Introduction to High Temperature Materials

Problem Set 4

Cap Morales, Shannon Nazareth
N25MA13

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1.1 Ni-Al system plotted using Thermo-Calc

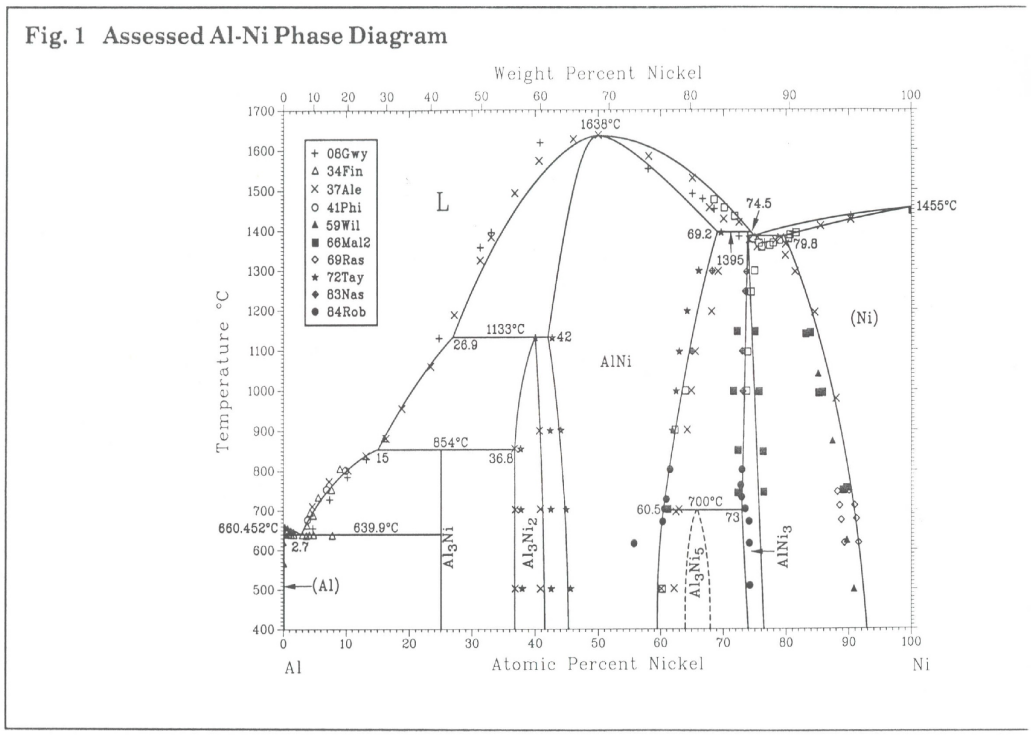
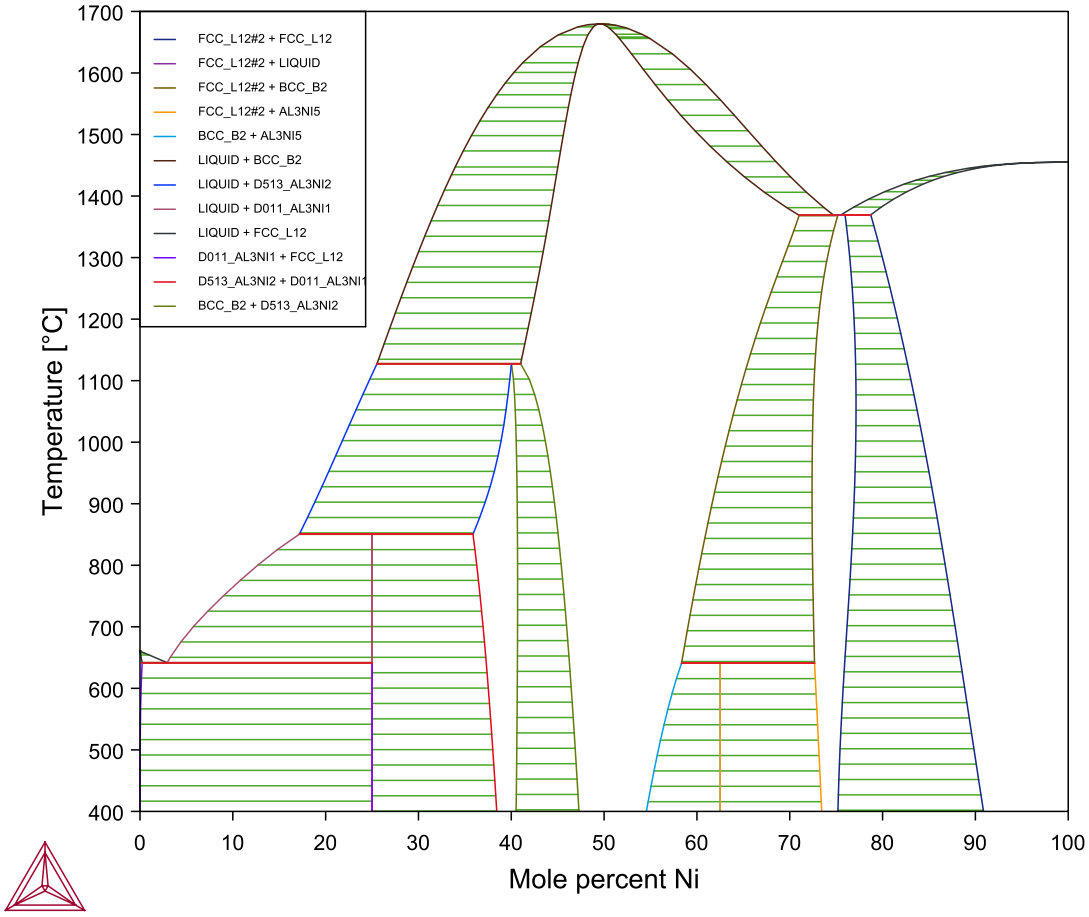


