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EFFECT THE CONCENTRATION OF RHENIUM ON THE MECHANICAL PROPERTIES AND DISLOCATION MECHANISMS OF TUNGSTEN-RHENIUM ALLOY

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Abstract- The tungsten-rhenium (W-Re) alloy is a high-performance material commonly used in various industrial applications- This alloy comprises tungsten and rhenium in varying proportions, with the most common composition being 75% tungsten and 25% rhenium. The addition of rhenium improves the ductility and strength of tungsten, making the alloy more resistant to wear and deformation at high temperatures. The tungsten-rhenium alloy is widely used in aerospace, electronics, and nuclear industries where high strength and durability are essential. The objective of this study is to enhance and optimize the mechanical properties and dislocation behavior of the W-Re alloy through an analysis of its mechanical characteristics. For this purpose, a series of nanoindentation tests is carried out on samples of (W-Re) alloys. Subsequently, a statistical analysis is applied to our different samples to indicate the quality of the simulation results and ensure appropriate agreement with experimental results.

Keywords: Nanoindentation, W-Re Alloy, Molecular Dynamics, Nanoindentation, Mechanical Properties, Dislocation Density.

1. INTRODUCTION

Composite materials, valued for their excellent mechanical properties and lightweight nature, play a crucial role in various industries such as automotive, aerospace, aviation, marine, and the sporting goods industry [1, 2]. However, tungsten faces challenges in demanding applications due to its lack of ductility at room temperature and high ductile-to-brittle transition temperature (DBTT) [3]. The DBTT refers to temperature at which a material changes from ductile to brittle behavior under stress, and for tungsten, it is relatively high, which limits its practical use in certain applications.

To overcome these challenges, researchers are exploring new techniques to enhance the ductility of tungsten at low temperatures and reduce the DBTT.

By doing so, they hope to expand the range of applications where tungsten can be used. In this context that studies in 1955 Geach and Hughes discovered that adding rhenium to tungsten could improve its ductility. To demonstrate this, they created a tungsten-rhenium alloy containing 35 at.% rhenium and cold-rolled the alloy at room temperature. The alloy could be rolled up to 11% reduction in thickness without cracking, while pure tungsten fractured during the rolling process. They also observed that tungsten could be easily worked at several hundred degrees Celsius [4].

Nanoindentation is a mechanical testing method that enables the determination of mechanical properties of materials at the nanoscale. It involves applying a gradually increasing load on a small point on the surface of a sample using an indenter with a known geometry. This technique is commonly used for characterizing the mechanical properties of thin films, as it allows for the manipulation of thickness at the nanoscale with loads below 1 μN. Parameters measured using this method include hardness, elastic modulus, and resilience. It is important to note that experimental results from nanoindentation can be influenced by various factors, and simulation modeling can be used to better understand the results. Several research studies have actually utilized nanoindentation simulation to explore the mechanical properties of materials, as evidenced by the reference [5]. Molecular dynamics is a numerical simulation method used to study the behavior of atoms and molecules in a given system. This technique relies on solving Newton's equations of motion numerically for individual particles, while considering their interactions with both their environment and each other [6].

The Embedded Atom Method (EAM) potential [7] is a molecular dynamics interatomic potential model that utilizes density functional theory to describe the correlation between potential energy and electron density. In the EAM potential, each atom is described as a positive nucleus surrounded by an electron cloud that is influenced by neighboring nuclei.

The EAM potential allows for the simulation of atomic-scale systems, taking into account both short and long-range interactions between atoms. The said potential is frequently employed to examine the mechanical and thermodynamic characteristics of various materials, encompassing properties such as thermal conductivity, diffusion, plasticity, fracture resistance, and more. Our research utilized MD simulation and EAM potential to study how incorporating Rhenium (Re) affects the structural and mechanical characteristics of Tungsten (W). To achieve this, we performed several nanoindentation experiments on samples of the alloy (W-Re), with a focus on how the addition of Re affected the dislocation mechanism and the mechanical characteristics of W, such as the reduced modulus of elasticity, hardness and yield stress. Our study also analyzed the total length of dislocation, number of dislocations, and dislocation density in samples with varying levels of Re addition. Additionally, we identified different types of dislocation structures.

