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Modelling of Super Alloy with Different Alloying Elements Using Multi-Scale Designer

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Abstract

Super alloys are alloys that can be used at 0.7 times of their melting temperature and will usually operate in the range of 1050°C to 1200°C. It becomes important that the high temperature alloys should possess high strength, creep resistance, resistance to oxidation, corrosion resistance and also good fatigue strength. The materials that exhibit these properties are usually termed as the super alloys and the nickel based alloys are the main class of super alloys and hence, they are widely used in the turbines, combustion chamber linings of jet engines, heat treatment plants, chemical plants and so on. Among the many nickel based alloys, Inconel 718 is one of the strongest alloy and is widely used because of the high corrosion resistance, oxidation resistance. Inconel 718 and Nimonic superalloy processing is important to understand and has relevance to the mineral processing and mining industry. In the present work, we are trying to characterize the Nimonic 80A base alloy using Altair Multi Scale Designer tool by adding alloying elements one at a time and observe the strengthening effects in approaching the final composition of Inconel 718. The alloying elements used in the study are Mo, Nb, Al and Ti.

Keywords: *IN718, Multi-scale Designer, Superalloys*

1.0 Introduction

The term "Super alloys" is used for certain group of materials that can function under high temperatures.

Superalloys are extensively used in the aircraft gas turbines like combustion chambers, exhaust systems, blades, steam turbine power plants, heat treating equipment, chemical industry applications that require high temperature, creep, corrosion and oxidation resistance.

Super alloys are complex and they contain 5 to 10 elements to get the enhanced properties of the alloy[1]. There are different kinds of super alloys that are used and they are classified based on the major constituent as:

- Nickel based,
- Iron based and
- Cobalt based.

Among these, nickel based alloys are the most widely used, complex and interesting class of alloys. There are a wide range of nickel based alloys that are designed for different applications and their benefits are as below.

- Inconel 600 is used in nuclear reactors, in chemical industry in heaters, condensors.
- Nimonic alloy 75 is used in furnace components and heat treatmentequipment.
- Alloy 601 is used in chemical processing, pollution control andaerospace industries.
- Alloy 718 is used in land-based gas turbine engines and in cryogenic tankage.

All the nickel based alloys have nickel weight percentage more than 40% and major alloying elements as Chromium, Iron, Cobalt and small quantities of alloying elements like Mo, Nb, Ti, Al[2]. The latest version

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of these alloys also contains expensive elements such as Rhenium, Ruthenium to get the required properties. The cost of the alloy increases because of this. However, the need and demand for these heat resistant alloys triggers more research in these alloys.

The main requirement of these materials is high melting point, stable microstructure, good oxidation resistance and corrosion resistance, high strength and good machinability and good weldability. For most of the materials, as the temperature increases the yield strength reduces as the metal becomes softer at higher temperatures. Hence the alloys play a vital role under those conditions.

In the development of super alloys, mechanical properties like tensile properties, creep and fatigue properties are of great importance.

The materials used in gas turbine applications are exposed to high temperatures, oxidation, fatigue, creep and rupture. Each alloying element has its own strengthening affect.

With the addition of chromium, we can prevent high temperature oxidation/sulphidation. Tungsten can prevent localized corrosion; weldability of the alloy also improves. The addition of Mo increases the resistance to non-oxidizing acids, improve the creep resistance of the alloy and solid solution strengthening of the alloy. Niobium also helps in improving the creep resistance of the alloy and also the yield strength of the alloy. Aluminum also helps in increasing the yield strength and the oxidation resistance of the alloy. When combined with Ti, it enhances the age hardening in some alloys. The resistanceto corrosion is reduced by adding carbon, as it reacts with the chromium in the alloy forming Chromium carbide and leads to sensitization during welding. The resistance to sulphidation and carburization is improved by the addition of Co.

The elements like Chromium, Molybdenum, Iron, Cobalt act as solid solution strengtheners. Ti, Nb, Al increases the solvus temperature of the alloy. These are the alloys that exhibit improved mechanical properties with the increase in temperature.

