Commentary on the Thermodynamics of a Super-alloy System (Al-Ni-Cr) Using the Thermocalc Databases

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Abstract: The present study aims to comprehend the thermodynamics of the Al-Ni-Cr superalloy system utilizing the latest Thermocalc 2022b databases. Thermocalc is a software that has a large database which has become vast over the years. The thermodynamic behavior and stability of the system were examined under varying conditions, including temperature and composition. The findings of this study provide crucial insight into the phase behavior and stability of the Al-Ni-Cr superalloy system, which can inform the optimization of its properties and performance for various industrial applications, compared to previous studies and research. The results of this study contribute to a deeper understanding of the thermodynamics of superalloy systems and can be of great benefit to the materials science and engineering communities. The databases used for the binary systems were NIDEMO v2.0 (Nickel Demo database v2.0, including Ni, Cr, and Al - a subset of TCNI) and TCBIN V1.1 (TC Binary Solutions Database, Version 1.0), while for the ternary systems, NIDEMO V2.0 and PURE 5SGTE V5.1 (Pure Elements - Unary Database, Scientific Group Thermodata Europe) were used. The results here demonstrate the great benefits of studying the thermodynamics of this alloy through available database systems and comparing the results with experimental studies.

Keywords: Thermodynamics, Super-alloys, Thermocalc, Al-Ni-Cr, Ternary, Binary

I. Introduction

Thermodynamics is an essential aspect of materials science and engineering, providing insight into the behavior and stability of materials at different temperatures and compositions. This information is crucial for optimizing the processing conditions and ensuring the reliability of materials in high-temperature and corrosive environments. One such material system is the Al-Ni-Cr super-alloy, which is composed of aluminum as the primary element and nickel and chromium as the main alloying elements. The Al-Ni-Cr alloy is a type of superalloy that is known for its high strength and corrosion resistance at elevated temperatures. It is commonly used in applications such as aerospace and power generation, where it is subjected to extreme environments and high mechanical stresses. Overall, Al-Ni-Cr alloys are a versatile and widely-used type of alloy that offers a combination of high strength, corrosion resistance [4], and good thermal and electrical conductivity. These properties make them an ideal material for a range of applications in a variety of industries.

The phase diagram for Al-Ni-Cr alloys is complex and involves several phases that can coexist in equilibrium at different temperatures and compositions [5]. At high temperatures, the alloys exist in a single-phase solid solution. As the temperature is lowered, various phases may form, including intermetallic, precipitates, and solid solutions. The phase diagram for Al-Ni-Cr alloys is important because it helps predict the microstructure and properties of the material at different temperatures and compositions [1].

One of the key phases found in Al-Ni-Cr alloys is the Ni3Al intermetallic compound, which has a high melting point and is known for its excellent corrosion resistance. The presence of Ni3Al in the microstructure of these alloys can significantly improve their corrosion resistance compared to pure aluminum alloys.

In every field, there is a paradigm shift towards conforming to the latest technology [2. Software is a necessary tool, and databases provide easy access to the best data for simulation. [3]. This study uses different databases from the latest Thermocalc 2022b database to reproduce some of the diagrams as found on the ASM Alloy Phase Diagram Database. Some diagrams were not found on ASM on this alloy system although several studies had initially been made on it. This database includes PURE 5SGTE V5.1, TCBIN V1.1 Database and NIDEMO V2.0 [13-15]. These databases contain the elements we need to form our alloy system. In the ASM Alloy Phase Diagram Center database, there are several binary phase diagrams, pseudo-binary phase diagrams, and ternary phase diagrams for this alloy system. We will be having a commentary view on the thermodynamics of this alloy system design with this database as given by Thermocalc.

II. The Work and Commentary

The thermodynamics of super-alloys is a crucial aspect in determining their performance and reliability in high-temperature and corrosive environments. One such super-alloy system is Al-Ni-Cr, which is a mixture of aluminum, nickel, and chromium. In this

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commentary, we are exploring the phase behavior of Al-Ni-Cr by considering two databases from Thermo-Calc and examining the phase diagram, liquidus temperature, pseudo-binary, and ternary aspects of the system.

