Simulation of the effects of Zr and Co addition on the properties of NiAl-Mo(Cr) alloy

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Abstract. The introduction of computational modelling during alloy development has significantly reduced the cost of production and the prolonged time spent by researchers doing trials and errors in the laboratory. In this study, computational software (JMat Pro) was used to simulate the effect of the addition of Zr and Co, on the material properties of NiAl-Mo(Cr) alloy such as the elastic modulus, hardness, thermal conductivity, bulk modulus and specific heat capacity. A significant improvement in the mechanical properties was observed in the developed alloys as compared to those without Zr and Co. Also, the addition of as low as 0.5 at. % Zr and 1.0 at. % Co to NiAl-Cr(Mo) resulted in improved compressive strength and plasticity of the alloy.

Keywords: Hardness, alloy, compressive strength, modulus of elasticity, simulation.

1 Introduction

The quest to enhance the thrust-weight ratio of aircraft engines and thus, improve the performance of such engines has called for the development and use of lightweight materials with high-temperature resistant properties for the fabrication of engine components such as the turbine blades in the engine of aircraft [1, 2]. In view of this, low-density NiAl-based alloys with approximately 2/3 the density of nickel-based alloy [3] are now being used as a replacement for nickel-based alloys in structural materials. This is because of their high resistance to oxidation at high temperatures, high thermal conductivity, high modulus of elasticity and high melting point [4-6]. Nevertheless, the low strength experienced by NiAl-based alloy at temperatures higher than 850 ℃ [7, 8], and the low plasticity reported at temperatures lower than 0.45 T_m are some of the limitations that prevent the widespread use of the alloy. Numerous techniques such as the use of alloying elements, composite material preparation, preparation technique optimization etc. have been adopted in a bid to improve the performance of NiAl-based alloy.

Of all the methods available, the alloying method appears to be cost-effective, and simpler with the capability of changing the bond type, electronic structure, and the degree of intermetallic compound long-range order. Previous research on intermetallic compounds like TiAl [9] and Ni3Al [10, 11] shows that their properties were significantly improved due to the addition of appropriate alloying elements. So far, extensive research has been conducted

on NiAl-based alloys using a number of alloying elements to improve their high-temperature strength and room-temperature plasticity. In some of the studies conducted, the addition of V, Mo, Cr and some other refractory metals to NiAl matrix tends to improve the strength and plasticity of the alloy [12-14]. Nonetheless, the addition of Mo to a system of NiAl-Cr would result in the formation of a layered microstructure of Cr(Mo), and then form an eutectic structured NiAl-Cr(Mo) alloy that possesses a considerable strength [15], considerable fracture toughness [16, 17], and antioxidant properties [18].

To further improve the properties of NiAl-based alloys, and make them suitable for vast applications, there is a dire need to conduct more studies on the alloying of NiAl matrix, and a cost-effective way to achieve this is via computational study. At the moment, only limited studies have been reported on Co and Zr addition in NiAl-Cr(Mo) alloy. Hence, this study would leverage material properties determination software, JMatPro (a software that uses the calculation of phase diagrams technique (CALPHAD)) to predict the effects of the addition of Zr and Co to NiAl-Cr(Mo) on the final properties of the newly developed alloy.

2 Alloy development

To develop the NiAl-based alloys, JMatPro alloys development, and material properties simulation software was used. The software integrates the functional calculations of phase diagrams and performance simulation of metallic materials such as general steels, cast iron [19], nickel alloys, magnesium alloy, aluminium alloy [20, 21] etc. Using this software, it is possible to design alloy compositions [20], develop new alloys, improve the different heat treatment processes [22], and generate support data for design flow processes and CAE software [20, 22].

Previous studies have shown that group 4(IVb) elements such as titanium (Ti) and hafnium (Hf) have been used to improve the strength of NiAl-based alloy. Zirconium, being an element in the same group as titanium and hafnium, has the potential to also increase the strength of the alloy. Colbat (Co) on the other hand is in the same group as iron (Fe), and it is expected to increase the NiAl-based alloy's plastic deformation. The atomic percentage composition of the NiAl-based alloy developed in the JMatPro software is shown in Table 1. In the development of the alloy, the percentage composition of Ni, Al and Cr are kept constant while that of Mo decreases with the addition of Zr and Co.