Sometimes small amounts of rare-earth metals like yttrium are added, to provide the oxidation resistance. Out of the Nickel based super alloys, Inconel class of alloys are stronger. During processing of Inconel and Nimonic alloys, many alloying elements are added to increase the strengthening effects and these are important in metallurgical and mineral processing of these alloys.

2.0 Inconel 718 and Nimonic 80A Alloys

Nimonic 80A alloys finds applications in the gas turbines, nuclear boiler parts. The Nimonic80A alloy is also being used in the parts of the vehicle and airplane industries. The Nimonic 80A alloy consists primarily of Nickel and Chromium. They can withstand high temperature, have low creep and good corrosion resistance.

Mathematical model establishes the correlation between the main alloying elements and the mechanical properties shown at 750°C; and all the selected parameters related to the chemical composition, affect the mechanical properties[3].

2.1 Inconel 718 Alloy

Inconel has been used widely in various fields. The major advantage of Inconel is that it can work well at elevated temperatures. It has an intrinsic ability to create oxide layer when exposed to heat. It provides exceptional welding quality. It provides high yield strength and good corrosion resistance thus making it a choice for gas turbine application. It is easier to machine.

The % of Nb, Ti, Al is in the range of 7- 7.5%, the yield strength and ultimate strength are the highest and also high content of Nb (5.4-5.5 wt%) contributes for better strength of the alloy[4]. Also for structural stability of 718 alloy, it requires precipitation of γ"+γ' and also the γ' precipitation and to meet this criteria the Al content has to be raised to 1- 1.15% wt, but Ti content is still kept at a nominal level (1% wt or less). This will increase the ratio of (Al+Ti)/Nb (in 1.1-1.4) and Al/Ti (higher than 1.5) for promoting the stable γ' precipitation.

Incorporating the Al, Ti and Nb, P and B into the alloy have helped in improving the stress rupture life of Inconel 718 and also helps in maintaining the properties at elevated temperatures. The best results can be achieved by increasing the P and B levels[5].

Upon adding Ru to the alloy, coarsening and rafting process of γ' precipitates reduces and Ru was there in the γ phase, also the lattice misfit of the alloy reduces with increase in Ru[6].

3.0 About Multi-scale Designer (MSD)

It is a complete framework for the development of material models for all materials from homogeneous isotropic to heterogenous anisotropic. It aims to reduce the time and cost and improve the design efficiency

[Altair Multiscale Designer user manual; 2021] has a well-defined methodology for the development of multiscale materials models[7]. MSD has two approaches for analysis

- Deterministic Approach
- Stochastic Approach

The deterministic approach follows a three-step process:

Representative Volume Element (RVE) Model Definition, Linear Material Characterization and Non-linear Material Characterization.

MSD uses 3D FEA Representative Volume Element (RVE)s with a Reduced Order Model (ROM) technique that allows for both predictive accuracy and computational efficiency. This technique uses a database to record material behaviour from the elastic and inelastic region by computing a one-time solution of the Representative Volume Element (RVE).

One non-linear material law is assigned to each phase of the FEA Representative Volume Element (RVE).

The damage laws are defined as follows: 2 piece and 3 piece damage for brittle materials, rate independent and rate dependent plasticity for ductile materials, and advanced hybrid damage and plasticity for materials showing dual behaviour.

For the forward homogenization problem, the homogeneous micro-phase material properties are user-defined and the corresponding macro homogeneous properties of the heterogeneous Representative Volume Element (RVE) are calculated. 6 different strain BCs are superimposed on the defined RVE within the linear elastic regime. 21 independent engineering constants specifying the anisotropic stiffness matrix [C] are determined. The stiffness matrix [C] is computed based on the 6 BCs on the Hooke's law equation.

For the nonlinear forward homogenization, MSD uses built-in Macro Simulation Models present in the MD library.

Virtual characterization using MSD of a NCF as reinforcement and an epoxy resin and observed that the results obtained from the tool are over predicting the results from experiments[8]. Also, MSD also couldn't capture fiber kinking phenomenon and the complexity in their architecture for their complex failures are also attributed for the major difference between the results.

4.0 Modelling Procedure

4.1 Modelling of Fibre-Matrix Interface

As discussed in the previous section, the, MSD separates the multiscale process in three steps, Representative Volume Element (RVE) Definition, Linear Material Characterization and Nonlinear Material Characterization.