The phase diagram of Al-Ni-Cr provides insight into the stability and behavior of the different phases present in the system at various temperatures and compositions. By examining the phase diagram, we can determine the conditions under which the different phases are in equilibrium, and predict the microstructure of the Al-Ni-Cr system. The liquidus temperature is also an important aspect to consider as it determines the temperature range at which the system is fully liquid, and thus, easy to cast and shape.

Pseudo-binary diagrams are a useful tool for understanding the effect of composition on the Al-Ni-Cr system. They provide a simplified representation of the system by assuming a binary relationship between two of the elements, and can help to understand the effect of adding nickel and chromium to aluminum on the phase behavior of the system.

Ternary diagrams provide a more comprehensive view of the Al-Ni-Cr system by considering the three elements in combination. These diagrams can help to understand the effect of the relative proportions of aluminum, nickel, and chromium on the phase behavior and stability of the system. We are going to reproduce these diagrams with the Thermocalc database.

A. Binary Phase

Here, two databases were used, NIDEMO v2.0 and TCBIN V1.1. References were made to the same phase diagram on ASM database. The available diagrams were reproduced while others were generated accordingly. The eutectic temperature (temperature where liquid and solid phases coexist) was consistently considered in all databases.

i. Al-Ni system:

The Al-Ni phase diagram shows the phases that are present in the Al-Ni alloy system at different compositions and temperatures. This phase diagram exhibits a eutectic reaction at 1365°C and different compositions, where liquid and solid phases coexist. [6] There is also an eutectic reaction also at 642°C. The solid phases present in this alloy system include the alpha-Al (fcc) (face-centred cubic) and gamma-Ni (fcc) phases, as well as the intermetallic phases Al3Ni and AlNi. As the temperature increases, the solid solution phase becomes unstable and undergoes a eutectoid reaction to form the Al2Ni (L12) intermetallic phase and the Ni (FCC) phase. At higher temperatures, the Al2Ni phase transforms into the AlNi (L10) intermetallic phase. [10]

ii. Al-Cr system:

This binary phase diagram in the database shows the phases that are present in the Al-Cr alloy system at different compositions and temperatures. This phase diagram exhibits a eutectic reaction at 870°C and different composition, where liquid and solid phases coexist [6][7]. The solid phases present in this alloy system include the alpha-Al (fcc) and gamma-Cr (bcc, body-centred cubic) phases, as well as the intermetallic phases Al3Cr and AlCr.

iii. Ni-Cr system:

The Ni-Cr binary phase diagram shows that at low temperatures, the alloy exists in the solid solution of Ni-Cr solid solution (FCC) phase. As the temperature increases, the solid solution phase becomes unstable and undergoes a eutectoid reaction to form the Ni2Cr (L12) intermetallic phase and the Cr (BCC) phase [8][9][11][12].

We are going to have the phase diagrams now reproduced from Thermocalc. The diagrams are marked with the eutectic temperature as calculated by Thermocalc. Looking at the TCBIN V1.1 database (TC Binary Solutions Database, Version 1.0), which is essentially for binary solutions, we can reproduce these diagrams.

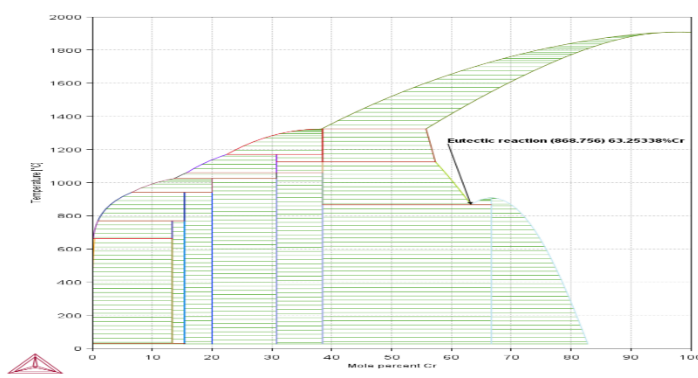

Fig 1: Al-Ni binary phase diagram (TCBIN V1.1)