Table 1 Special Points of the Assessed Al-Ni Phase Diagram

(a) Binary Ni-Al ASM Materials Handbook

Figure 1: Ni-Al binary phase diagram



(b) Ni-Al system obtained using *ThermoCalc* (Andersson et al., 2002)

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

In figure 1 the plots for the binary system of Ni-Al is presented. 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% using *ThermoCalc* (Andersson et al., 2002)

From 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.

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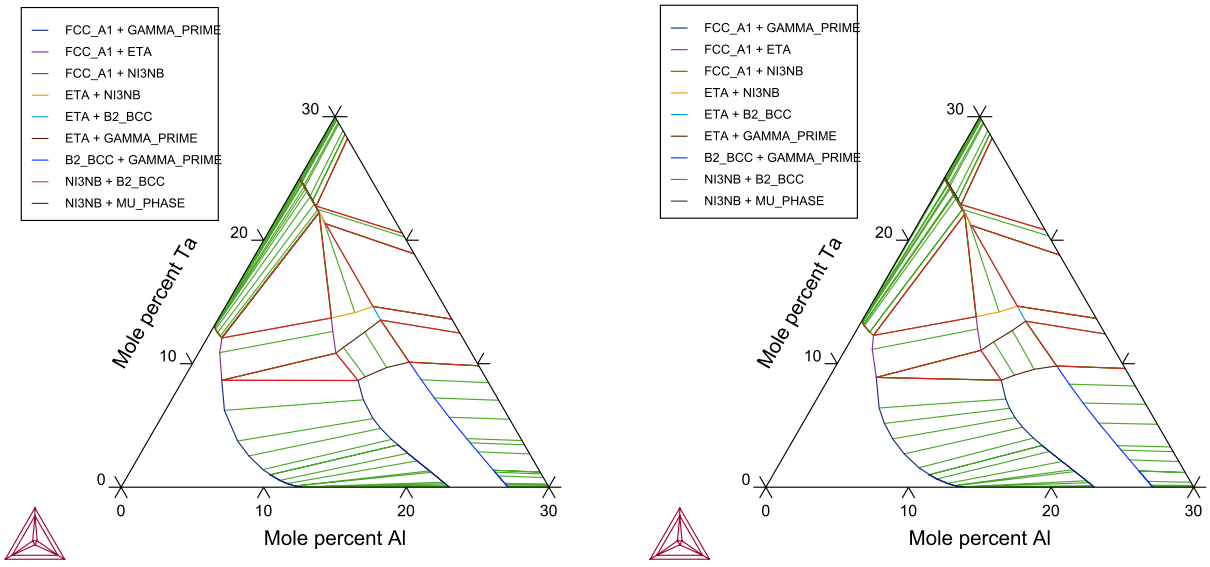
2.1 Examine the Ni-Al-Ta ternary phase diagram, is there a strong temperature dependence?

To evaluate eif 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 xxx in figure 2a, to xxx Al fraction axis in figure 2b.