Table 1. summary of the key properties of the Re EAM potential [7] and W EAM potential [8], E_c: cohesive energy (eV/atom); a: lattice parameter (Å); B: bulk modulus (GPa); C_{ij}: elastic constants (GPa); T_m: melting point (K); $E_{f(v)}$ and $E_{m(v)}$ are the vacancy formation energy (eV) and the vacancy migration energy (eV)

Property	E_c	a_0	B	$E_{f(v)}$	$E_{m(v)}$	C_{11}	C_{12}	C_{44}	T_m
W	-8.9	3.1652	309	3.58	3.58	520	204	161	4100±50
Re	8.03	2.7609	382	3.49	1.81	611	299	159	4836

2. INTERATOMIC POTENTIAL

In this study, the EAM potential is used to analyze various W-Re alloys compounds with different stoichiometric coefficients. The aim is to model and investigate the interactions between W and Re atoms, and characterize the elastic properties of these compounds, including the distinct interatomic interactions (W-W, Re-Re, and W-Re). Selecting the appropriate interatomic potential function for MD simulations is vital. This function determines the potential energy between two atoms, which is calculated through a sum of separation functions between atoms and their neighbors. The "EAM potential," which was created by Daw and Baskes [9] for studying metal defects, is used to determine the E_{tot} of an N-atom system, and it is defined by Equation (1):

$$E_{tot} = \sum_i F_i(\rho_i) + \frac{1}{2}\sum_{i\neq j}\varphi_{i,j}(r_{i,j}), \rho_i = \sum_{j\neq i} f_i(r_{ij}) \quad (1)$$

The equation for the total energy E_{tot} of the system involves the pair interaction energy $\varphi_{i,j}(r_{i,j})$ between atoms i and its neighboring atom j, the electronic density function $f_i(r_{ij})$, and an embedding function $F_i(\rho_i)$ that considers the influence of the metal's liberated electrons.

2.2. Simulation Procedure

This study examined the structural behavior of ($W_{(1-x)}$-Re_x) alloys with x=5, 10, and 25 at %Re using the LAMMPS open-source code [10] and the EAM potential suggested by Bonny and Bakaev [9]. The Cubic Body Center Structure (BCC), which has 512191 atoms, was the only component of the MD model, which was housed in a simulation box with the dimensions 200×200×200^3. The model comprised a 30Å radius spherical diamond indenter, in the x and y dimensions, periodic boundary conditions are implemented, as well as a freed surface in the z direction. The simulation box contains fixed, thermostatic, and Newtonian atoms, with a time step of 1fs. The upper substrate layer was immobilized during the simulation and a constant temperature of 300K was maintained in the thermostat atoms layer. The indenter's speed was set to 3 Å/ps. The centrosymmetric parameter (CSP) [11], the dislocation extraction algorithm (DXA) [12], and the common neighbor analysis (CNA) [13] were utilized to evaluate the MD simulation data using the OVITO program [14], and to study the dislocation processes that emerged during the nanoindentation process. Model for the simulation is shown in Figure 1.

We first built the atomistic system at the identical temperature and pressure settings, then we minimized and relaxed the model before continuously loading and unloading it during the nanoindentation procedure. In order to facilitate the deformation process, we chose one of the surface-free atoms as the "the initial contact atom" and positioned the spherical indenter above it (Figure 1). When the indenter made contact with the first contact atom, the loading process started, and when the desired deformation was attained, the unloading process started [15].