4.1.1 Representative Volume Element (RVE) Definition

In the Representative Volume Element (RVE) Model Definition step, a parameter based model of the RVE is to be evolved. The model option is 'fibrous' and the RVE option is a 'Honeycomb'. As input data, the 'Geometric data' option is chosen where the fiber volume fraction in the alloy is chosen. A two-phase parametric Representative Volume Element (RVE) is generated depending on the volume fraction of the matrix and the fiber. In the present work, we have chosen 4 alloying elements Ti, Al, Mo, Nb for understanding the effect of these elements on the alloy.

4.1.2 Linear Material Characterization

In the Linear Material Characterization step, a forward homogenization technique is adopted. The properties are mentioned for two different phases. The matrix is taken as an ***isotropic phase*** whose properties are taken from the handbook [ASM metal hand book; 1988].

The fibre is considered as ***isotropic*** with the corresponding properties. For both phases, the compressive Young's Modulus is assumed to be the same as in tensile.

In addition to the micro material properties, a single ply laminate with 0^{o} direction is defined as a lay-up in the Linear Material Characterization.

4.1.3 Non-Linear Material Characterization

The next step after completing the linear material characterization is to run the Non-linear Material Characterization step to get the nonlinear elastic properties of the homogenized model.

Even though we chose a simulation model for Nonlinear Characterization model, the material model obtained is independent of the test we have chosen and can be used as material model for any kind of non-conventional simulations.

The virtual test model chosen in this case is the (Unnotched tension/compression) ***UNTC model***. The loading is as shown in the Figure 1. A nonlinear material will have the linear regime and the nonlinear regime and finally the ultimate failure region as shown in Figure 2.

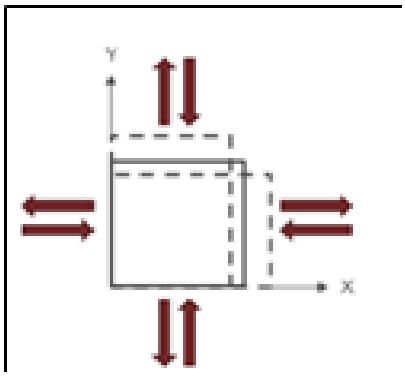


Figure 1. Loading for UNTC.

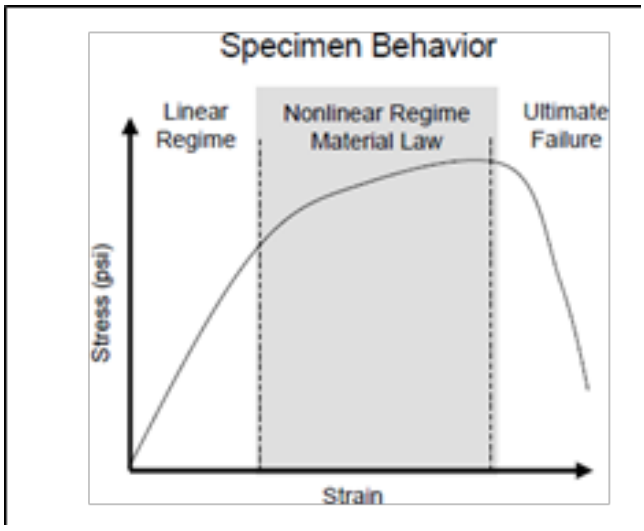


Figure 2. Stress-strain behavior of any homogenized specimen.

We have to select appropriate damage law and hence a suitable damage law which can to an extent accurately predict the nonlinear behaviour. In the present work, ***Isotropic damage and RI plasticity model*** is selected to define the matrix behaviour and ***RI plasticity model*** to define the fiber side.

5.0 Results

Here, we are giving the properties of Nimonic 80A Alloy and trying to strengthen the alloy taking into account the composition of Inconel 718 alloy. Here we are trying to match Nimonic 80A alloy to the strength of that of Inconel 718 after adding the alloying elements.