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System

Moles	1.00000	
Mass	42.80420	[g]
Temperature	1141.90598	[K]
Total Gibbs Energy	-61870.21623	[J]
Enthalpy	15315.86362	[J]
Volume	0.00000	[m³]

Component	*Mole Fraction*	*Mass Fraction*	*Activity*	*Potential*
Al	0.36747	0.23164	0.09534	-22314.73234
Cr	0.63253	0.76836	0.34081	-10219.92245

Stable Phases

	Moles	*Mass*	*Volume Fraction*	
BCC_A2#1	1.00000	42.80420	0.00000	Composition

Composition

Component	*Mole Fraction*	*Mass Fraction*
Cr	0.63253	0.76836
Al	0.36747	0.23164

Fig 2: Al-Ni binary phase description at 1141.9 K Eutectic (TCBIN V1.1)

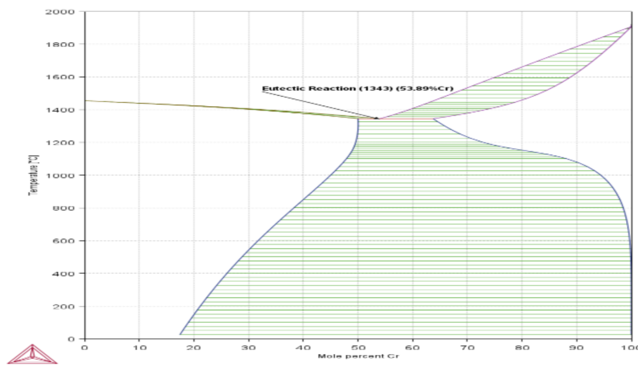

Fig 3: Ni-Cr binary phase diagram (TCBIN V1.1)

System

Moles	1.00000	
Mass	55.08247	[g]
Temperature	1616.29863	[K]
Total Gibbs Energy	-91757.09309	[J]
Enthalpy	49396.14825	[J]
Volume	0.00000	[m³]

Component	*Mole Fraction*	*Mass Fraction*	*Activity*	*Potential*
Ni	0.46108	0.49128	0.34491	-14305.04930
Cr	0.53892	0.50872	0.78989	-3169.68534

Stable Phases

	Moles	*Mass*	*Volume Fraction*	
BCC_A2#1	0.28044	15.26062	0.00000	Composition

Composition

Component	*Mole Fraction*	*Mass Fraction*
Cr	0.63842	0.61002
Ni	0.36158	0.38998

Fig 4: Ni-Cr binary phase description at 1616.3K Eutectic (TCBIN V1.1)

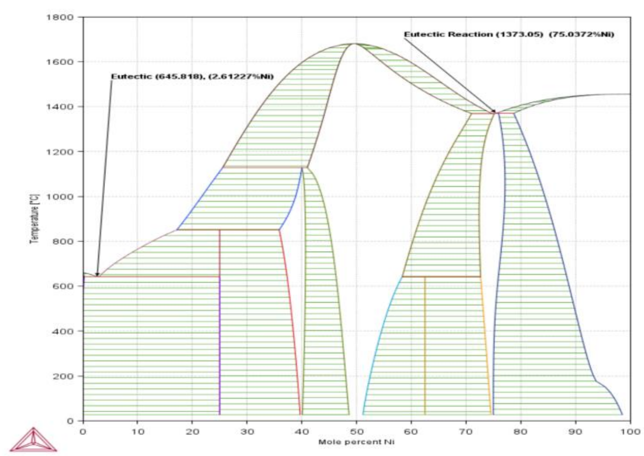

Fig 5: Al-Ni binary phase diagram (TCBIN V1.1)

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Moles	1.00000			
Mass	50.87895	[g]		
Temperature	1646.19661	[K]		
Total Gibbs Energy	-1.25645E5	[J]		
Enthalpy	25023.55428	[J]		
Volume	0.00000	[m³]		
Component	*Mole Fraction*	*Mass Fraction*	*Activity*	*Potential*
Al	0.24634	0.13064	0.00032	-1.10083E5
Ni	0.75366	0.86936	0.54271	-8365.50114
Stable Phases				
	Moles	*Mass*	*Volume Fraction*	
LIQUID#1	1.00000	50.87895	0.00000	Composition
Composition				
Component	*Mole Fraction*	*Mass Fraction*		
Ni	0.75366	0.86936		
Al	0.24634	0.13064		

