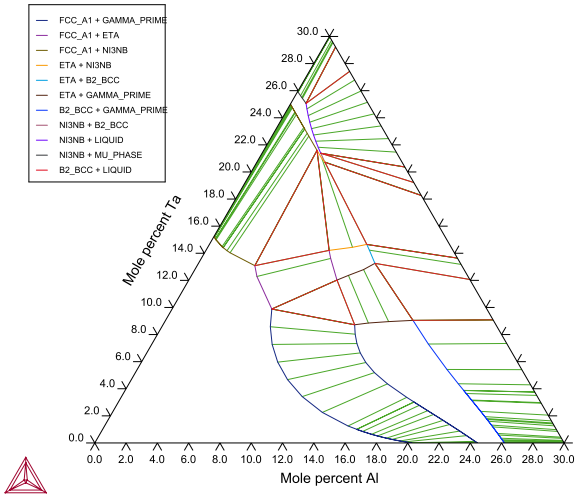
(c) 1000°C



(d) 1100°C



(e) 1200°C



(f) 1300°C

Figure 2: Ni-Al-Ta ternary diagram at different temperatures generated with *ThermoCalc* (Andersson et al., 2002) (continued)

Along with the increase of the area that is ocuppied by the γ phase, there is also a decrease on the area of the γ' phase. These changes can indicate that there is a dependence on temperature on the equilibrium of the γ and γ' phases in the Ni-Al-Ta alloy.

2.2 Ni-Al-Ta alloys for which γ' phase fraction is optimal

The optimal fraction is that for which γ' is 75%. To find the optimal fractions for γ' the calculation tool *One axis* was used, the results obtained are presented in table 2:

Mole % Ni	**Mole % Al**	**Mole % Ta**
78.8510	21.1490	7.6838e-10
79.5936	19.4064	1
80.3959	17.6041	2
81.1163	15.8837	3
81.6316	14.3684	4
81.9001	13.0999	5
81.9378	12.0622	6
81.7829	11.2171	7
81.4782	10.5218	8
81.1562	10.0517	8.7921

Table 2: Results obtained from the

The fractions of Ni, Al and Ta for which the γ' fraction is optimal presented in table 2 were plotted ternary phase diagram, figure 3.