In the current work, we are trying to study the effect of alloying elements Mo, Nb, Al, Ti by taking a basic nickel-based alloy NIMONIC 80A and strengthening of the alloy with each alloying element and comparing the results with the base Nimonic 80A alloy.

5.1 Step 1: Representative Volume Element (RVE)

For the current work, we have chosen fibrous honey comb structure (Figure 3) with different volume fraction of the fiber inside the matrix.

The Representative Volume Element (RVE) model created is as below for 6% volume fraction of Mo and 94% volume fraction of Nimonic 80A alloy (Figure 4).

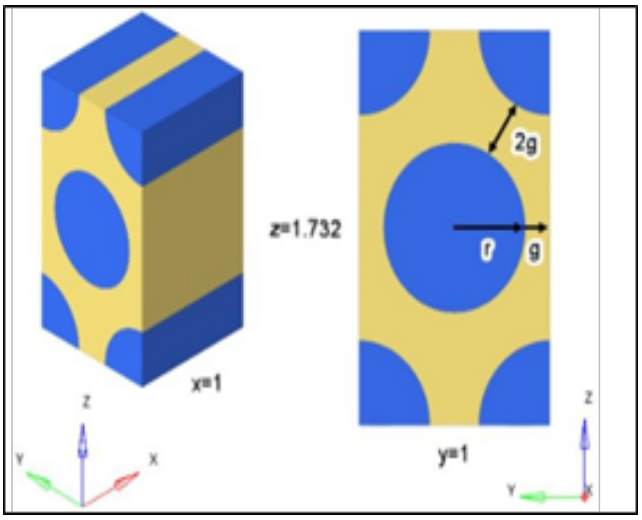


Figure 3. Representative Volume Element (RVE) (Honeycomb) considered.

Representative Volume Element (RVE)_mesh

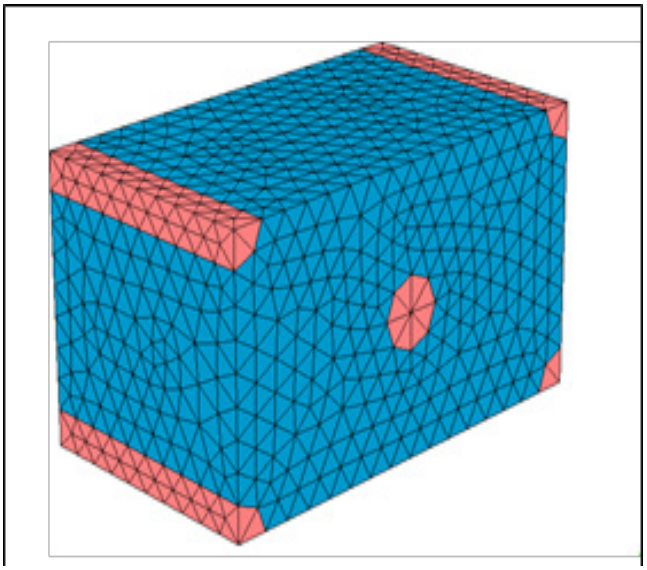


Figure 4. Representative Volume Element (RVE) generated in MSD.

The Representative Volume Element (RVE) created has the following number of elements for matrix phase and also for fiber phase as tabulated below in Tables 1,2.

Table 1. Elements of Representative Volume Element (RVE) In MSD

Spatial Dimensions	**3**
Number_of_Nodes	13641
Number_of_Elements	8576
Type_of_Elements	C3D10

Representative Volume Element (RVE)_phase

Table 2. Unit cell phases

Number_of_Phases	2

Phase_ID	**2**
Phase_Name	Fiber
Number_of_Elements	785
Phase_Volume	1.03868E-01
Volume_Fraction	6.00%

Phase_ID	**1**
Phase_Name	Matrix
Number_of_Elements	7791
Phase_Volume	1.62813E+00
Volume_Fraction	94.00%

5.2 Step 2: Linear Material Homogenization

After the Representative Volume Element (RVE) is generated, we start with the linear material homogenization step by inputting the matrix as well as the fiber properties as given in the Tables 3 and 4.