Fig 6: Al-Ni binary phase description at 1646.19K Eutectic 1 (TCBIN V1.1)

System				
Moles	1.00000			
Mass	27.81030	[g]		
Temperature	918.96832	[K]		
Total Gibbs Energy	-41002.26768	[J]		
Enthalpy	24552.72385	[J]		
Volume	0.00000	[m³]		
Component	*Mole Fraction*	*Mass Fraction*	*Activity*	*Potential*
Al	0.97388	0.94487	0.99473	-40.36926
Ni	0.02612	0.05513	3.04528E-9	-1.49833E5
Stable Phases				
	Moles	*Mass*	*Volume Fraction*	
LIQUID#1	1.00000	27.81030	0.00000	Composition
Composition				
Component	*Mole Fraction*	*Mass Fraction*		
Al	0.97388	0.94487		
Ni	0.02612	0.05513		

Fig 7: Al-Ni binary phase description at 918.96 Eutectic 2 (TCBIN V1.1)

Now, we reproduce these on the NIDEMO v2.0 (Nickel Demo database v2.0) Database.

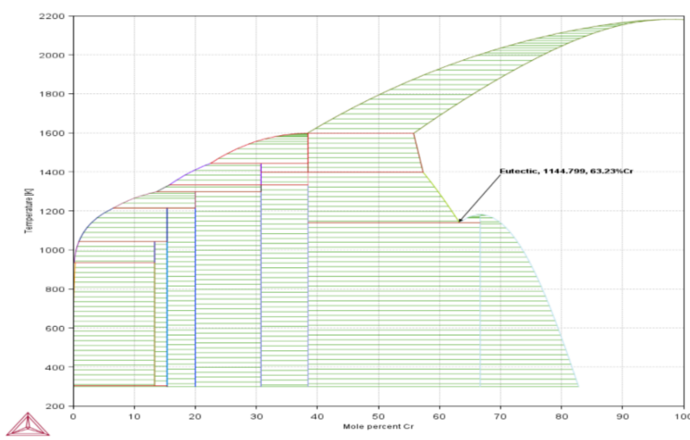

Fig 8: Al-Cr binary phase diagram (NIDEMO v2.0)

Moles	1.00000			
Mass	42.79917	[g]		
Temperature	1144.38960	[K]		
Total Gibbs Energy	-62041.84834	[J]		
Enthalpy	15397.71582	[J]		
Volume	8.25815E-6	[m³]		
Component	*Mole Fraction*	*Mass Fraction*	*Activity*	*Potential*
Al	0.36767	0.23179	0.09576	-22321.15541
Cr	0.63233	0.76821	0.34105	-10235.48141
Stable Phases				
	Moles	*Mass*	*Volume Fraction*	
BCC_B2#2	1.00000	42.79917	1.00000	Composition
Composition				
Component	*Mole Fraction*	*Mass Fraction*		
Cr	0.63233	0.76821		
Al	0.36767	0.23179		

Fig 9: Al-Cr binary phase description at 1144.38K Eutectic (NIDEMO v2.0)

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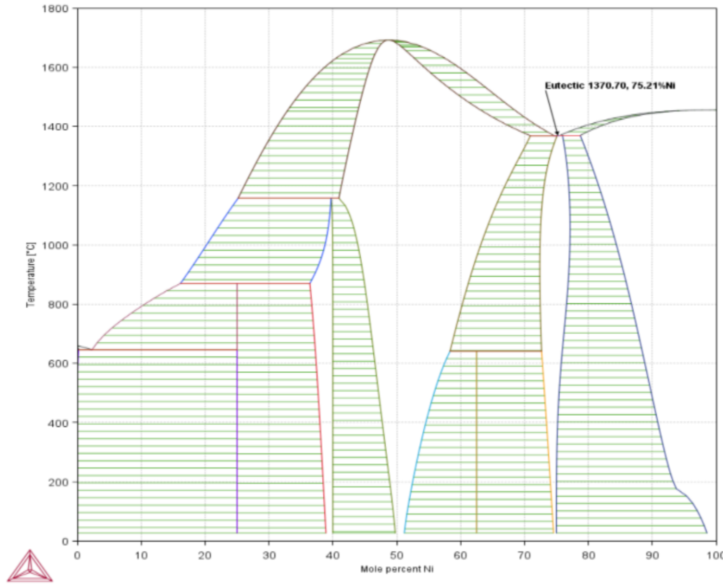