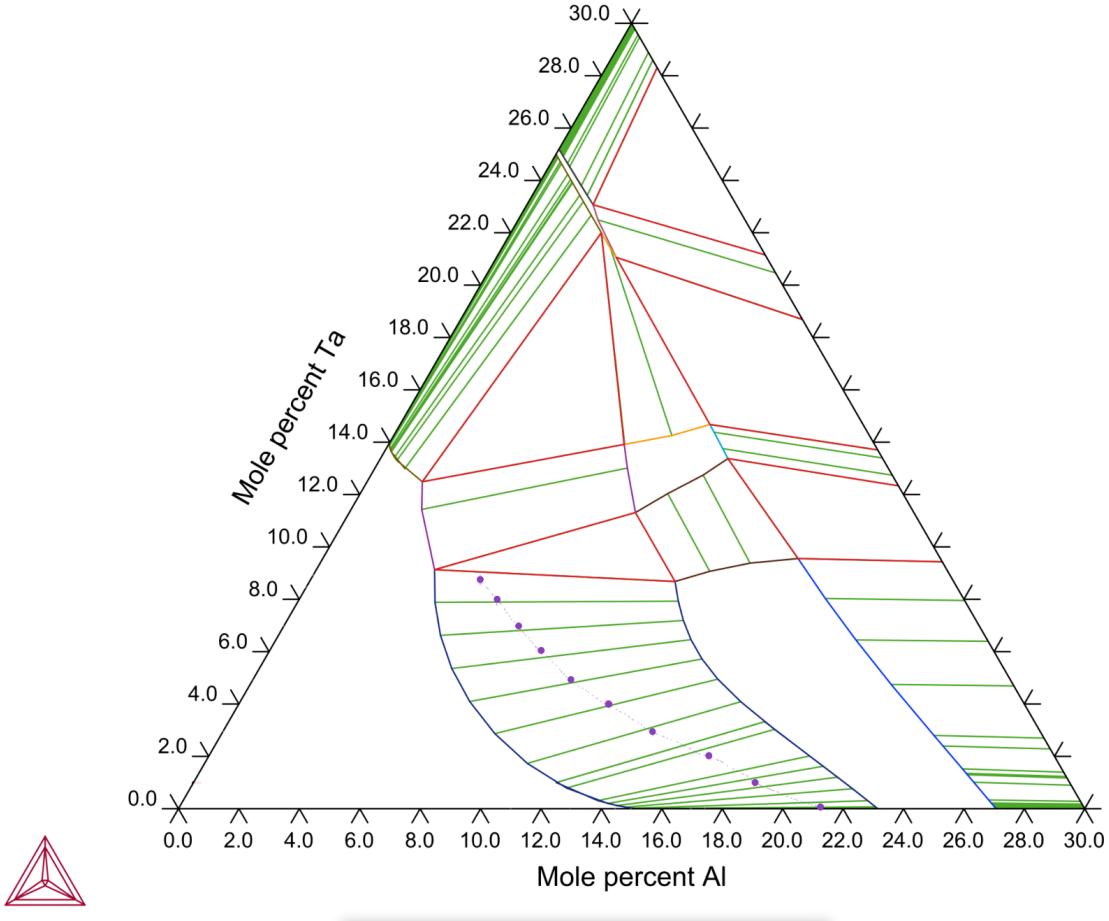


Figure 3: Ni-Al-Ta ternary phase diagram with compositions for optimal γ' phase fraction, 75%, generated using *ThermoCalc* (Andersson et al., 2002).

3

3.1 Show that the alloys chosen are not ideal

Lattice parameters:

$$\begin{aligned} a_{\gamma} &= 3.523 + 0.179Al + 0.700Ta + 0.110Cr + 0.444W + 0.441Re \\ &\quad + 0.478Mo + 0.096Co \\ a_{\gamma'} &= 3.558 + 0.500Ta \cdot 0.004Cr + 0.194W + 0.262Re + 0.208Mo \end{aligned} \tag{1}$$

Lattice misfit equation

$$\delta = 2 \times \left[\frac{a_{\gamma'} - a_{\gamma}}{a_{\gamma'} + a_{\gamma}} \right] \tag{2}$$

Using the *One axis* tool in *ThermoCalc* the composition of the different phases of the alloy were calculated. Using these values and equation 1, the lattice parameter of the γ and γ' phases were calculated. Then, the lattice misfit, δ, was calculated using equation 2. The results obtained are presented in table 3:

Ni_{γ}	Al_{γ}	Ta_{γ}	$Ni_{\gamma'}$	$Al_{\gamma'}$	$Ta_{\gamma'}$	a_{γ}	$a_{\gamma'}$	δ
0.8633	0.1317	0.0050	0.7842	0.1908	0.0250	3.5501	3.5705	0.0057
0.8721	0.1156	0.0123	0.7909	0.1732	0.0359	3.5523	3.5760	0.0066
0.8789	0.0979	0.0232	0.7954	0.1590	0.0456	3.5568	3.5808	0.0067
0.8826	0.0809	0.0365	0.7978	0.1477	0.0545	3.5630	3.5853	0.0062
0.8830	0.0661	0.0509	0.7982	0.1388	0.0630	3.5705	3.5895	0.0053
0.8803	0.0541	0.0655	0.7970	0.1315	0.0715	3.5786	3.5937	0.0042
0.8751	0.0448	0.0800	0.7947	0.1253	0.0800	3.5870	3.5980	0.0030
0.8696	0.0391	0.0913	0.7922	0.1210	0.0868	3.5939	3.6014	0.0021
0.8696	0.0391	0.0913	0.7922	0.1210	0.0868	3.5939	3.6014	0.0021
0.8696	0.0391	0.0913	0.7922	0.1210	0.0868	3.5939	3.6014	0.0021
0.8696	0.0391	0.0913	0.7922	0.1210	0.0868	3.5939	3.6014	0.0021
0.8696	0.0391	0.0913	0.7922	0.1210	0.0868	3.5939	3.6014	0.0021
0.8633	0.1317	0.0050	0.7842	0.1908	0.0250	3.5501	3.5705	0.0057
0.8547	0.1439	0.0013	0.7763	0.2108	0.0129	3.5497	3.5644	0.0041
0.8485	0.1515	0.0000	0.7685	0.2315	0.0000	3.5501	3.5580	0.0022

Table 3: Lattice misfit, δ, calculated for the Ni-Al-Ta alloy using the compositions (molar fractions) of the elements present in γ and γ' phases obtained using *ThermoCalc* (Andersson et al., 2002). The calculations of a_{γ}, $a_{\gamma\prime}$ and δ were performed in Python (Cap Morales, 2025)

From table 3 it can be seen that the values of δ are not equal to zero, which can indicate that the alloy is not ideal for the different compositions.

3.2 With additions of Cr, W, Re, Mo or mixture, find alloy for which the lattice misfit is close to zero

The values of the lattice misfit for both γ and γ' phases were calculated using the molar fractions of the γ and γ' phases of different alloys of Ni-Al-Ta-X, where X is Cr, Mo, Re and W, obtained from a *ThermoCalc* calculations and equations 1 and 2. The results obtained are presented in tables 9, ,10, 11 and 12 in the Appendix 6.