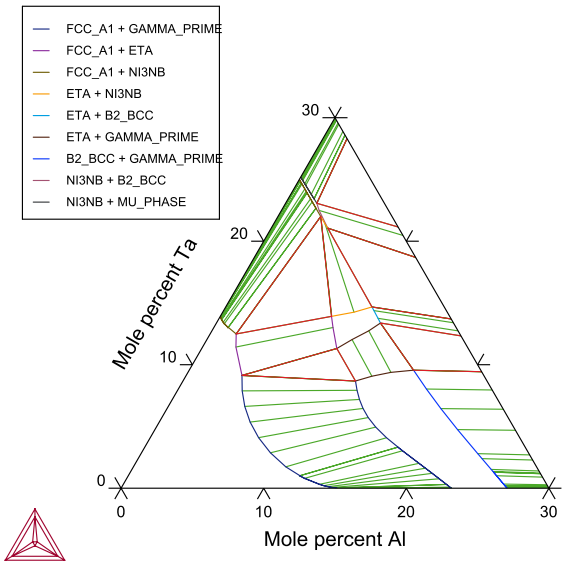
(a) 800°C

(b) 900°C

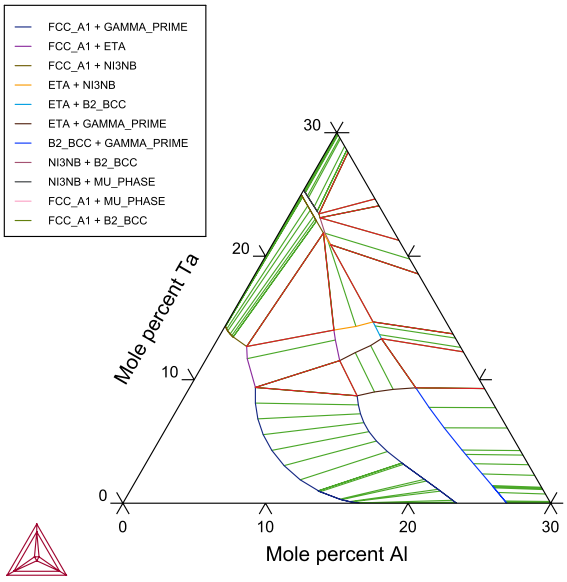
Figure 2: Ni-Al-Ta ternary diagram at different temperatures generated with *ThermoCalc* (Andersson et al., 2002)

As temperature increases, the increase on the γ phase is more evident, where the bondary linw of the γ phase moves from xxx fraction at 10000°C, in figure 2c, to $xxxx$ at 1100°C, in figure 2d. There is also a decrease in the region of the γ' phase; where the boundaries go from yyy Al fraction to yyy. 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 the decrease of the region of γ' phase is more evident.

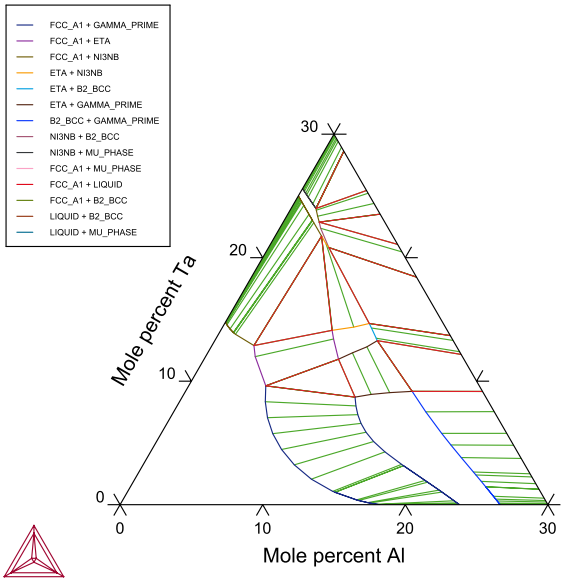
This indicates that there is a dependence on temperature on the equilibrium of the *gamma* and γ' phases in the Ni-Al-Ta alloy.



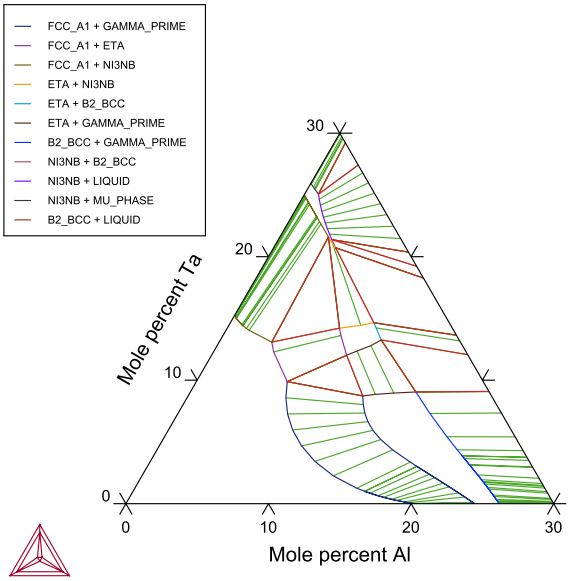
(c) 1000°C



(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)

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

The optimal fraction is that for which γ' is 75%. The

Mole percent Ni	Mole percent Al	Mole percent Ta
78.85099667	21.14900333	7.68378e-10
79.59362927	19.40637073	1
80.39594974	17.60405026	2
81.11631779	15.88368221	3
81.63158462	14.36841538	4
81.90005914	13.09994086	5
81.93775742	12.06224258	6
81.78294354	11.21705646	7
81.47817335	10.52182665	8
81.15616469	10.05173194	8.792103367