Fig 10: Al-Ni binary phase diagram (NIDEMO v2.0)

Moles	1.00000			
Mass	50.83041	[g]		
Temperature	1643.85071	[K]		
Total Gibbs Energy	-1.25576E5	[J]		
Enthalpy	24731.09201	[J]		
Volume	7.64949E-6	[m³]		
Component	*Mole Fraction*	*Mass Fraction*	*Activity*	*Potential*
Al	0.24787	0.13158	0.00033	-1.09723E5
Ni	0.75213	0.86842	0.53868	-8455.44530
Stable Phases				
	Moles	*Mass*	*Volume Fraction*	
LIQUID#1	1.00000	50.83041	1.00000	Composition
Composition				
Component	*Mole Fraction*	*Mass Fraction*		
Ni	0.75213	0.86842		
Al	0.24787	0.13158		

Fig 11: Al-Ni binary phase description 1643.85K Eutectic (NIDEMO v2.0)

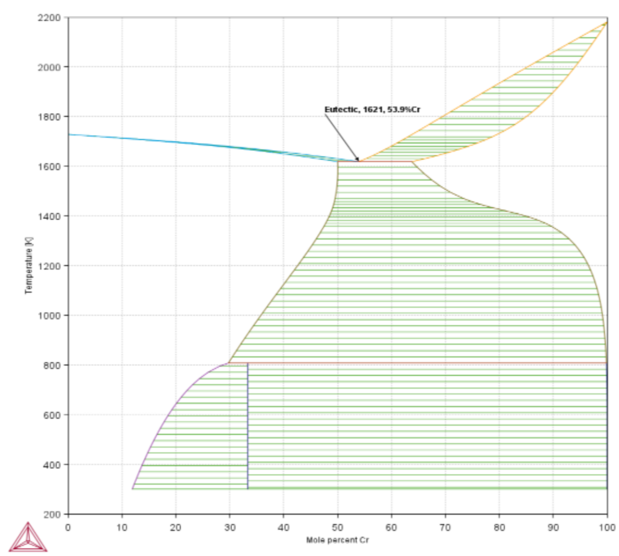
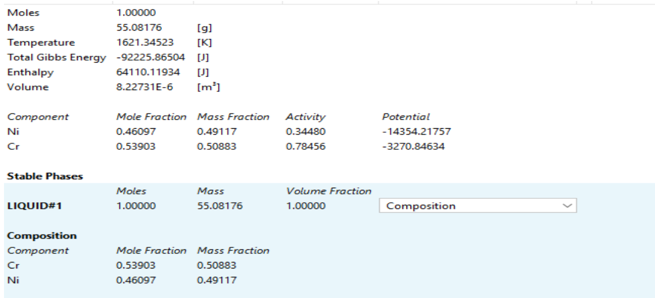


Fig 12: Ni-Cr binary phase diagram (NIDEMO v2.0)



Moles	1.00000			
Mass	55.08176	[g]		
Temperature	1621.34523	[K]		
Total Gibbs Energy	-92225.86504	[J]		
Enthalpy	64110.11934	[J]		
Volume	8.22731E-6	[m³]		
Component	*Mole Fraction*	*Mass Fraction*	*Activity*	*Potential*
Ni	0.46097	0.49117	0.34480	-14354.21757
Cr	0.53903	0.50883	0.78456	-3270.84634
Stable Phases				
	Moles	*Mass*	*Volume Fraction*	
LIQUID#1	1.00000	55.08176	1.00000	Composition
Composition				
Component	*Mole Fraction*	*Mass Fraction*		
Cr	0.53903	0.50883		
Ni	0.46097	0.49117		

Fig 13: Ni-Cr binary phase description at 1621.34K Eutectic (NIDEMO v2.)