Table 3. Matrix properties

ID	**Parameter**	**Value**
1	E	222
2	ν	0.31
3	E_C	222
4	σ	12.7E-06
5	ρ	8.19E-06

Table 4. Fiber properties

ID	**Parameter**	**Value**
1	E	329
2	ν	0.31
3	E_C	329
4	σ	4.8E-06
5	ρ	10.28E-06

The linear material homogenization was run by taking Nimonic 80A properties on the matrix side and the molybdenum properties on the fiber side. We get the homogenized material matrix after linear homogenization as shown (Table 5).

Table 5. Material matrix generated in linear material homogenization

Homogenized Material Matrix

$$\begin{bmatrix} 3.16E+02 & 1.41E+02 & 1.41E+02 & 8.57E-05 & -7.66E-07 \\ 1.41E+02 & 3.14E+02 & 1.41E+02 & 1.81E-04 & -1.67E-05 \\ 1.41E+02 & 1.42E+02 & 3.14E+02 & 9.54E-05 & 1.357E-05 \\ 8.57E-05 & 1.81E-04 & 9.64E-05 & 8.66E-01 & 1.48E-05 \\ -7.66E-07 & -1.67E-05 & 1.36E-05 & 1.48E-05 & 8.67E-01 \end{bmatrix}$$

5.3 Step 3: Nonlinear Material Homogenization

After the linear material homogenization, we go to the nonlinear material homogenization step.

Here we input the (Unnotched tension/compression) UNT/C test simulation parameters as given in Table 8. There are many damage laws in the database of MDS for predicting the behavior of the matrix as well as the fiber.

In the current work, ***Isotropic damage and RI plasticity model*** was chosen on the matrix side and ***RI plasticity model*** on the fiber side.

Material properties on the matrix side and the fiber side are as given below in Tables 6 and 7.

Matrix damage law: Isotropic damage and RI plasticity

Table 6. Damage parameters used for the matrix (Nimonic80A)

ID	Parameter	Value
1	σy	0.78
2	σ1	1.25
3	δ	3
4	H	0.1
5	q	0
6	β1	0.0
7	β2	0.0
8	εpo	0.25
9	εp1	0.27
10	σmean	0.7
11	J1	0.1
12	C	1.0
13	w_max	1.0

Fiber damage law: Rate Independent plasticity

Input parameters

Table 7. Damage parameters used for the fiber (Niobium)

ID	Parameter	Value
1	σy	0.88
2	σ1	1.25
3	δ	3
4	H	0.1
5	θ	0
6	β1	0.0
7	β2	0.0
8	εpo	0.25
9	εp1	0.27
10	w_max	1.0

Simulation Parameters

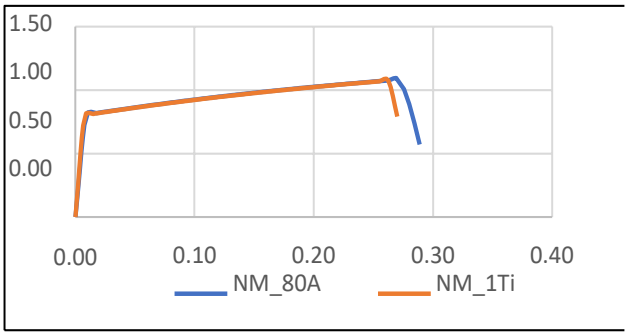


Figure 5. UNTC behavior of Nimonic 80A Alloy before and after adding 1% Ti.

Table 8. Simulation parameters input for UNTC test

ID	Parameter	Value
1	Test time(s)	1
2	Maximum strain	0.3
3	Delta Temperature	0
4	Minimum Thermal Increments	0
5	Minimum Mechanical Increments	40

The model was run for different alloying elements and the results are as shown in Figures 5-9.