Table 2: Results obtained from the

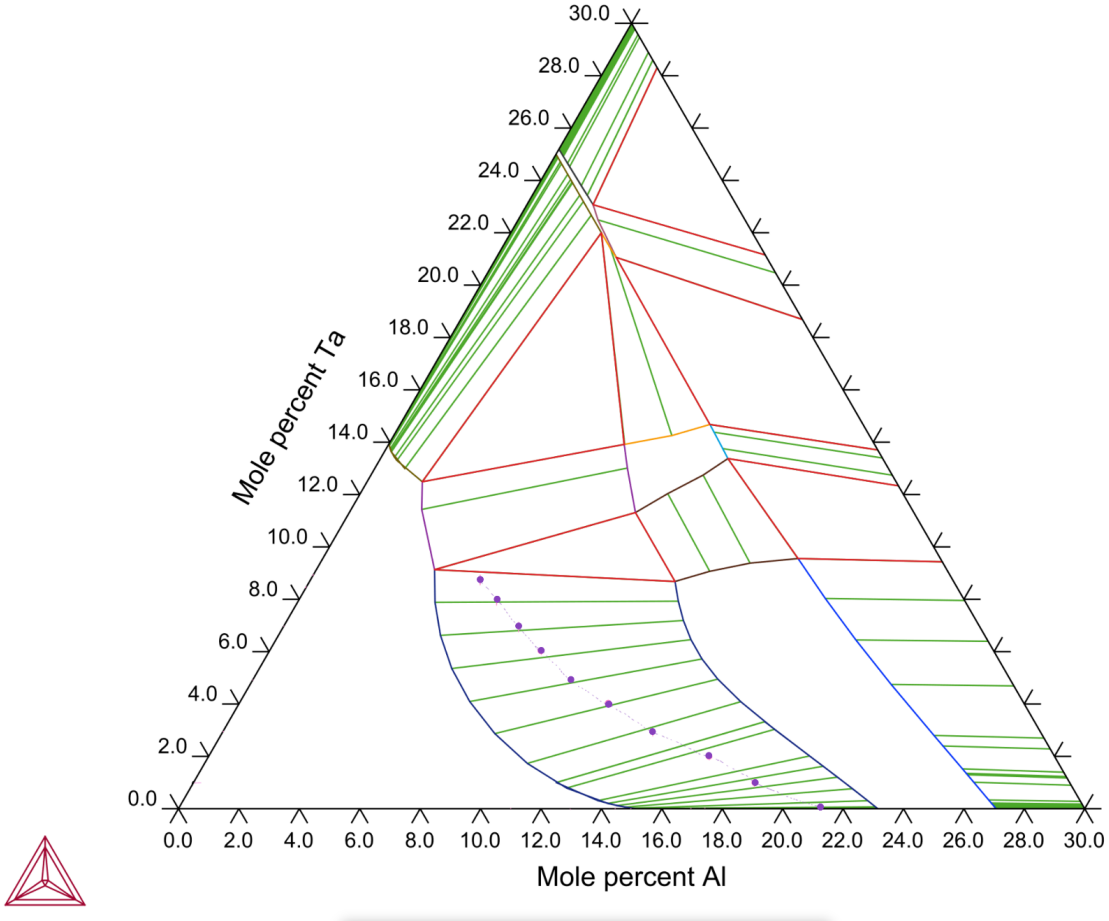


Figure 3: Ni-Al-Ta ternary phase diagram with compositions for optimal γ' phase fraction, 75%, generated using *ThermoCalc* (Andersson et al., 2002).

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

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

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. The results obtained are presented in tables 6, ,7, 8 and 9 in the Appendix 5.

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
0.7434	0.0862	0.0077	0.1627	0.7528	0.1741	0.0347	0.0384	3.5617	3.5752	0.0038
Ni_γ	Al_γ	Ta_γ	Mo_γ	$Ni_{\gamma'}$	$Al_{\gamma'}$	$Ta_{\gamma'}$	$Mo_{\gamma'}$	a_γ	$a_{\gamma'}$	δ
0.8430	0.0843	0.0196	0.0530	0.7731	0.1641	0.0307	0.0320	3.5772	3.5734	0.0011
Ni_γ	Al_γ	Ta_γ	Re_γ	$Ni_{\gamma'}$	$Al_{\gamma'}$	$Ta_{\gamma'}$	$Re_{\gamma'}$	a_γ	$a_{\gamma'}$	δ
0.8303	0.1157	0.0087	0.0453	0.7790	0.1798	0.0340	0.0072	3.5698	3.5769	0.0020
Ni_γ	Al_γ	Ta_γ	W_γ	$Ni_{\gamma'}$	$Al_{\gamma'}$	$Ta_{\gamma'}$	$W_{\gamma'}$	a_γ	$a_{\gamma'}$	δ
0.8711	0.0797	0.0199	0.0293	0.7871	0.1588	0.0300	0.0241	3.5642	3.5777	0.0038