From the values of lattice misfit obtained for each alloy, the minimum value was extracted in order to know which composition gives a lattice misfit closer to zero, the results are presented in table 4:

Ni_γ	Al_γ	Ta_γ	Cr_γ	$Ni_{\gamma'}$	$Al_{\gamma'}$	$Ta_{\gamma'}$	$Cr_{\gamma'}$	a_γ	$a_{\gamma'}$	δ
0.743	0.086	0.008	0.163	0.753	0.174	0.035	0.038	3.562	3.575	0.004
Ni_γ	Al_γ	Ta_γ	Mo_γ	$Ni_{\gamma'}$	$Al_{\gamma'}$	$Ta_{\gamma'}$	$Mo_{\gamma'}$	a_γ	$a_{\gamma'}$	δ
0.843	0.084	0.020	0.053	0.773	0.164	0.031	0.032	3.577	3.573	0.001
Ni_γ	Al_γ	Ta_γ	Re_γ	$Ni_{\gamma'}$	$Al_{\gamma'}$	$Ta_{\gamma'}$	$Re_{\gamma'}$	a_γ	$a_{\gamma'}$	δ
0.830	0.116	0.009	0.045	0.779	0.180	0.034	0.007	3.570	3.577	0.002
Ni_γ	Al_γ	Ta_γ	W_γ	$Ni_{\gamma'}$	$Al_{\gamma'}$	$Ta_{\gamma'}$	$W_{\gamma'}$	a_γ	$a_{\gamma'}$	δ
0.871	0.080	0.020	0.029	0.787	0.159	0.030	0.024	3.564	3.578	0.004

Table 4: Minimum values of lattice misfit, δ, for each alloy calculated using Python (Cap Morales, 2025)

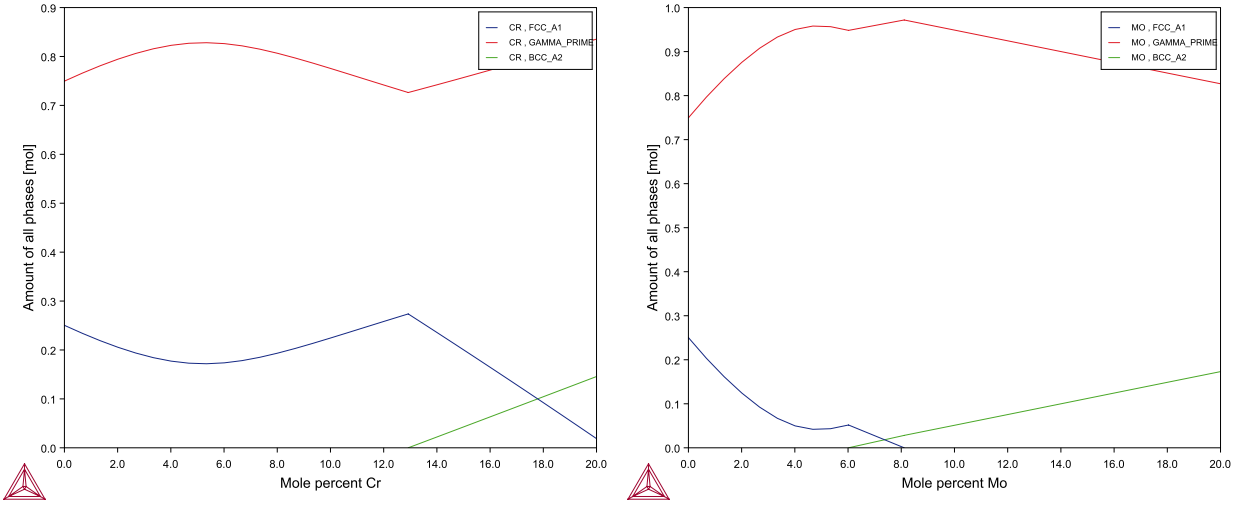
From the values presented in table 4, the minimum value of all the alloys was extracted, which is shown in table 5, with a misfit value of 0.0011, being the closet value for all the alloys.

Ni_γ	Al_γ	Ta_γ	Mo_γ	$Ni_{\gamma'}$	$Al_{\gamma'}$	$Ta_{\gamma'}$	$Mo_{\gamma'}$	a_γ	$a_{\gamma'}$	δ
0.843	0.084	0.020	0.053	0.773	0.164	0.031	0.032	3.577	3.573	0.001

Table 5: Minim value of lattice misfit from all alloys, corresponding to the Ni-Al-Ta-Mo alloy. Table generated using Python (Cap Morales, 2025).

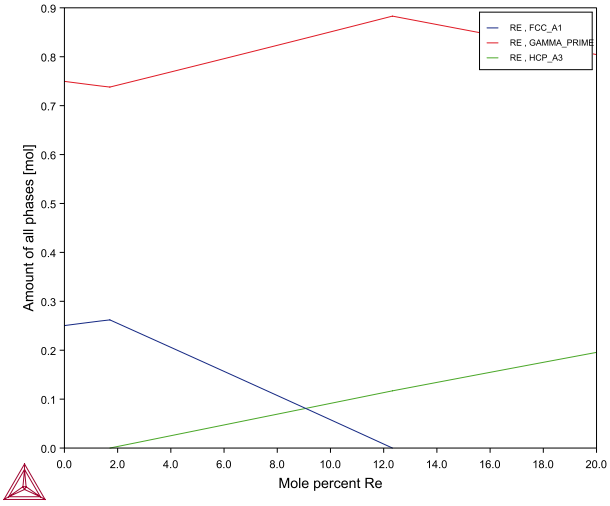
3.3 Do Cr, W, Re and Mo alter significantly the fraction of γ' present?

