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An Analysis of the structure and properties of the HEA NbTaMoW

Abstract
This paper aims to showcase the structure and mechanical properties of the high-entropy alloy NbTaMoW. This was done by investigating how the material acts under stress, looking at its fracture toughness, and exploring strengthening mechanisms that could potentially increase its refractory abilities. Furthermore, by analyzing its behavior when it undergoes different phases we were able to determine that NbTaMoW exhibits extraordinary potential for conditions that are high temperature and high stress as it has an exceptionally high yield strength and ductility.

Introduction
Research into high-entropy alloys in today's world has a high emphasis on transition metals such as Ni, Co, Cu, and Fe. The material NbTaMoW was chosen as we wanted to look into HEAs that primarily consisted of highly refractory elements. This is so because one of the main potential uses of HEAs is in high-load and temperature-bearing situations. Hence, exploring HEAs made up of metals with high melting temperatures has a compelling rationale.
Overall, it is established that NbTaMoW is stable at extremely high temperatures. The material might not be as ductile in the low-temperature range as its pure BCC metal equivalents but it is very applicable for high-temperature structural applications, such as those in the nuclear and aerospace sectors, because they maintain very high strengths at high temperatures.[1] After conducting further research, it was evident that NbTaMoW could be and has been employed in the manufacturing of industrial components such as a high-performance blade that can not only be used to cut soft metals such as brass or copper but also, hard metals such as stainless or mild steel.[23] This is due to the mechanical properties that allow it to bear low residual stresses while maintaining fracture-free printed parts and low density. To fabricate a high-performance blade that employs NbTaMoW, the process of near-net-shape manufacturing is utilized. This manufacturing process is a general term used to describe manufacturing procedures that seek to create products with properties that closely resemble the final shape and composition of the component.[4]

Base Crystal Structure
NbTaMoW exhibits a single-phase body-centered cubic structure with a Bravais lattice. In a lattice such as this one, per lattice point, there is one atom placed at the corners of the cube. NbTaMoW consists of 4 elements that all have BCC structure so the fact that it also has the same structure is not surprising; the similar atomic radii and valence numbers of the elements could be the cause of this.
The Pittsburgh Materials Technology, Inc. experimented, using vacuum arc melting, by mixing equimolar amounts of the elements to determine the weight and atomics percentages of the constituent elements. The results were as follows;

Table 1:Chemical composition of NbTaMoW.[5]

Element	Nb	Ta	Mo	W

wt%/at%	15.2/22.7	31.7/24.4	17.8/25.6	36.0/27.3

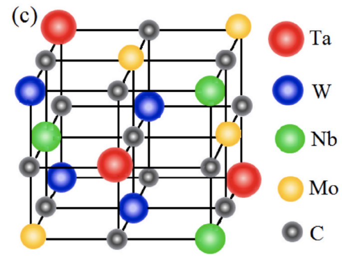

Image 1: BCS after sintering with carbon.[6]

Slip System in a BCC Structure

Slip system in body-centered cubic (BCC) metals is very complicated and occurs in the <111> direction at the closest pack with an a/2 <111> Burgers vector. It is more difficult to pinpoint the precise planes in bcc metals where slide occurs. The maximum interplanar distance is found in the planes {110}, {112}, and {123}. BCC metals have been found to experience twinning along with adiabatic shear banding at low temperatures and high strain. At low temperatures, BCC metals have a behavior of parabolic hardening but as the temperature is increased they exhibit mechanical behaviors of classic three-stage hardening. Stage 0: the initial rounding at higher temperatures, is mostly caused by the activation of mixed dislocations. Stage I: abnormal slip, which is the activation of a dominating slip system with a low resolved shear stress and typically involves 110 planes. Single crystals of pure bcc metals are typically quite ductile.[7]

Shear Stress

At room temperature:

At 20°C, when a sample of NbTaMoW is analyzed using a scanning electron microscope it is revealed that it undergoes fracture by splitting across planes that are almost parallel to the compression direction. When a higher magnification of the microscope is used, it is evident that the fracture patterns showcase river-like markings along the flat facets.[8] This shows that it undergoes tensile stress rather than shear stress at this temperature.