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

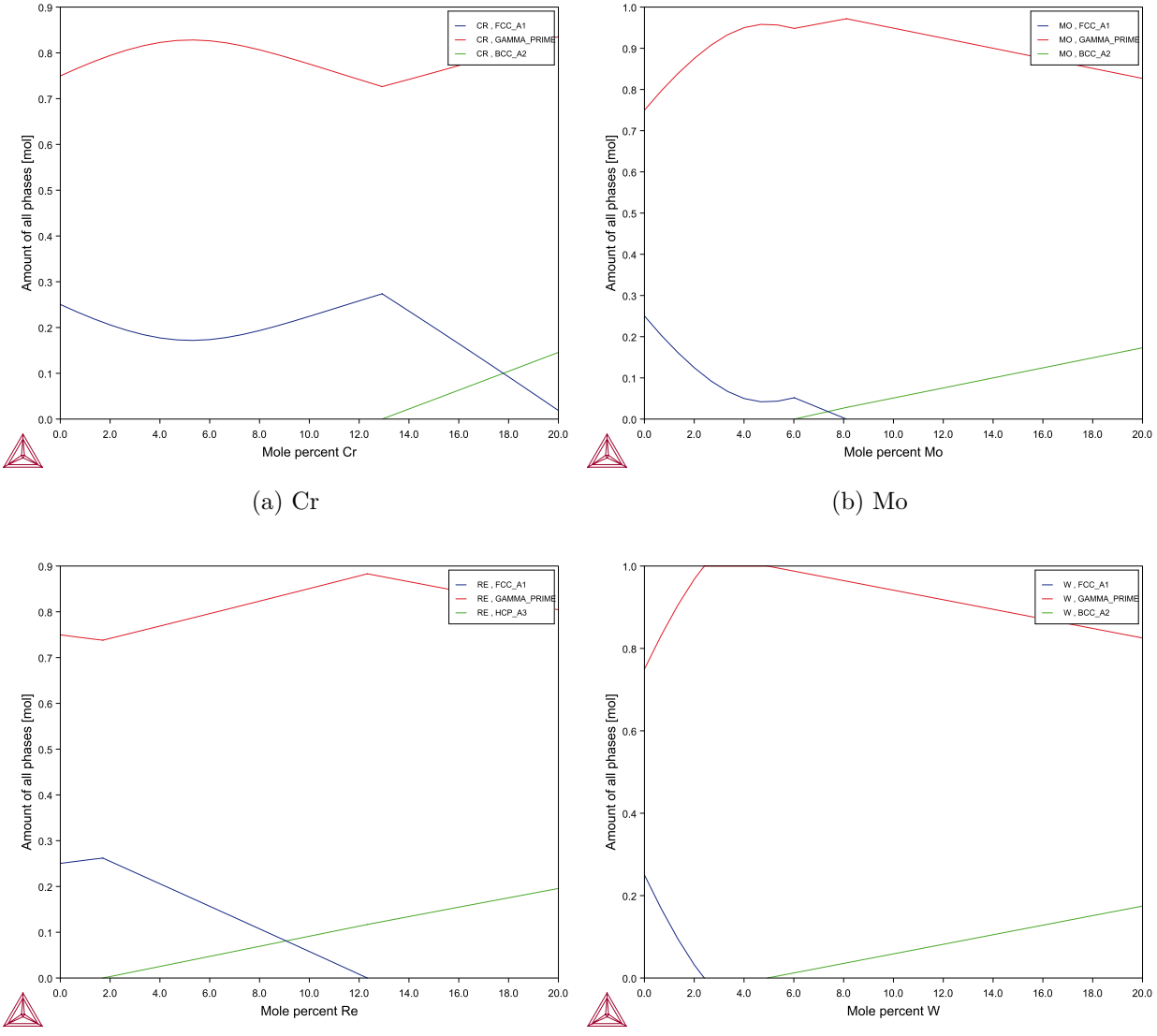
From the values presented in table 4, the minimum value of all the alloys was extracted, which is shown in table 5, with a misfit value of 0.0011, being the closet value for all the alloys.

Ni_γ	Al_γ	Ta_γ	Mo_γ	$Ni_{\gamma'}$	$Al_{\gamma'}$	$Ta_{\gamma'}$	$Mo_{\gamma'}$	a_γ	$a_{\gamma'}$	δ
0.8430	0.0843	0.0196	0.0530	0.7731	0.1641	0.0307	0.0320	3.5772	3.5734	0.0011

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. 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).

