

WELDABILITY OF NICKEL-BASED ALLOYS: SOLVING PROBLEMS WITH THE ASSISTANCE OF COMPUTATIONAL TECHNIQUES

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INTRODUCTION

Nickel-based alloys are valued for their excellent combination of strength and corrosion resistance. However, weldability concerns can limit their potential. Engineers must select the right combination of joint geometry, welding process, alloy type and heat treatment to avoid potential problems, something often determined only after costly trial and error testing. In the last 30 years, computational thermodynamics tools have become invaluable to help solve the challenges related to the welding of nickel-based (Ni-based) alloys.

This paper highlights four areas where the use of computational thermodynamic software has been an important part of the engineer's toolbox to help solve weldability challenges.

Challenge 1: Resistance to Weld Cracking

Many Ni-based alloys are susceptible to different weld cracking phenomena that can be sensitive to alloy chemistry. During the solidification of weld metal, the alloying elements segregate to either the liquid or the solid and cause local composition differences. Segregation of aluminium (Al), titanium (Ti) and/or niobium (Nb) causes local variances in gamma prime (γ') and gamma double prime (γ'') precipitation kinetics and volume fractions, leading to a loss of creep strength^[1]. Depending on alloy chemistry, this segregation can also cause formation of low melting point eutectics, which can then cause solidification cracking^[2].

Challenge 2: Post Weld Heat Treatments

The segregation during solidification is typically unavoidable during welding. A solution heat treatment can be applied to smooth the composition gradients, but this is not always practical. Choosing the right time and temperature can be a time consuming trial and error process.

Challenge 3: Pitting Corrosion Resistance

The segregation of alloying elements during solidification can also be detrimental to other properties such as pitting corrosion resistance. For example, the segregation of molybdenum (Mo) during solidification can lead to local pitting corrosion in areas depleted of Mo, which can cause local corrosive attack.

Challenge 4: HAZ Liquation Cracking

Weldability challenges are not always limited to the weld metal. In the heat affected zone (HAZ), liquation cracking can occur depending on the alloy chemistry, weld thermal cycle and the pre-existing microstructure.

DESIGN NEW ALLOYS WITH RESISTANCE TO WELD CRACKING

The nuclear power industry now uses Ni-based filler metals with 30wt%Cr (AWS ENiCrFe-7) to mitigate primary water stress corrosion cracking issues discovered with 20wt%Cr alloys (AWS ENiCrFe-3). These high Cr filler metals are

susceptible to either solidification cracking or ductility dip cracking (DDC). Susceptibility is related to the Nb content. Nissley and Lippold showed that alloys with higher Nb (2-3wt%) are generally resistant to DDC as a eutectic is formed at the end of solidification, creating tortuous solidification grain boundaries [3]. However, Dupont and Alexandrov showed that the higher Nb causes an expansion of the solidification temperature range, increasing susceptibility to solidification cracking [4, 5]. Alloys with lower Nb (0-2wt%), have the opposite problem: these are resistant to solidification cracking but susceptible to ductility dip cracking.

There does not seem to be a level of Nb in these high Cr Ni-based filler metals that can be used to simultaneously diminish both forms of weld cracking. However, alternative eutectic forming elements could potentially generate sufficient eutectic to resist DDC, while maintaining a narrow solidification temperature range (STR) to prevent solidification cracking. Hope and Lippold devised a methodology to select and optimise a filler metal composition using a combination of computational and experimental techniques [6].

Hope and Lippold calculated pseudo-binary phase diagrams with various eutectic forming elements in a Ni-30Cr system [6]. They showed the eutectics that may form as well as determined the lowest terminal eutectic temperature possible for each element. Systems with low terminal eutectic temperatures are likely to have a wide STR as compositions are not near the eutectic composition. The plots in Figure 1 are calculated using Thermo-Calc and Table 1 summarises the terminal eutectic temperatures of systems containing the elements tantalum (Ta) and hafnium (Hf), chosen as potential candidates and compared to Nb.

After identifying potential candidates, the Scheil simulation determined the STR and fraction eutectic for more specific alloy chemistries. The authors used this simulation in combination with a design of experiment methodology to help reduce the number of alloys that needed to be

created in the lab [7]. Some compositions were tested experimentally, with a novel arc melting/thermocouple plunging technique to determine the non-equilibrium STR. The fraction eutectic was verified using metallographic image analysis. Using this combined experimental and computational technique, the authors optimised a few filler metal compositions with improved weldability, which can be produced and tested on a commercial scale.