At 800°C:

SEM pictures of the same samples at this temperature showed that because it undergoes localized shear stress, it can maintain its ductility.

Strengthening Mechanisms

Co-sputtering using various nitrogen ratio flows

(NbTaMoW)Nx films can be created through a reaction of co-sputtering using various nitrogen ratio flows. There is an increase in the stoichiometric ratio x of (NbTaMoW)Nx as the ratio flow Rn2 increases along with a BCC metal phase change to the FCC covalent nitride phase. Co-sputtering using nitrogen flows can increase the GPa or hardness of NbTaMoW by 6.8 GPa by increasing the hardness value of the metallic films from 24GPa to 30.8 GPa at maximum when the stoichiometric ratio x has a value of 0.48. If the stoichiometric value of x is increased to 0.72 the hardness of NbTaMoW will decrease to 20 GPa. This is because the addition of nitrogen to HEA films can change the bonds of the structure from metallic to covalent in turn increasing the strength and improving the mechanical properties of the HEA. The results can change greatly due to various stoichiometric ratio values.

Enhanced by adding titanium

NbTaMoW can also be enhanced by adding titanium through alloying. This addition of titanium to the high entropy alloy can cause changes in the phase structure, density, elastic properties, electronic structure, and lattice parameters. The alloying of titanium does not change the BCC structure of NbTaMoW and does not change whether it is electrically conductive or not. The metallic characteristics of NbTaMoW are not changed either. The addition of titanium enhanced the strength and the ductility of NbTaMoW while also increasing the amount of Ti to Ti metallic bonds which in turn decreases the number of covalent bonds which enhances the atomic interaction in the high entropy alloy.[9]

Comparison with NbTaMoW

For precipitation hardening, 304 stainless steel is part of Austenitic stainless steel and NbTaMoW is part of second-phase strengthening. The HEA is soluble at high temperatures but its solubility in lower temperatures is more bounded. Regarding grain size reduction, 304 stainless steel's grain sizes can be acquired through cryogenic rolling and reversion annealing. NbTaMoW has columnar grains and this is made when metals solidify slowly in a sharp temperature gradient.[10]

Mechanical Properties

Table 2: Yield strength and ductility at room temperature (23°C).[11]

Plastic Strain(ε_p) %	Yield Stress/MPa	Maximum Yield Strength/MPa	Ductility/%
0.95	1058	1211	2.0

Fracture in NbTaMoW

S-N Curve

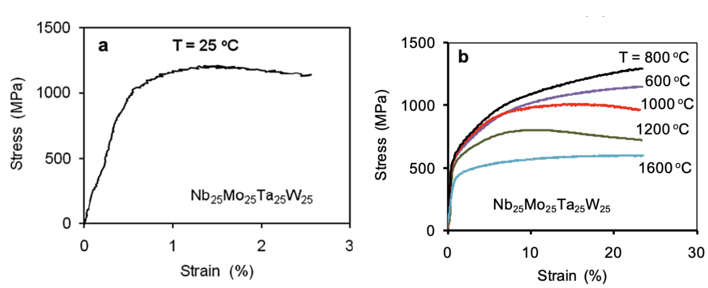

Figure 2 : (a) Basic stress-strain curve for NbTaMoW, fracture occurs between 2-3 at end of the curve. (b) Stress-strain curve for NbTaMoW at elevated temperatures, fracture occurs between 20-30 at end of the curve.

Fracture toughness:

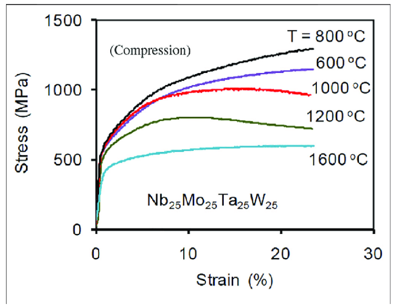

Figure 3: Engineering stress vs Engineering strain curve for NbMoTaW.[12]

An engineering stress vs strain curve at varying temperatures can be used to analyze a material's fracture toughness. At temperatures such as 800°C shows exceptional yield strengths of about 1350MPa. While the yield strength is comparatively lower at higher temperatures such as 1600°C, NbTaMoW still maintains a constant yield strength of about 400MPa even as crack initiation occurs and also during stable crack growth.