Figure 4 shows the graphs of the amount of all phases as a function of the mole percent of Cr, Mo, Re and W, obtained usinig *ThermoCalc*. The red line is the γ' composition and as it can be seen in all four plots the behavior of the γ' phase line is different with each system. From these plots it can be said that the presence of Cr, W, Re and Mo do have an effect ont he fraction of γ' present.

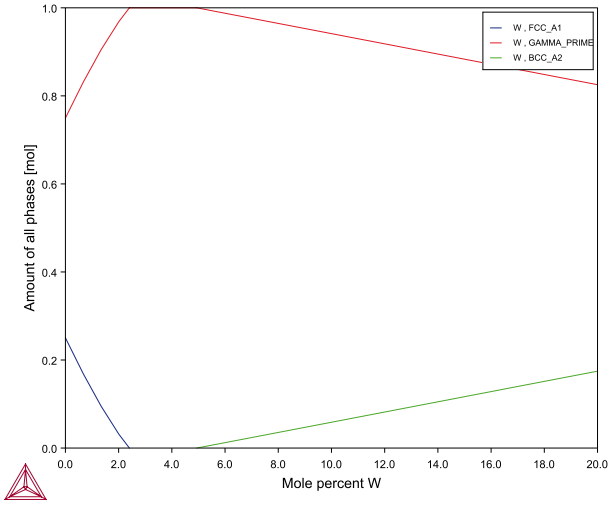


(a) Cr

(b) Mo



(c) Re



(d) W

Figure 4: Amount of phase as function of mole percent of a) Cr, b) Mo, c) Re and d) W generated with *ThermoCalc* (Andersson et al., 2002).

4

4.1 a) Suitable solutioning temperature and extent of the heat treatment window, and b) primary ageing temperature for new alloy

To obtain a plot that can be used to find the solution temperature and treatment window, a calculation using *One axis* with the following compositions was used:

x_{Al}	x_{Ta}	x_{Cr}	x_{Re}	x_{W}	x_{Co}
18	2.24	0.2	0.5	0.5	15

Table 6: Molar fraction composition of the Ni-Al-Ta-Cr-Re-W-Co.