Table 1: Summary of terminal eutectic temperatures determined from calculated pseudo-binary phase diagrams [6].

	γ -MC eutectic (°C)	γ -Laves eutectic (°C)	γ -Ni ₇ Hf ₂ eutectic (°C)
Nb	1280	1160	
Ta	1330	1190	
Hf	1310		1250

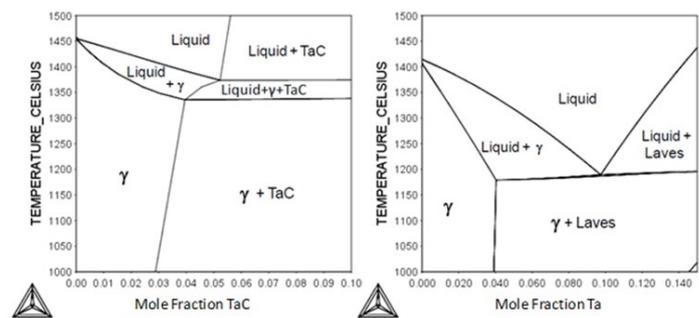


Figure 1: Pseudo-binary phase diagrams for a Ni-30Cr-Ta bearing system. Calculated with Thermo-Calc and TTN17 database [10].

SIMULATE POST WILD HEAT TREATMENTS OF SUPERALLOY WELDS

The power generation industry aims to design power plants with higher operating temperatures and pressures, with a goal to improve efficiency and reduce CO₂ emissions. For example, an Advanced Ultra Supercritical (A-USC) plant is designed to run at temperatures between 700-760°C and at pressures of 35-45MPa. These conditions demand the use of γ' strengthened Ni-based alloys for the hottest sections of the power plant, making the creep strength and coal ash corrosion resistance an important material property concern.

The Special Metals Corporation (New Hartford, U.S.A.) developed the INCONEL[®] alloy 740H to fill this need. It is based on an aircraft alloy, NIMONIC[®] alloy 263, with modifications to improve coal ash corrosion resistance. However, even after aging treatment, welds made on this alloy have a lower creep strength than the base material^[8]. Extensive investigations done by Bechetti, Tung, and others found that segregation during solidification plays a major role in the reduction of weld metal creep strength^[9-11]. These authors used Thermo-Calc Scheil simulation results in a Diffusion module (DICTRA) simulation and determined an optimal homogenisation treatment.

The Scheil simulation for INCONEL[®] alloy 740H is shown in Figure 2. Bechetti et al. found that the results closely aligned with energy dispersive spectroscopy (EDS) scans across dendrites in the weld metal^[10]. Such a composition profile, along with the width of the dendrite obtained from the EDS scans, is used as the starting condition for a DICTRA homogenisation model^[9]. Figure 3 also shows the Nb concentration across a half dendrite for a simulated heat treatment at 1100°C for different time conditions. Only the slowest diffusing element, Nb, is displayed on the plot and it shows that at least one hour is needed to homogenise the material. This solutionising treatment is performed before the aging treatment and leads to a more even γ' distribution in the weld.

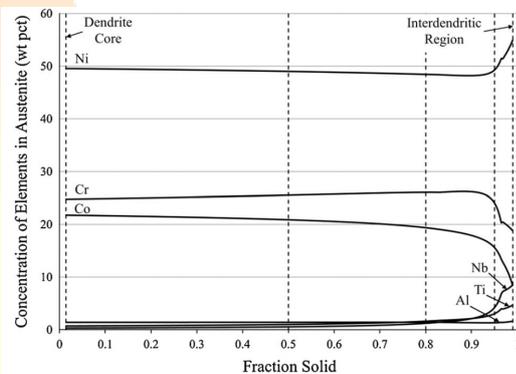


Figure 2: A Thermo-Calc Scheil simulation using the TTNI7 database showing elemental segregation across a half dendrite in INCONEL[®] alloy 740H^[10].