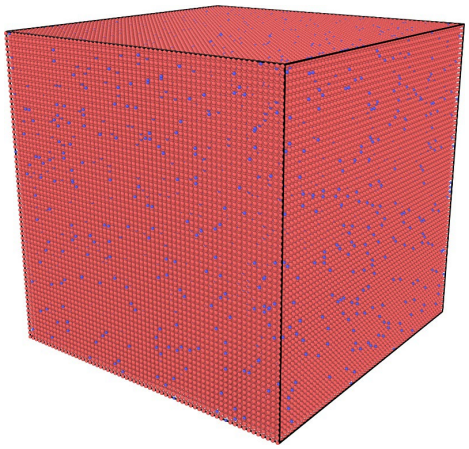

Figure 1. Sample of tungsten- 5% at Rhenium contained 512191 atoms (red color atoms of tungsten and blue color atoms of Rhenium)

3. RESULTS AND DISCUSSIONS

3.1. Force-Displacement Behavior

We performed nanoindentation tests at four different percentages of Re: 0%, 5%, 10%, and 25% at %Re. Throughout the tests, the temperature remained fixed at 300K, and we used a loading rate of 3Å/ps, using MD simulation with the EAM potential.

The simulation box size (200Å×200Å×200Å) contains single crystals of isotropic crystallographic orientations of body-centered cubic (bcc) lattice. The simulation box was equilibrated by the NVT ensemble. A rigid spherical indenter with a radius of 30 Å was used for the simulations. The lower 20 Å of the substrate remained fixed, and the region from 20 Å to 40 Å was designated as the thermostat atoms. The upper surface of the sample was considered a free surface.

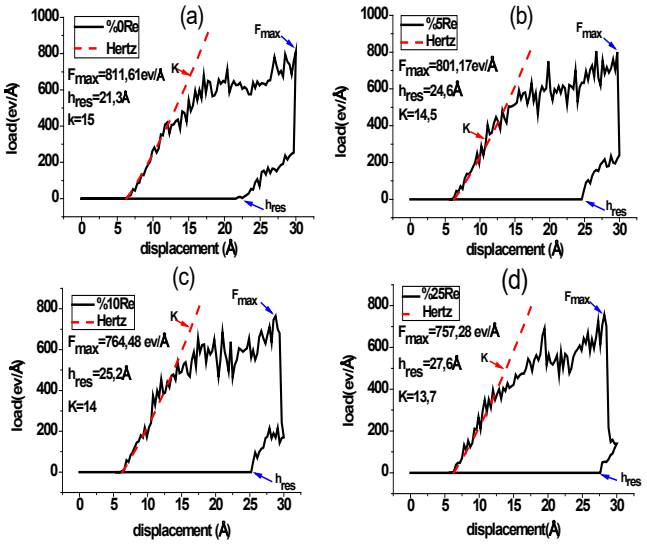

Figure 2. Load-Displacement curves of varying %Re

Table 2. Maximum indentation forces for different %Re

%Re	0%	5%	10%	25%
Maximum indentation forces (ev/Å)	811.61	801.17	764.48	757.28

The force-depth (*F-h*) curve of nanoindentation for ($W_{(1-x)}$-Re_x) with Re atomic fractions ranging from 5 to 25% at %Re is presented in Figure 2. All samples showed similar load-unload responses during nanoindentation. Discontinuous plastic events of (W-Re), representing the pop-in phenomenon, were observed. Indentation forces gradually increased with increasing depth of nanoindentation until reaching the maximum depth of 30 Å. Furthermore, the fluctuation of the *F-h* curves increased during the loading process due to hardening and plastic rearrangements. In the initial unloading phase, the nanoindentation force dropped sharply due to the immediate change in direction of the indenter movement. Eventually, when the indenter completely detaches from the substrate atoms, the force returns to zero, leaving behind residual plastic deformation. Interestingly, a decrease in the maximum indentation forces was observed with increasing Re concentration, as shown in Table 2.

The analysis of Charge-Displacement curves in this research yielded several mechanical properties of the material under study, such as the hardness (*H*), yield stress (*y*) and reduced elastic modulus (E_r). The Hertzian force was determined by calculating the average indenter force during the last 100 fs before the indenter's descent.