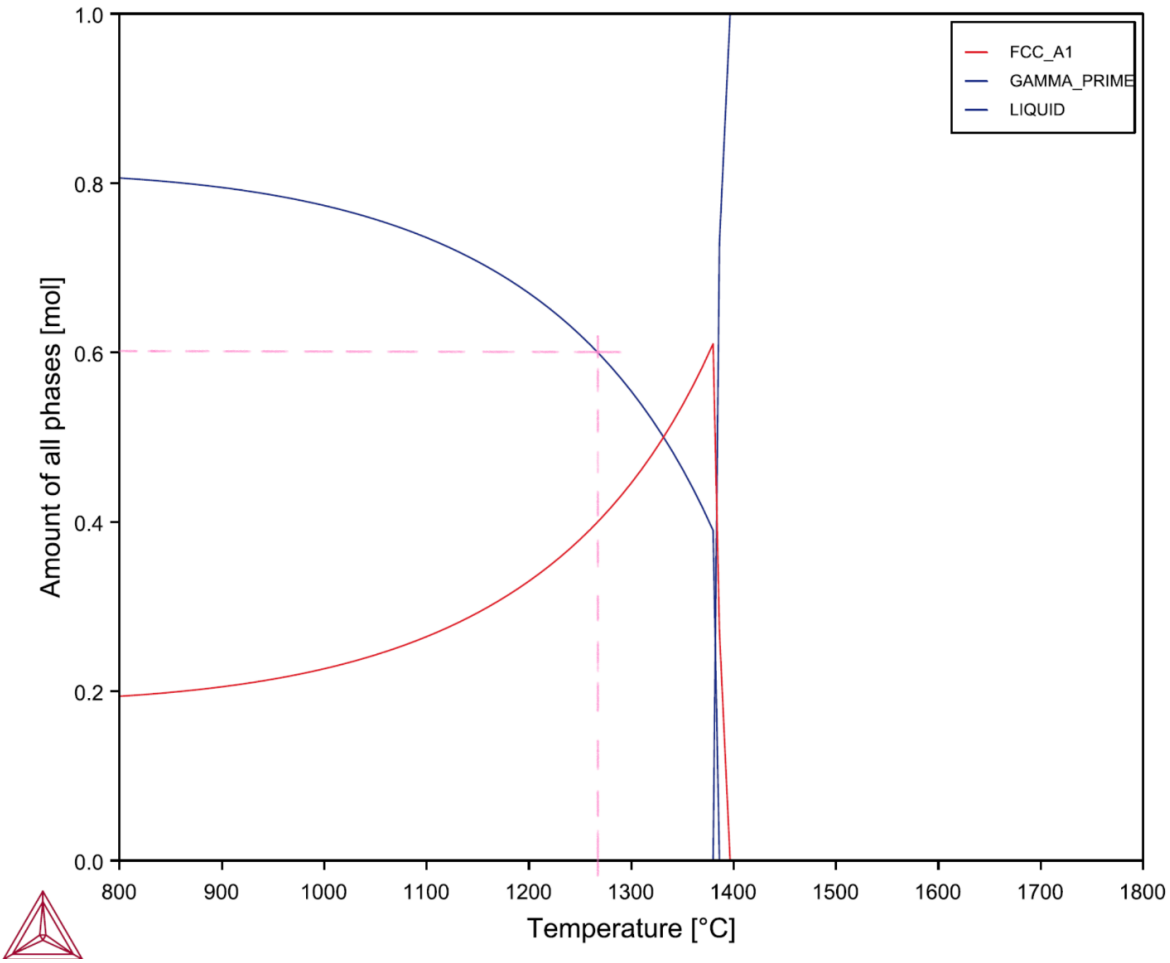


Figure 5: Amount of all phases as a function of temperature generated with *ThermoCalc* (Andersson et al., 2002)

a) In figure 5 the amount of all phases is plotted as a function of temperature for the alloy system Ni-Al-Ta-Cr-Re-W-Co. It shows that the γ' curve starts at a composition near 0.8 value and decreases as the temperature increases, reaching a composition of value 0 around 1388°C. The temperature where the composition of the $gamma'$ phase becomes zero is the solutioning temperature.

The liquid curve corresponds to an approximate temperature of 1380°C, this temperature corresponds to the solidus temperature, where the liquid phase begins to form.

The hear treatment window corresponds to de window that exists between the solutioning temperature, 1388°C, to the solidus temperatures, 1380°C, which gives a window of approximately 8°C; so in this range of temperature the γ' can be dissolved without partial melting of the alloy.

b) The primary ageing temperature is found at a γ' fraction of 0.60, which corresponds to a temperature of approximately 1270°C, as it is shown in figure 5. This is temperature at which a stable amount of precipitate can form and strengthen the alloy.

5

5.1

Alloy density:

$$\rho = \frac{4(\sum x_i * M_i)}{N_A \left(a_\gamma^3 f_\gamma + a_{\gamma'}^3 f_{\gamma'}\right)} \tag{3}$$

The molar fraction of the elements of the Ni-Al-Ta-Cr-Re-W-Co alloy was obtained using *ThermoCalc*. With these values and using equation 3, the density of the alloy was calculated using *Python*. The results are presented in table 7 in the Appendix section 6.

From the results obtained, the average and minimum density wer calculated:

ρ_{avg} (g/cm^3)	ρ_{avg} (g/cm^3)
8.6261	8.2376

Table 7: Average and minimum density values calculated for the Ni-Al-Ta-Cr-Re-W-Co alloy.

5.2

To calculate the cost of the alloy the following equation can be used:

$$\text{Cost per kg} = \sum_i w_i P_i, \tag{4}$$

where w_i is the weight fraction of the element i in the alloy and P_i is the price.

The data for the prices of the different alloy elements is presented in table 8:

Element	Price ($/lb)	Price ($/kg)
Al	1.30	2.866
Cr	5.60	12.3459
Co	12.00	26.4555
Ni	7.70	16.9756
Re		1370.00
Ta		170.00[1]
W	250.00[2]	31.5

Table 8: jfsofdjso [1] dollars per kg of Ta2O5, [2] dollar per metric ton of tungsten trioxide, metric ton of tungsten trioxide contains 7.93kg of tungsten.
Source: Data obtained from U.S. Geological Survey (U.S. Geological Survey, 2025)

Using the prices in table 8 and the weights of the elements the price of the alloy was calculated, the results are shown in table

6 Appendix

6.1 Results obtained for problem 4

Lattice misfit calculated for different alloy systems.