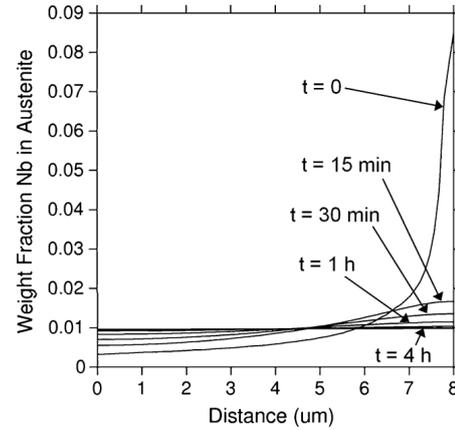


Figure 3: A DICTRA simulation of the homogenisation of Nb in INCONEL[®] alloy 740H with a half-dendrite at 1100°C for different times^[9].

OPTIMISE PITTING CORROSION RESISTANCE OF WELD METAL

Many commercially available stainless steels and Ni-based alloys contain significant amounts of Mo (>5wt%) for good corrosion and pitting corrosion resistance. When arc welding autogenously or with matching filler metals on these materials, Mo segregates to the liquid during solidification. This leaves the dendrite core depleted in Mo, causing preferential local corrosive attack in the weld metal. Ni-based weld metals such as INCONEL[®] alloys 625 (IN625) and 622 (IN622) are widely used to mitigate this issue as these alloys have higher levels of Mo (~9 and ~14wt%, respectively).

The segregation of Mo still occurs during solidification. However, the level of Mo at the dendrite core is high enough to lessen preferential attack, but such alloys can be expensive because of the added cost of Mo.

For engineers developing or selecting materials with good pitting corrosion resistance, there are empirical relationships developed that seek to rank alloys based on composition. The *Pitting Resistance Equivalent Number* (PREN) is one example^[12]. The following equation is specific to Ni-based alloys:

$$PREN = \%Cr + 3.3(\%Mo + 0.5\%W)$$

This relationship shows that tungsten (W) is also more effective than chromium (Cr) in preventing pitting corrosion. However, unlike Mo, W segregates to the solid during solidification. Since it also increases pitting corrosion resistance, additions of W can help counteract the loss of corrosion resistance associated with low Mo in the dendrite cores.

Segregation during welding can easily be predicted using the Scheil equation coupled with thermodynamic databases. Thuvander et al. varied concentrations of W and Mo in different weld mock-ups and measured segregation using EDS^[13]. They also predicted the segregation using the Scheil module in Thermo-Calc and found good agreement with the EDS results.

Conceivably, one can optimise an alloy composition for cost and corrosion resistance by simulating a matrix of compositions with the Thermo-Calc Scheil module. A 'good' PREN value is typically >40. By calculating the PREN at all points from the dendrite core to the dendrite boundary (taken from the Scheil results), compositions are identified that satisfy this condition.

Based on the alloying content these compositions can then be evaluated for cost. An example of a Scheil calculation for a Ni-30Cr-3Mo-3W is shown in Figure 4, where the maximum extent of segregation during solidification across a hypothetical dendrite is predicted.

The dendrite core composition is at fraction solidified, $f_s=0$, while the dendrite boundary composition is at $f_s=1$. From Figure 5, a wrought alloy with 20Cr and 6Mo is expected to have a PREN of 40, but segregation during solidification reduces the corrosion resistance of the dendrite core. By substituting 3Mo for 3W, the PREN of the wrought composition drops to 35, but due to the segregation effect it is above 40 everywhere across the dendrite.

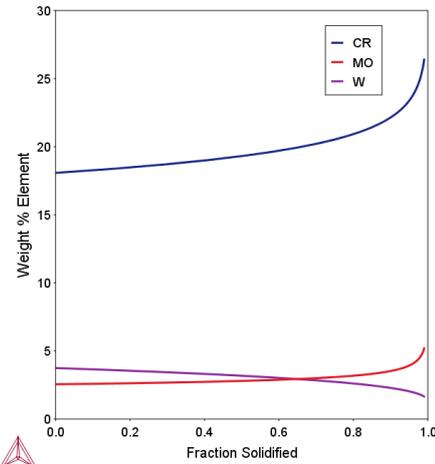


Figure 4: A Scheil simulation performed in Thermo-Calc using the TCNI8 database, showing elemental segregation due to solidification across a dendrite for a Ni-20Cr-3Mo3W alloy.