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

In figure 5 the amount of all phases is plotted as a function of temperature for the alloy system. Figure **??** 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 1380°C. This temperature is the solutioning temperature.

For the Liquid curve, it appears at an approximate temperature of 1370°C, this temperature corresponds to the solidus area. The heat treatment window is from the solutioning to the solidus temperature, which is aproximately.

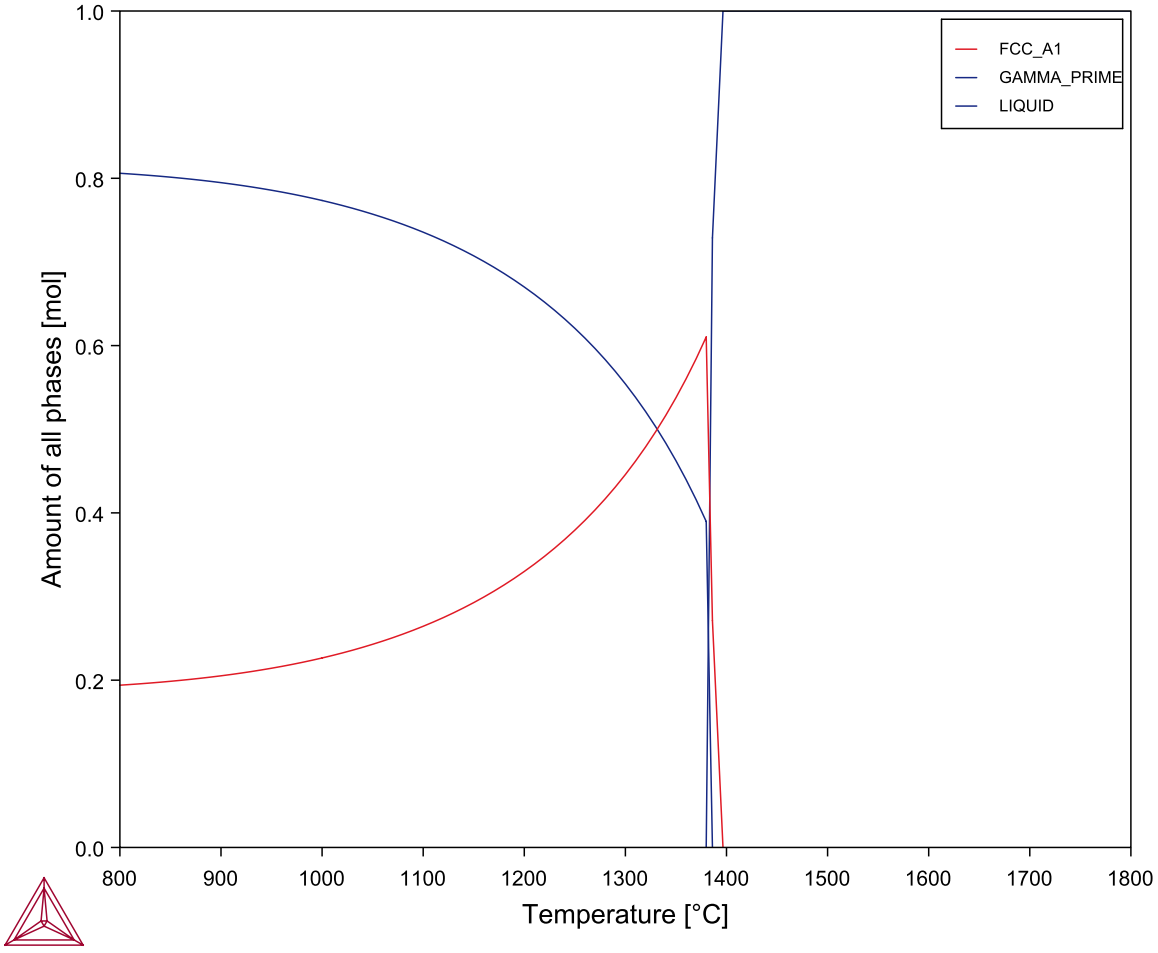

Figure 5: Amount of all phases as a function of temperature generated with *ThermoCalc* (Andersson et al., 2002)