Ni_γ	Al_γ	Ta_γ	Cr_γ	$Ni_{\gamma'}$	$Al_{\gamma'}$	$Ta_{\gamma'}$	$Cr_{\gamma'}$	a_γ	$a_{\gamma'}$	δ
0.872	0.116	0.012	0.000	0.791	0.173	0.036	0.000	3.552	3.576	0.007
0.869	0.114	0.012	0.005	0.790	0.173	0.036	0.001	3.552	3.576	0.007
0.866	0.113	0.012	0.009	0.789	0.173	0.036	0.002	3.553	3.576	0.007
0.862	0.112	0.012	0.014	0.787	0.173	0.036	0.004	3.553	3.576	0.006
0.859	0.111	0.012	0.019	0.786	0.173	0.035	0.005	3.553	3.576	0.006
0.855	0.109	0.012	0.024	0.785	0.173	0.035	0.006	3.553	3.576	0.006
0.852	0.108	0.011	0.029	0.784	0.173	0.035	0.007	3.553	3.576	0.006
0.848	0.107	0.011	0.034	0.783	0.173	0.035	0.009	3.554	3.576	0.006
0.845	0.106	0.011	0.039	0.782	0.173	0.035	0.010	3.554	3.576	0.006
0.841	0.104	0.011	0.044	0.780	0.173	0.035	0.011	3.554	3.575	0.006
0.837	0.103	0.011	0.049	0.779	0.173	0.035	0.013	3.554	3.575	0.006
0.833	0.102	0.011	0.054	0.778	0.173	0.035	0.014	3.555	3.575	0.006
0.829	0.101	0.011	0.060	0.777	0.173	0.035	0.015	3.555	3.575	0.006
0.825	0.100	0.010	0.065	0.775	0.173	0.035	0.017	3.555	3.575	0.006
0.821	0.099	0.010	0.070	0.774	0.173	0.035	0.018	3.556	3.575	0.006
0.816	0.098	0.010	0.076	0.773	0.173	0.035	0.019	3.556	3.575	0.005
0.812	0.096	0.010	0.082	0.772	0.173	0.035	0.021	3.556	3.575	0.005
0.808	0.095	0.010	0.087	0.770	0.173	0.035	0.022	3.557	3.575	0.005
0.803	0.094	0.010	0.093	0.769	0.173	0.034	0.024	3.557	3.575	0.005
0.798	0.093	0.010	0.099	0.768	0.173	0.034	0.025	3.557	3.575	0.005
0.794	0.093	0.009	0.105	0.766	0.173	0.034	0.026	3.558	3.575	0.005
0.789	0.092	0.009	0.110	0.765	0.173	0.034	0.028	3.558	3.575	0.005
0.784	0.091	0.009	0.116	0.764	0.173	0.034	0.029	3.558	3.575	0.005
0.779	0.090	0.009	0.122	0.762	0.173	0.034	0.030	3.559	3.575	0.005
0.774	0.089	0.009	0.128	0.761	0.173	0.034	0.031	3.559	3.575	0.004
0.769	0.089	0.009	0.134	0.759	0.173	0.034	0.033	3.560	3.575	0.004
0.764	0.088	0.008	0.140	0.758	0.173	0.034	0.034	3.560	3.575	0.004
0.759	0.088	0.008	0.146	0.757	0.174	0.035	0.035	3.560	3.575	0.004
0.753	0.087	0.008	0.151	0.755	0.174	0.035	0.036	3.561	3.575	0.004
0.748	0.087	0.008	0.157	0.754	0.174	0.035	0.037	3.561	3.575	0.004
0.743	0.086	0.008	0.163	0.753	0.174	0.035	0.038	3.562	3.575	0.004
0.872	0.116	0.012	0.000	0.791	0.173	0.036	0.000	3.552	3.576	0.007
0.872	0.116	0.012	0.000	0.791	0.173	0.036	0.000	3.552	3.576	0.007

Table 9: Lattice missfit, δ, calculated for the Ni-Al-Ta-Cr alloy using the compositions (molar fractions) of the elements in γ and γ' phases obtained using *ThermoCalc* (Andersson et al., 2002). The calculations of a_γ, $a_{\gamma\text{t}}$ and δ were performed in Python (Cap Morales, 2025)

Ni_γ	Al_γ	Ta_γ	Mo_γ	$Ni_{\gamma'}$	$Al_{\gamma'}$	$Ta_{\gamma'}$	$Mo_{\gamma'}$	a_γ	$a_{\gamma'}$	δ
0.872	0.116	0.012	0.000	0.791	0.173	0.036	0.000	3.552	3.576	0.007
0.871	0.109	0.014	0.006	0.787	0.171	0.034	0.007	3.555	3.575	0.006
0.868	0.103	0.015	0.014	0.784	0.170	0.033	0.013	3.559	3.574	0.004
0.863	0.097	0.017	0.023	0.781	0.168	0.032	0.020	3.563	3.574	0.003
0.855	0.090	0.018	0.036	0.777	0.166	0.031	0.026	3.569	3.574	0.001
0.843	0.084	0.020	0.053	0.773	0.164	0.031	0.032	3.577	3.573	0.001
0.826	0.079	0.020	0.075	0.768	0.163	0.030	0.038	3.587	3.573	0.004
0.804	0.075	0.021	0.101	0.763	0.162	0.030	0.044	3.599	3.573	0.007
0.778	0.072	0.020	0.129	0.757	0.163	0.030	0.050	3.612	3.573	0.011
0.778	0.072	0.020	0.129	0.757	0.163	0.030	0.050	3.612	3.573	0.011
0.751	0.072	0.020	0.158	0.751	0.164	0.031	0.055	3.625	3.573	0.014
0.750	0.072	0.020	0.158	0.751	0.164	0.031	0.055	3.625	3.573	0.014
0.750	0.072	0.020	0.158	0.751	0.164	0.031	0.055	3.625	3.573	0.014
0.750	0.072	0.020	0.158	0.751	0.163	0.031	0.055	3.625	3.573	0.014
0.750	0.071	0.020	0.158	0.751	0.163	0.031	0.055	3.625	3.573	0.014
0.872	0.116	0.012	0.000	0.791	0.173	0.036	0.000	3.552	3.576	0.007
0.872	0.116	0.012	0.000	0.791	0.173	0.036	0.000	3.552	3.576	0.007