All the phase diagrams have a table description that shows the mole and mass fraction of the binary formation of these compounds.

B. Ternary Phase Diagram

The ASM Alloy Phase Diagram Center database also includes a ternary phase diagram for the Al-Ni-Cr alloy system, which shows the phase relationships among the three main constituents at various temperatures and compositions [4]. This phase diagram exhibits a eutectic reaction at 1410°C and a composition of 54.5% Al, 33.5% Ni, and 12% Cr, where liquid and solid phases coexist.

The solid phases present in this phase diagram are the γ-Ni, γ-Fe, and γ-Cr phases, which form a three-phase region at low temperatures, and the ε-AlNi, ε-AlNiCrFe, and θ-AlCr phases, which form at higher temperatures. The diagram shows that at low concentrations of aluminum and nickel, the dominant phase is a solid solution of chromium in aluminum and nickel, with small amounts of the intermetallic phases Al3Cr, AlCr, and Cr3Al. As the concentration of aluminum and nickel increases, the dominant phase becomes a solid solution of aluminum in nickel and chromium, with small amounts of the intermetallic phases Al3Ni, AlNi, and AlNi3 [10].

Ternary, liquidus projection

This projection is useful for understanding the phase diagram for these alloys, which can help predict their behavior during solidification and cooling. In general, as the temperature decreases, the alloys will start to solidify at a certain temperature, known as the liquidus temperature [10].

On Thermocalc, NIDEMO V2.0 and PURE 5SGTE V5.1 are the databases used for the following ternary diagrams. These databases contain the three elements needed in the formation of the alloy-system.

i. NIDEMO V2.0 (Nickel Demo database v2.0):

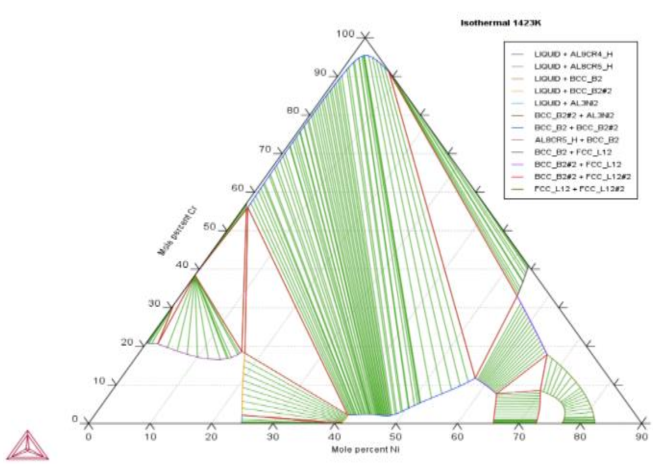


Fig 14: Al-Ni-Cr ternary phase diagram (NIDEMO v2.0)

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Fig 14 shows the isothermal phase diagram (1423K) for the Al-Ni-Cr for the ternary alloy system. The legend reveals different phases in the ternary system. The formation of Al-Ni-Cr takes different phases, forming the solidus and liquidus as well. The mole percent of the constituent elements were also revealed.

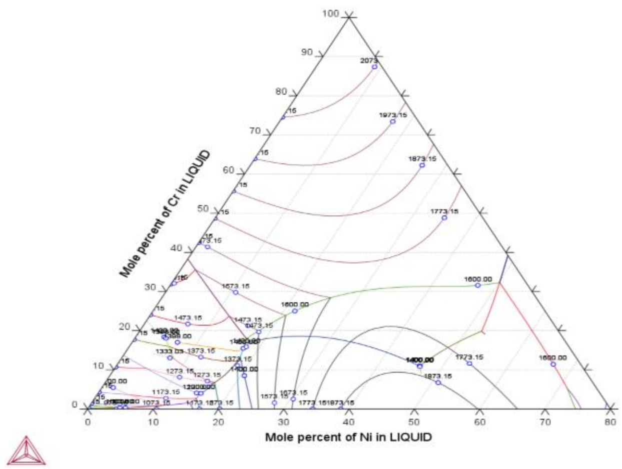

Fig 15: Al-Ni-Cr liquidous projection (NIDEMO v2.0)