The primary ageing temperature is found at a γ' fraction of approximately 0.60, this

is following the gamma prime curve

5 Appendix

Ni_γ	Al_γ	Ta_γ	Cr_γ	$Ni_{\gamma'}$	$Al_{\gamma'}$	$Ta_{\gamma'}$	$Cr_{\gamma'}$	a_γ	$a_{\gamma'}$	δ
0.8720	0.1156	0.0123	0.0002	0.7908	0.1732	0.0359	0.0001	3.5523	3.5760	0.0066
0.8688	0.1143	0.0121	0.0048	0.7897	0.1732	0.0358	0.0012	3.5525	3.5759	0.0066
0.8656	0.1131	0.0120	0.0094	0.7886	0.1733	0.0357	0.0024	3.5527	3.5758	0.0065
0.8623	0.1118	0.0118	0.0141	0.7875	0.1733	0.0356	0.0036	3.5528	3.5758	0.0064
0.8589	0.1106	0.0117	0.0188	0.7864	0.1733	0.0355	0.0049	3.5530	3.5757	0.0064
0.8555	0.1093	0.0116	0.0237	0.7852	0.1733	0.0354	0.0061	3.5533	3.5757	0.0063
0.8519	0.1081	0.0114	0.0286	0.7840	0.1733	0.0353	0.0074	3.5535	3.5756	0.0062
0.8483	0.1068	0.0113	0.0336	0.7829	0.1733	0.0352	0.0087	3.5537	3.5756	0.0061
0.8446	0.1056	0.0111	0.0386	0.7817	0.1732	0.0351	0.0100	3.5540	3.5755	0.0061
0.8409	0.1044	0.0110	0.0437	0.7804	0.1732	0.0350	0.0113	3.5542	3.5755	0.0060
0.8370	0.1032	0.0109	0.0489	0.7792	0.1732	0.0350	0.0126	3.5545	3.5754	0.0059
0.8331	0.1020	0.0107	0.0542	0.7780	0.1732	0.0349	0.0140	3.5547	3.5754	0.0058
0.8290	0.1008	0.0106	0.0595	0.7767	0.1731	0.0348	0.0153	3.5550	3.5753	0.0057
0.8249	0.0997	0.0104	0.0649	0.7755	0.1731	0.0347	0.0167	3.5553	3.5753	0.0056
0.8207	0.0986	0.0103	0.0704	0.7742	0.1731	0.0347	0.0181	3.5556	3.5753	0.0055
0.8164	0.0975	0.0101	0.0760	0.7729	0.1731	0.0346	0.0194	3.5559	3.5752	0.0054
0.8120	0.0964	0.0100	0.0816	0.7716	0.1730	0.0346	0.0208	3.5562	3.5752	0.0053
0.8075	0.0954	0.0098	0.0872	0.7703	0.1730	0.0345	0.0222	3.5566	3.5752	0.0052
0.8029	0.0944	0.0097	0.0929	0.7689	0.1730	0.0345	0.0235	3.5569	3.5752	0.0051
0.7983	0.0935	0.0095	0.0987	0.7676	0.1730	0.0345	0.0249	3.5573	3.5751	0.0050
0.7935	0.0926	0.0094	0.1045	0.7663	0.1731	0.0344	0.0262	3.5576	3.5751	0.0049
0.7887	0.0917	0.0092	0.1103	0.7649	0.1731	0.0344	0.0276	3.5580	3.5751	0.0048
0.7838	0.0909	0.0090	0.1162	0.7636	0.1731	0.0344	0.0289	3.5584	3.5751	0.0047
0.7789	0.0901	0.0089	0.1221	0.7622	0.1732	0.0344	0.0302	3.5588	3.5751	0.0046
0.7739	0.0894	0.0087	0.1280	0.7609	0.1733	0.0344	0.0314	3.5592	3.5751	0.0045
0.7688	0.0888	0.0085	0.1339	0.7595	0.1734	0.0345	0.0327	3.5596	3.5751	0.0044
0.7637	0.0881	0.0083	0.1398	0.7581	0.1735	0.0345	0.0339	3.5600	3.5751	0.0042
0.7586	0.0876	0.0082	0.1457	0.7568	0.1736	0.0345	0.0351	3.5604	3.5751	0.0041
0.7535	0.0870	0.0080	0.1515	0.7554	0.1737	0.0346	0.0363	3.5608	3.5751	0.0040
0.7483	0.0866	0.0078	0.1573	0.7541	0.1739	0.0346	0.0374	3.5613	3.5752	0.0039
0.7434	0.0862	0.0077	0.1627	0.7528	0.1741	0.0347	0.0384	3.5617	3.5752	0.0038
0.8720	0.1156	0.0123	0.0002	0.7908	0.1732	0.0359	0.0001	3.5523	3.5760	0.0066
0.8721	0.1156	0.0123	0.0000	0.7909	0.1732	0.0359	0.0000	3.5523	3.5760	0.0066