Table 10: Lattice missfit, δ, calculated for the Ni-Al-Ta-Mo alloy using the compositions (molar fractions) of the elements in γ and γ' phases obtained using *ThermoCalc* (Andersson et al., 2002). The calculations of a_γ, $a_{\gamma t}$ and δ were performed in Python (Cap Morales, 2025)

Ni_γ	Al_γ	Ta_γ	Re_γ	$Ni_{\gamma'}$	$Al_{\gamma'}$	$Ta_{\gamma'}$	$Re_{\gamma'}$	a_γ	$a_{\gamma'}$	δ
0.872	0.116	0.012	0.000	0.791	0.173	0.036	0.000	3.552	3.576	0.007
0.856	0.114	0.012	0.018	0.787	0.174	0.036	0.003	3.559	3.577	0.005
0.841	0.113	0.011	0.036	0.783	0.175	0.037	0.006	3.567	3.578	0.003
0.832	0.112	0.011	0.045	0.781	0.176	0.037	0.007	3.571	3.578	0.002
0.832	0.112	0.011	0.045	0.781	0.176	0.037	0.007	3.571	3.578	0.002
0.832	0.112	0.011	0.045	0.780	0.176	0.037	0.007	3.570	3.578	0.002
0.831	0.113	0.010	0.045	0.780	0.177	0.036	0.007	3.570	3.578	0.002
0.831	0.114	0.009	0.045	0.779	0.179	0.035	0.007	3.570	3.577	0.002
0.830	0.116	0.009	0.045	0.779	0.180	0.034	0.007	3.570	3.577	0.002
0.872	0.116	0.012	0.000	0.791	0.173	0.036	0.000	3.552	3.576	0.007
0.872	0.116	0.012	0.000	0.791	0.173	0.036	0.000	3.552	3.576	0.007

Table 11: Lattice missfit, δ, calculated for the Ni-Al-Ta-Re alloy using the compositions (molar fractions) of the elements in γ and γ' phases obtained using *ThermoCalc* (Andersson et al., 2002). The calculations of a_γ, $a_{\gamma t}$ and δ were performed in Python (Cap Morales, 2025)

Ni_γ	Al_γ	Ta_γ	W_γ	$Ni_{\gamma'}$	$Al_{\gamma'}$	$Ta_{\gamma'}$	$W_{\gamma'}$	a_γ	$a_{\gamma'}$	δ
0.872	0.116	0.012	0.000	0.791	0.173	0.036	0.000	3.552	3.576	0.007
0.873	0.113	0.013	0.001	0.791	0.172	0.035	0.002	3.553	3.576	0.007
0.874	0.110	0.014	0.002	0.790	0.171	0.034	0.005	3.553	3.576	0.006
0.875	0.108	0.014	0.003	0.790	0.170	0.033	0.007	3.554	3.576	0.006
0.876	0.105	0.015	0.005	0.790	0.168	0.033	0.009	3.554	3.576	0.006
0.876	0.102	0.015	0.006	0.790	0.167	0.032	0.011	3.555	3.576	0.006
0.876	0.099	0.016	0.008	0.790	0.166	0.032	0.013	3.556	3.576	0.006
0.876	0.096	0.017	0.011	0.789	0.165	0.031	0.014	3.557	3.576	0.006
0.876	0.093	0.017	0.013	0.789	0.164	0.031	0.016	3.558	3.577	0.005
0.875	0.090	0.018	0.017	0.789	0.162	0.031	0.018	3.559	3.577	0.005
0.874	0.087	0.019	0.020	0.788	0.161	0.030	0.020	3.561	3.577	0.005
0.873	0.083	0.019	0.025	0.788	0.160	0.030	0.022	3.562	3.577	0.004
0.871	0.080	0.020	0.029	0.787	0.159	0.030	0.024	3.564	3.578	0.004
0.872	0.116	0.012	0.000	0.791	0.173	0.036	0.000	3.552	3.576	0.007
0.872	0.116	0.012	0.000	0.791	0.173	0.036	0.000	3.552	3.576	0.007

Table 12: Lattice missfit, δ, calculated for the Ni-Al-Ta-W alloy using the compositions (molar fractions) of the elements in γ and γ' phases *ThermoCalc* (Andersson et al., 2002). The calculations of a_γ, $a_{\gamma\mathrm{t}}$ and δ were performed in Python (Cap Morales, 2025)