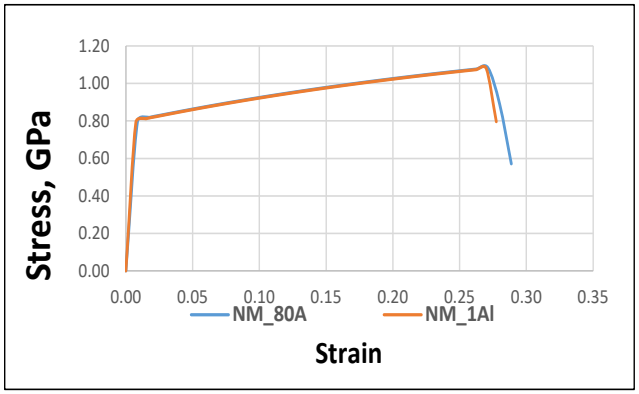


Figure 6. UNTC behaviour of Nimonic80A Alloy before and after adding 1% Al.

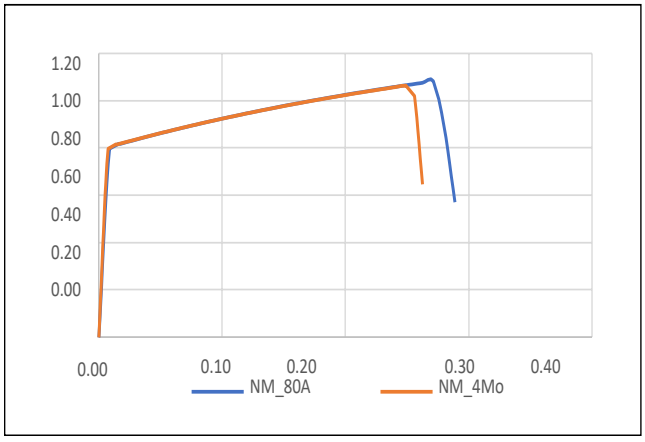


Figure 7. UNTC behaviour of Nimonic80A Alloy before and after adding 4% Mo.

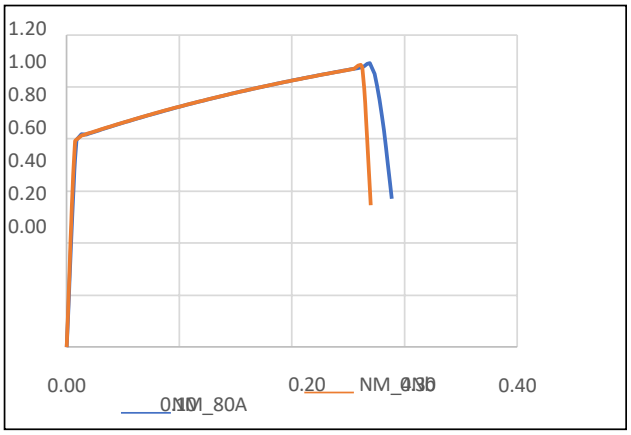


Figure 8. UNTC behaviour of Nimonic80A Alloy before and after adding 4% Nb.

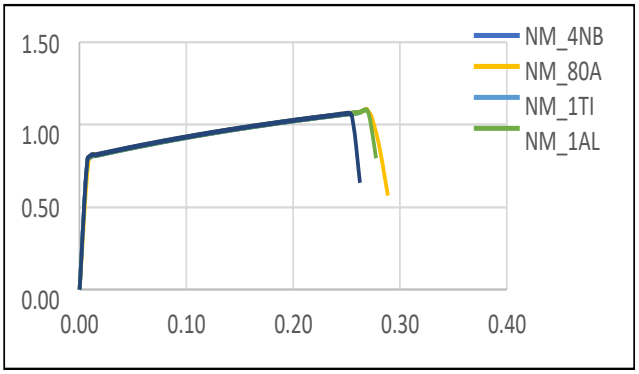


Figure 9. UNTC behaviour of Nimonic80A Alloy before and after adding 4 alloying elements one at a time.

The strengthening effect can be seen from the plots in Figures 5-9. It can be seen that Mo and Nb provide more strengthening effect to the alloy.

6.0 Conclusion

The UNTC behavior of the NIMONIC 80A material with alloying elements like Ti, Al, Mo and Nb was determined using MSD. It can be seen that Mo and Nb provide more strengthening effect to the alloy and approach properties of Inconel 718. We can also determine the effect of alloying element with one alloy considered at a time. The strengthening effect of the elements in individual and combined fashion is important to understand as they affect the metallurgical and mineral processing conditions for the Nimonic superalloy.

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