Table 6: 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, $a_{\gamma\mathrm{t}}$ 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
0.8721	0.1155	0.0123	0.0001	0.7908	0.1732	0.0359	0.0001	3.5523	3.5759	0.0066
0.8710	0.1093	0.0138	0.0059	0.7874	0.1714	0.0341	0.0070	3.5550	3.5751	0.0056
0.8682	0.1030	0.0153	0.0135	0.7842	0.1695	0.0328	0.0134	3.5586	3.5744	0.0044
0.8631	0.0966	0.0169	0.0234	0.7809	0.1676	0.0319	0.0196	3.5633	3.5739	0.0030
0.8550	0.0904	0.0184	0.0362	0.7772	0.1658	0.0312	0.0258	3.5694	3.5736	0.0012
0.8430	0.0843	0.0196	0.0530	0.7731	0.1641	0.0307	0.0320	3.5772	3.5734	0.0011
0.8261	0.0790	0.0205	0.0745	0.7682	0.1630	0.0305	0.0383	3.5871	3.5732	0.0039
0.8039	0.0749	0.0207	0.1005	0.7627	0.1625	0.0304	0.0444	3.5990	3.5732	0.0072
0.7779	0.0724	0.0204	0.1293	0.7569	0.1627	0.0304	0.0500	3.6120	3.5732	0.0108
0.7779	0.0724	0.0204	0.1293	0.7569	0.1627	0.0304	0.0500	3.6120	3.5732	0.0108
0.7507	0.0716	0.0196	0.1581	0.7511	0.1636	0.0306	0.0548	3.6251	3.5733	0.0144

Table 7: 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, $a_{\gamma\mathrm{t}}$ 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
0.8719	0.1156	0.0123	0.0003	0.7908	0.1732	0.0359	0.0000	3.5524	3.5760	0.0066
0.8564	0.1141	0.0117	0.0177	0.7866	0.1741	0.0363	0.0030	3.5594	3.5769	0.0049
0.8409	0.1125	0.0111	0.0355	0.7827	0.1750	0.0366	0.0057	3.5666	3.5778	0.0031
0.8323	0.1116	0.0107	0.0455	0.7806	0.1756	0.0368	0.0070	3.5705	3.5783	0.0022
0.8323	0.1116	0.0107	0.0455	0.7806	0.1756	0.0368	0.0070	3.5705	3.5783	0.0022
0.8321	0.1119	0.0106	0.0454	0.7804	0.1759	0.0366	0.0070	3.5705	3.5781	0.0021
0.8315	0.1132	0.0099	0.0454	0.7800	0.1772	0.0357	0.0071	3.5702	3.5777	0.0021
0.8308	0.1145	0.0093	0.0454	0.7795	0.1786	0.0348	0.0071	3.5700	3.5773	0.0020
0.8303	0.1157	0.0087	0.0453	0.7790	0.1798	0.0340	0.0072	3.5698	3.5769	0.0020
0.8719	0.1156	0.0123	0.0003	0.7908	0.1732	0.0359	0.0000	3.5524	3.5760	0.0066
0.8721	0.1156	0.0123	0.0000	0.7909	0.1732	0.0359	0.0000	3.5523	3.5760	0.0066

Table 8: 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, $a_{\gamma\mathrm{t}}$ 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
0.8722	0.1155	0.0123	0.0000	0.7908	0.1732	0.0359	0.0001	3.5523	3.5760	0.0066
0.8732	0.1130	0.0129	0.0008	0.7906	0.1720	0.0349	0.0025	3.5527	3.5759	0.0065
0.8741	0.1105	0.0136	0.0019	0.7904	0.1709	0.0341	0.0047	3.5531	3.5760	0.0064
0.8749	0.1078	0.0142	0.0031	0.7902	0.1697	0.0334	0.0067	3.5536	3.5760	0.0063
0.8755	0.1052	0.0148	0.0046	0.7900	0.1685	0.0327	0.0087	3.5542	3.5761	0.0061
0.8759	0.1024	0.0154	0.0063	0.7899	0.1673	0.0322	0.0107	3.5549	3.5762	0.0060
0.8762	0.0995	0.0160	0.0083	0.7897	0.1661	0.0317	0.0126	3.5557	3.5763	0.0058
0.8762	0.0965	0.0167	0.0107	0.7895	0.1648	0.0313	0.0144	3.5567	3.5764	0.0055
0.8759	0.0934	0.0173	0.0134	0.7892	0.1636	0.0309	0.0163	3.5578	3.5766	0.0053
0.8753	0.0901	0.0180	0.0166	0.7888	0.1624	0.0306	0.0182	3.5591	3.5768	0.0050
0.8744	0.0867	0.0186	0.0203	0.7884	0.1611	0.0304	0.0201	3.5606	3.5771	0.0046
0.8729	0.0832	0.0193	0.0246	0.7878	0.1599	0.0302	0.0221	3.5623	3.5774	0.0042
0.8711	0.0797	0.0199	0.0293	0.7871	0.1588	0.0300	0.0241	3.5642	3.5777	0.0038
0.8722	0.1155	0.0123	0.0000	0.7908	0.1732	0.0359	0.0001	3.5523	3.5760	0.0066
0.8721	0.1156	0.0123	0.0000	0.7909	0.1732	0.0359	0.0000	3.5523	3.5760	0.0066

Table 9: 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)

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