6.2 Results obtained for problem 5

x_{Ni}	x_{Al}	x_{Ta}	x_{Cr}	x_W	x_{Re}	x_{Co}	x_γ	$x_{\gamma'}$	a_γ	$a_{\gamma'}$	ρ
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.227	0.773	3.579	3.574	8.287
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.229	0.771	3.579	3.574	8.286
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.233	0.767	3.579	3.574	8.286
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.236	0.764	3.579	3.574	8.286
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.239	0.761	3.579	3.574	8.285
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.243	0.757	3.579	3.574	8.285
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.247	0.753	3.580	3.574	8.284
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.251	0.749	3.580	3.574	8.284
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.255	0.745	3.580	3.574	8.284
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.260	0.740	3.580	3.574	8.283
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.264	0.736	3.580	3.574	8.282
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.269	0.731	3.580	3.574	8.282
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.275	0.725	3.580	3.574	8.281
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.280	0.720	3.580	3.575	8.281
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.286	0.714	3.580	3.575	8.280
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.293	0.707	3.580	3.575	8.279
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.299	0.701	3.580	3.575	8.278
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.306	0.694	3.580	3.575	8.277
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.314	0.686	3.580	3.575	8.277

(continued on next page)

(continued from previous page)

x_{Ni}	x_{Al}	x_{Ta}	x_{Cr}	x_{W}	x_{Re}	x_{Co}	x_{γ}	$x_{\gamma'}$	a_{γ}	$a_{\gamma'}$	ρ
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.322	0.678	3.580	3.575	8.276
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.330	0.670	3.580	3.575	8.275
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.339	0.661	3.581	3.575	8.273
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.348	0.652	3.581	3.575	8.272
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.358	0.642	3.581	3.575	8.271
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.368	0.632	3.581	3.576	8.270
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.379	0.621	3.581	3.576	8.268
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.391	0.609	3.581	3.576	8.267
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.404	0.596	3.582	3.576	8.265
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.417	0.583	3.582	3.576	8.263
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.431	0.569	3.582	3.576	8.262
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.446	0.554	3.582	3.576	8.260
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.462	0.538	3.583	3.577	8.257
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.479	0.521	3.583	3.577	8.255
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.497	0.503	3.583	3.577	8.253
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.517	0.483	3.583	3.577	8.250
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.538	0.462	3.584	3.577	8.247
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.560	0.440	3.584	3.578	8.244
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.584	0.416	3.584	3.578	8.241
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.610	0.390	3.585	3.578	8.238
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.610	0.390	3.585	3.578	8.238
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.607	0.386	3.585	3.578	8.294
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.271	0.000	3.585	3.580	30.284
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.227	0.773	3.579	3.574	8.287
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.224	0.776	3.580	3.574	8.287
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.221	0.779	3.580	3.574	8.287
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.219	0.781	3.580	3.574	8.287
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.216	0.784	3.580	3.574	8.288
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.214	0.786	3.580	3.574	8.288
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.212	0.788	3.580	3.574	8.288
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.210	0.790	3.580	3.574	8.288
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.208	0.792	3.580	3.574	8.288
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.207	0.793	3.580	3.574	8.288
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.205	0.795	3.580	3.574	8.288
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.204	0.796	3.580	3.574	8.289
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.202	0.798	3.580	3.574	8.289
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.201	0.799	3.580	3.574	8.289
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.200	0.800	3.580	3.574	8.289
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.199	0.801	3.580	3.573	8.289
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.198	0.802	3.581	3.573	8.289
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.197	0.803	3.581	3.573	8.289
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.196	0.804	3.581	3.573	8.289

(continued on next page)

(continued from previous page)

x_{Ni}	x_{Al}	x_{Ta}	x_{Cr}	x_{W}	x_{Re}	x_{Co}	x_{γ}	$x_{\gamma'}$	a_{γ}	$a_{\gamma'}$	ρ
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.195	0.805	3.581	3.573	8.289
0.636	0.180	0.022	0.002	0.005	0.005	0.150	0.194	0.806	3.581	3.573	8.289

Table 13: Density in (g/cm^3) calculated using *Python* (Cap Morales, 2025) for the compositions of the Ni-Al-Ta-Cr-Re-W-Co alloy, compositions obtained using *ThermoCalc* (Andersson et al., 2002).

References

Andersson, J. O., Helander, T., Höglund, L., Shi, P. F., & Sundman, B. (2002). Thermo-Calc and DICTRA, computational tools for materials science. *Calphad*, *26*(2), 273–312. doi: 10.1016/S0364-5916(02)00037-8

Cap Morales, S. N. (2025). *Github repository: High temperature materials.* `https://github.com/ShannonNCM/High_temp_materials/blob/main/codes.ipynb`. (Source code for data processing and visualization)

U.S. Geological Survey. (2025). *Mineral commodity summaries 2025.* Reston, Virginia. Retrieved from `https://pubs.usgs.gov/periodicals/mcs2025/mcs2025.pdf` doi: 10.3133/mcs2025