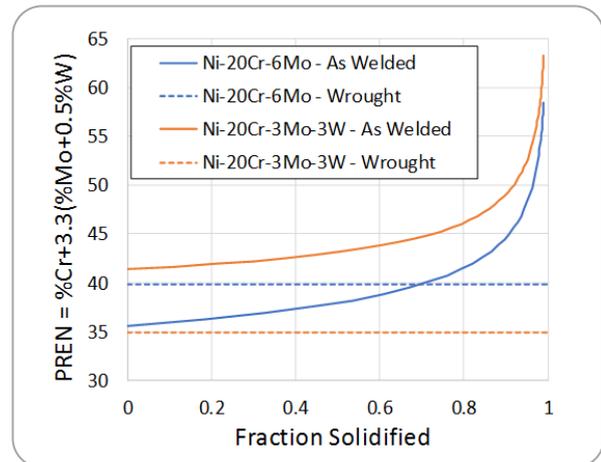


Figure 5: A PREN calculation across a dendrite using a composition from a Scheil simulation for a Ni-20Cr-3Mo-3W alloy and a Ni-20Cr-6Mo alloy. PREN for the wrought compositions is plotted with dashed lines.

CHOOSE WELDING PARAMETERS TO AVOID HAZ LIQUATION CRACKING

Typically, welds on γ' -strengthened alloys are done in the solution annealed condition. Sometimes this is not practical due to part geometries or other constraints. Depending on the welding process parameters, γ' in the heat affected zone (HAZ) can liquate and cause liquid film formation at grain boundaries, which leads to cracking. This is known as constitutional liquation and involves the partial dissolution of a particle. The subsequent enrichment of solute

around the particle depresses the melting point to be lower than the nominal melting temperature^[14]. This is an inherently non-equilibrium phenomena that occurs under high heating rates. If the heating rate is slow enough, solute diffuses away from the particle, which prevents local enrichment and melting.

Tancret describes a process using Thermo-Calc and DICTRA to predict liquation for a given alloy composition and thermal cycle^[15]. The thermodynamic modelling can be used to determine the maximum possible heating rate to prevent liquation. When this limit is known, finite element modelling can be used to optimize the welding parameters to stay below this critical heating rate.

SUMMARY

Solving weldability challenges does not have to be a reactive process. Proper planning and exploration using a combination of computational modelling and experimental trials can prevent issues before they arise. For long term research and development, these techniques can speed up the development cycle, reduce the number of experiments that need to be performed as well as reduce costs.

REFERENCES

1. Siefert, J., et al., Science and Technology of Welding and Joining, 2016. **21**(5): p. 397-427.
2. Lippold, J.C. 2014: Wiley.
3. Nissley, N. and J. Lippold, Welding Journal, 2008. **87**(10): p. 257s-264s.
4. Alexandrov, B.T., et al., Welding in the World, 2011. **55**(3-4): p. 65-76.
5. DuPont, J., C. Robino, and A. Marder, Welding Journal, 1998.
6. Hope, A.T. and J.C. Lippold, Welding in the World, 2017. **61**(2): p. 325-332.
7. Fusner, E., A. Hope, and J. Lippold, Welding journal, 2014. **93**(5).
8. Tortorelli, P., et al. in *Advances in Materials Technology for Fossil Power Plants: Proceedings from the Seventh International Conference, October 22-25, 2013 Waikoloa, Hawaii, USA*. 2014. ASM International.
9. Bechetti, D.H., J.N. DuPont, and B.A. Baker, Metallurgical and Materials Transactions A, 2014. **45**(7): p. 3051-3063.
10. Bechetti, D.H., et al., Metallurgical and Materials Transactions A, 2015. **46**(2): p. 739-755.
11. Tung, D.C. and J.C. Lippold, Superalloys 2012, 2012: p. 563-567.
12. Szklarska-Smialowska, Z. and ZS-Smialowska. 2005: NACE International Houston, TX.
13. Thuvander, M., L. Karlsson, and B. Munir, Stainless Steel World, 2004. **16**: p. 52-57.
14. Owczarski, W., D. Duvall, and C. Sullivan, WELD J, 1966. **45**(4): p. 145.
15. Tancret, F., Computational Materials Science, 2007. **41**: p. 13-19.



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