From Fig 15, the liquidus projection is calculated with Thermocalc for the Al-Ni-Cr alloy. The green lines are univariant equilibria and red lines are isotherms. These temperatures are very important in the formation of the alloy.

ii. PURE 5SGTE V5.1 (Pure Elements (Unary) Database Scientific Group Thermodata Europe):

This database contains almost all elements in the periodic table. It is a database for pure unary elements, but can also be used to evaluate ternary diagrams.

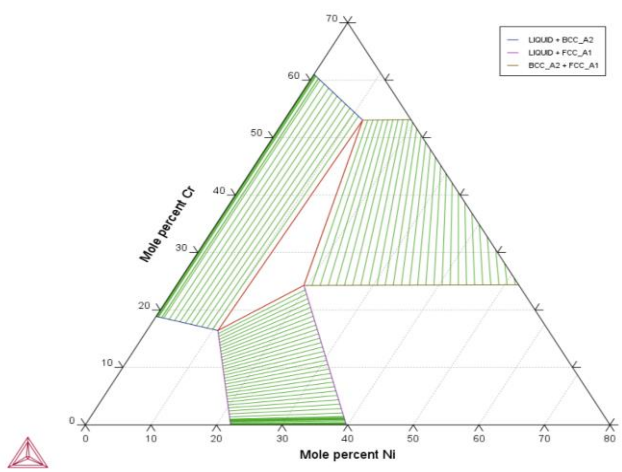

Fig 16: Al-Ni-Cr ternary diagram (PURE 5SGTE V5.1.)

Fig 16 shows the isothermal phase diagram (1423K) for the Al-Ni-Cr for the ternary alloy system in the PURE 5SGTE V5.1 database. This database does not give more information about the transformation as NIDEMO because it was not designed for metal-based alloys but pure elements.

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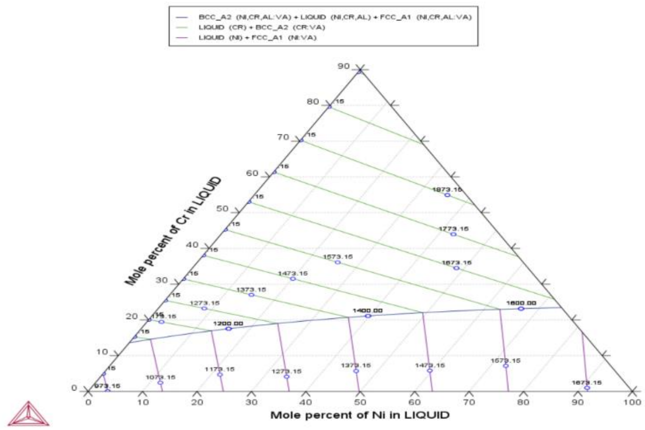

Fig 17: Al-Ni-Cr liquidous projection (PURE 5SGTE V5.1.)

III. Conclusion

In conclusion, the Al-Ni-Cr super-alloy system is a complex and important aspect of materials science and engineering. Thermocalc provides free educational access to a comprehensive database for studying this system, allowing for improvements over previous works. Comparing the results obtained from different databases showed that while there were some variations, the results from Thermocalc were more reliable than those from experimental methods, as they were calculated and less prone to human errors. A deep understanding of the thermodynamics of this system is crucial for optimizing processing conditions, ensuring the reliability of the super-alloy in various applications, and conducting further research in this area. The phase diagram, liquidus temperature, pseudo-binary and ternary diagrams, and other thermodynamic parameters provide valuable information about the behavior and stability of the Al-Ni-Cr super-alloy, and are essential for understanding the behavior of this system. Further research in this area is necessary to advance our understanding of the Al-Ni-Cr super-alloy system and to develop new and improved alloys for use in high-temperature and corrosive environments.

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