Table 1. Composition of elements used in the alloy development (at. %)

Ni	Al	Cr	Mo	Zr	Co
55.0	20.0	18.0	7.0	0.0	0.0
55.0	20.0	18.0	6.0	0.5	0.5
55.0	20.0	18.0	5.5	1.0	0.5
55.0	20.0	18.0	5.0	1.0	1.0
55.0	20.0	18.0	4.0	2.0	1.0
55.0	20.0	18.0	4.0	1.0	2.0
55.0	20.0	18.0	3.0	2.0	2.0

In the design and development of the NiAl-based alloy, nickel-based superalloy was selected on the JMatPro material design and properties prediction software, after which the different percentage compositions of the elements that make up the alloy are appropriately assigned. To compute and predict the hardness and compressive strength of the alloy to be developed, the default heat treatment temperature of 720 ℃ was used and the default phase which includes liquid, gamma (γ), gamma prime (γ'), gamma prime-prime (γ'') etc was activated. For the determination of the other thermo-mechanical properties of the developed

alloy, thermophysical and physical properties analysis was selected, and a default heat treatment temperature of 600 ℃ for nickel-based alloys with an upper limit of 1400 ℃, and a step of 10 ℃ was selected. The analysis takes all the possible phases into account, and the effect of the Zr and Co addition on the properties of the developed alloy is predicted.

3 Results and discussions

The compressive strength of the developed alloys with the addition of different at. % Zr and Co are shown in Fig. 1. From the figure, it was observed that the compressive strength of the alloy increases with an increase in the at, % of Zr, while the addition of Co improves the ductility of the alloy. At 0 at. % Zr and 0 at. % Co, the developed alloy exhibits its lowest strength, with the highest ductility. Whereas, at 2 at. % Zr and 1 at. % Co, the developed alloy gave the highest compressive strength but with a lesser ductility. The strengthening behaviour exhibited by the alloy is because the Co and part of Zr form a solid solution in the NiAl and Cr(Mo) phase, thus resulting in lattice distortion and internal stress field generation. As a result of the solid solution strengthening that occurs in the alloy with Zr and Co addition, it is hard for the internal stress field to be overcome by direct dislocations slip [23].

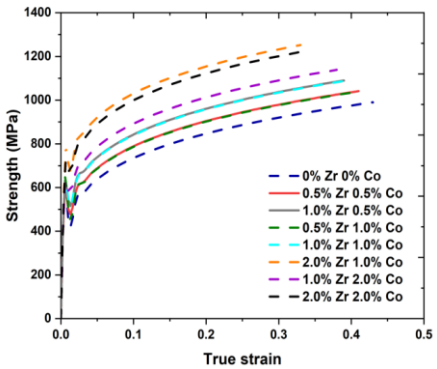

Fig. 1. Compressive strength of the developed alloys at different at. % of Zr and Co

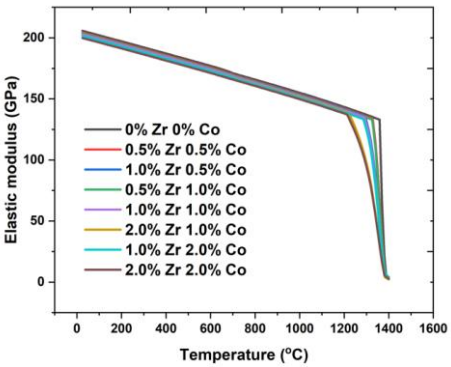

Fig. 2. Elastic modulus of developed alloy as a function of temperature

As depicted in Fig. 2., the elasticity modulus of the alloys decreases with an increase in the operating temperature. At room temperature, the alloy with 0 at. % Zr and 0 at. % Co has the highest elastic modulus and the value decreases with an increase in the at. % of Zr and Co.