Electron micrograph of failure type (Fracture/compression deformation):

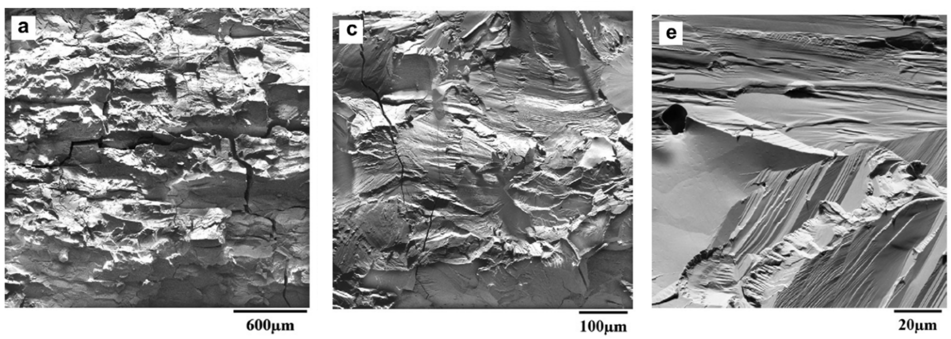

Figure 4: SEM images of fracture surfaces of Nb25Mo25Ta25W25 alloy after compression deformation at 25 °C. (a) River pattern cracking (e) Flat Facet cracking.[13]

Eutectic Reaction

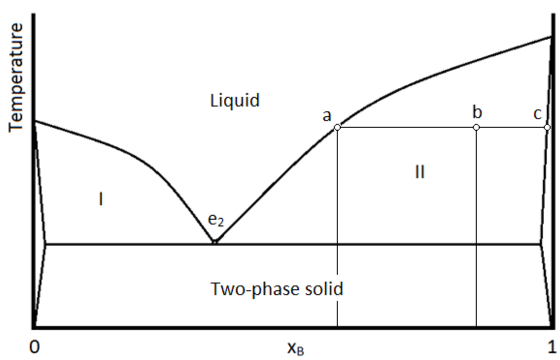

Figure 5: Generalized graph of eutectic reaction in High Entropy Alloys (e_2 represents the point at which the eutectic reaction occurs)

It is important to note that, this graph's information does not pertain specifically to NbTaMoW but rather it is a generalized representation of the reaction in a BCC high-entropy alloy. The graph shows that the temperature has reached a point where it must remain constant and that the maximum amount of phases is in equilibrium. Crystals start to precipitate out of the liquid. The size of eutectic particles can be controlled by increasing their cooling rates of them. Furthermore, the weight of the material changes, and the temperatures do as well.[14]

Phase Diagram:

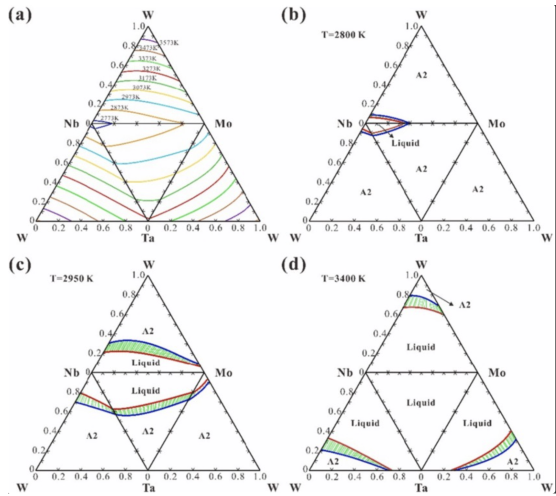

Figure 6: Phase Diagram (pseudo-ternary systems) of NbTaMoW.

The quaternary system of NbTaMoW consists of 6 pseudo-binary systems that are as follows: NbMO, MoTa, MoW, NbTa, NbW, and TaW. It also has 4 pseudo-ternary systems that comprise of NbMoTa, NbMoW, MoTaW, and NbTaW.[15] After analyzing the thermodynamic properties and the data from the phase diagrams a critical review showed that the 6 pseudo-binary systems have very similar phase diagrams at higher temperatures and tend to remain in liquid phases and maintain an A2 continuous solid solution.

Transformation Kinetics in Conventional Alloys as compared to High Entropy Alloys

Table 3: Comparing conventional alloys against High Entropy Alloys.[16]

	HEAs	Conventional Alloys
Rate of Phase Transformation	Slower in HEAs	Relatively Faster
Precipitates	Slow kinetics of atomic movements lead to the formation of nanosized precipitates.	Usually no nanosized precipitates.
Intermetallic Phases	HEAs contain one or more dispersed ordered intermetallic phases to various extents.	Do not contain dispersed ordered intermetallic phases.
Role of Base Metals	By using refractory metals and a suitable alloy as the base, there is a significant increase in the strength of the solid solution in the matrix. Additionally, this causes a much more stable second-phase dispersion for the arresting grain yielded by the materials even at high temperatures such as 1000C.	Usually have only one base metal that cannot necessarily survive very high temperatures.
Pressure-specific phase transitions	Pressure is the driving force for the formation of defects and strains, which leads to the sliding of the atomic layer. The FCC and HCP crystal structures are closely stacked, and the transition only requires	It has been found that pressure alters the phase diagrams of binary alloys. The variation is controlled by the

	atoms moving along the 111-plane and a small amount of thermal activation energy. Therefore, pressure can cause deformation to rise, flaws to occur, and the martensitic transition to be promoted. Pressure can collapse the lattice, alter the stacking density of the lattice, and induce phase transitions. Pressure buildup inhibits a metal's magnetic properties, and high pressure results in the collapse of a magnetic moment. Additionally, the pressure reduces the density of the Fermi energy level and broadens 3D valence bands, which prevents the magnetic moment.	very well-known pressure dependence of the elemental end members and the relatively unstudied excess interaction within the framework of solution-type models. For the pressure and temperature dependence of the interaction parameters in an alloy solution, precise thermodynamic relationships are created and connected to the composition dependence of the excess thermodynamic values derived at ambient conditions. To ascertain the role of the surplus volume in phase diagrams and solubility limits, the effects of altering the value of the interaction parameter for pressure are examined in model systems.
Heat-specific phase transitions	The phase transition of HEAs is also influenced by the heat treatment or sintering temperature. In the process of high-temperature sintering or heat treatment, the internal stress in the solid solution formed after alloying is released, changing the metastable structure into a stable one.	With heat and pressure treatment, the phases that are present in many common alloys can be changed. Phase transformation is the process of creating one or more phases from another phase. Phase changes can happen when an alloy is heated or while it is cooling off from a high temperature.

The phase change is slower in HEAs compared to normal alloys.[17] This is so because each lattice site often has various surrounding atoms. Every site has unique local energy as a result of its unique bonding and local atomic configuration. An atom becomes "stuck" and its likelihood of re-jumping decreases when it enters a low-energy location. The atom is more likely to return to its original site if the site is low energy, on the other hand. Both of these possibilities impede the diffusion process. The atom is more likely to return to its initial site if the site is low energy, on the other hand. Both of these possibilities slow the diffusion process. Nanosized precipitates frequently occur in HEAs due to the sluggish kinetics of atomic motion. Such precipitates support the enhanced creep capabilities and good diffusion barrier performance of HEA coatings.

Conclusions

By looking at the microstructure, mechanical properties, and phase transitions of NbTaMoW, it was determined that this specific HEA has major advantages over other conventional alloys. Initially, it could be seen that even though the material, at lower temperatures, was able to maintain its high-stress endurance, it was unable to maintain higher levels of ductility. However, this low level of ductility can be overcome by adding titanium to the material. Analysis of the phase diagrams showed that at high temperatures the HEA's pseudo-binary system can maintain a stable liquid phase which could potentially make the manufacturing process of this particular alloy relatively easier in comparison to other HEAs. What makes NbTaMoW stand out amongst its other HEA equivalents is that it mainly constitutes elements that are highly refractory. Analyzing materials such as NbTaMoW could have scope in a sub-category in the research of HEAs that is concentrated on the examination of HEAs that correspond with highly refractory metals.

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