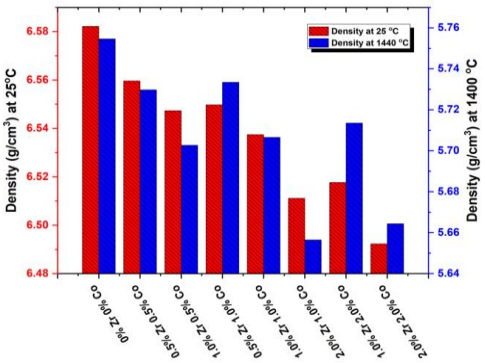

Fig. 3. Density of alloy at different at. % of Zr and Co

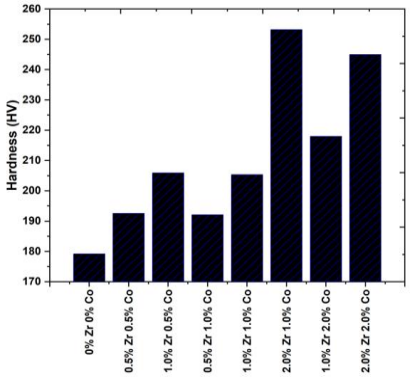

Fig. 4. Hardness of alloy at different at. % of Zr and Co

The density of the alloy decreases with an increase in the at. % of Zr both at room temperature and high temperature, while the addition of a significant at. % Co and a significant reduction of the at. % Zr slightly increase the density as experienced in the composition 0.5 at. % Zr-1.0 at. % Co and 1.0 at. % Zr-2.0 at. % Co, for both temperatures as shown in Fig. 3. Also, the increase in the at. % of Zr results in a significant increase in the hardness value of the developed alloys, while a higher at. % of Co as compared to Zr results in a significant drop in the hardness value as shown in Fig. 4. The increase in hardness experienced with the addition of Zr is due to the solid solution strengthening of Zirconium, which makes it difficult for the movement of dislocation through the alloy [24]. Similar results were reported when Zr was added to NiAl and Ni3Al [25, 26].

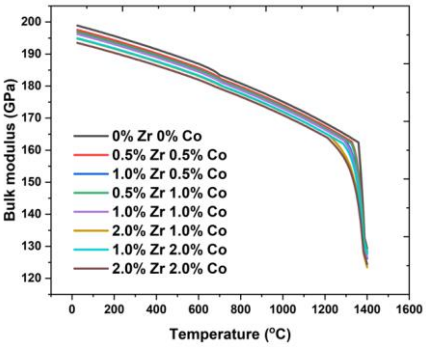

Fig. 5. Bulk density of developed alloy as a function temperature

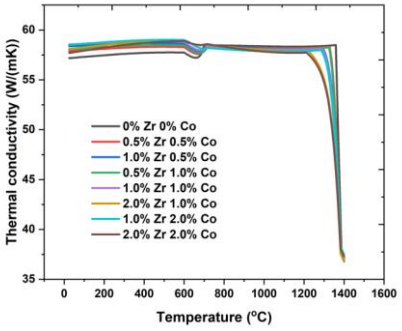

Fig. 6. Thermal conductivity of developed alloy as a function of temperature

Just like the elastic modulus, the bulk modulus of the developed alloy decreases with an increase in the at. % of Zr and Co, both at room and high temperatures, such that the alloy with 0 at. % Zr and Co, has the highest bulk modulus, while alloy with 2 at. % Zr and Co has the lowest bulk modulus both at room and high temperatures as shown in Fig. 5.

The thermal conductivity of the developed alloys increases with an increase in temperature up to about 1 300℃ for the different compositions of the developed alloys, after a further increase in temperature results in a drastic drop in the thermal conductivity of the alloys. At room temperature, the thermal conductivity of the alloy was observed to increase

with the addition of Zr, while the addition of Co slightly reduces the thermal conductivity as depicted in Fig. 6.

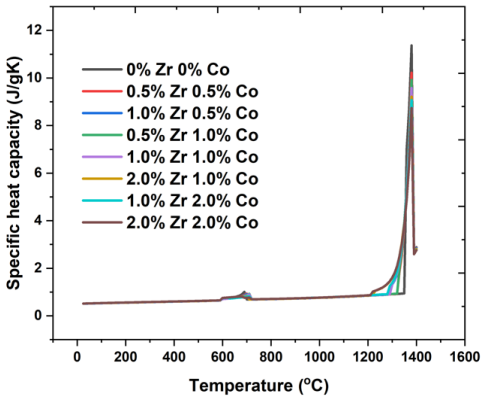

Fig. 7. Specific heat capacity of alloy as a function of temperature

The specific heat capacity of the alloy increased with an increase in the at. % of Zr and Co and temperature up to 1 370 ℃. At a temperature higher than 1 370 ℃, the specific heat capacity of the alloy decreases with a further increase in temperature as depicted in Fig. 7. The decrease in the specific heat capacity of the alloys at elevated temperatures (above 1 370 ℃) could be a result of the heterogeneity of the alloys which may likely change their crystallization mode [27].

4 Conclusions

In this study, a computational-based technique that uses the CALPHAD method was employed in the prediction of the effect of Zr and Co addition on the properties of NiAl-Mo(Cr) alloy. For the simulation, materials properties and alloy development software, JMatPro was used and the effects of the addition of Zr and Co were predicted. The addition of Zr significantly improves the compressive strength and hardness of the alloy while the ductility of the alloy improves with an increase in the at. % of Co. The trend of the thermomechanical properties predicted is similar to those obtained during experiments [1]. Hence, computational-based simulation is a cost-effective way of determining the properties of new alloys prior to their manufacturing in the laboratory.

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