The Hertzian force can be calculated using the formula provided below [16]:

$$F = \frac{4}{3}(K.h^{\frac{3}{2}}),\ K = E_r.R^{\frac{1}{2}} \quad (2)$$

where, *R* representing the radius of the indenter (30Å), *h* is the depth of indentation, *K* is the slope of the elastic portion of the load-depth curve, and E_r is the reduced elastic modulus. Expressing the hardness value (*H*) can be done in the following manner:

$$H = \frac{F_{\max}}{A} \quad (3)$$

The maximum load, denoted by $F_{\max}$, represents the greatest force applied during the test and the equation below is employed to calculate the projected contact area, A [16, 17]:

$$A \approx 2\pi R h_{res} \quad (4)$$

The residual depth is represented by h_{res}, and *R* is the indenter's radius. The Table 3 presents the results of the calculated hardness, yield stress and reduced elastic modulus values for various %Re, for the purpose of comparison and study.

Table 3. Measurements of reduced elastic modulus and hardness (in GPa) were taken for all %Re

%Re	0%	5%	10%	25%
Reduced elastic modulus E_r (GPa)	350.8	329.07	322.66	307.28
Hardness *H* (GPa)	35.8	35.44	32.3	31.9
Yield stress *y* (GPa)	11.93	11.81	10.76	9.1

The results of our investigation indicate that adding %Re to W causes a reduction in hardness, decreased Young's modulus, and yield stress, as demonstrated in Table 3. Specifically, we compared the value of the reduced Young's modulus of tungsten pure sample, which was found to be approximately 350.8 GPa, with the value for solid W [18], which is approximately 410 GPa. In another study, Kang, et al. [19] experimentally found a Young's modulus value of approximately 323.6 GPa for polycrystalline W using nanoindentation and Nano scratch tests [20]. Furthermore, our simulations indicate that hardness generally decreases with increasing %*Re*, with values ranging from 31.9 to 35.8 GPa. We compared the value of 35.8 GPa, found for the hardness of a pure tungsten (W-0%Re) sample, with a value of approximately 35 GPa, which is almost equal to that found by Saurav Goel, et al. [21], namely *H* = 35 GPa. The study conducted by Peter et al. [22] highlighted an interesting phenomenon concerning BCC alloys at low temperatures. The results showed that the yield strength of W at 77 K decreased with increasing Re content.

3.1. Effect of Re Fraction in W on Dislocation Density

This section will employ the Ovito software to examine how the addition of %Re to W metal affects three key properties: dislocation density, number of dislocation segments and total dislocation length. Moreover, different types of dislocation structures were identified for various %Re, including 0%, 5%, 10%, and 25%, at a depth of *h*=30 Å, utilizing the DXA technique.

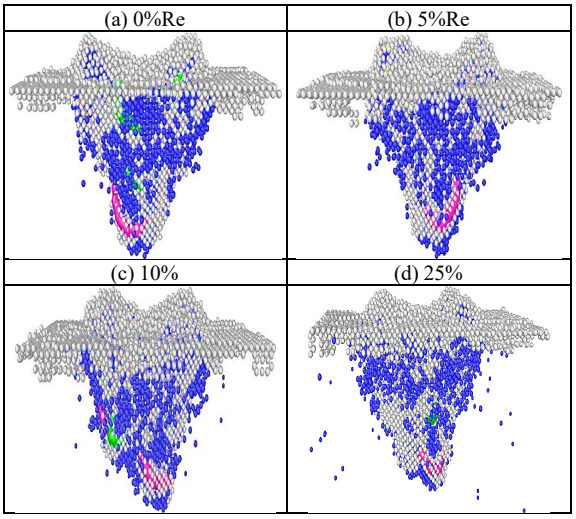

Figure 3. snapshots the dislocation network that formed at the maximum indentation depth of 30Å for different %Re

The dislocation density ρ_{disl} was determined using the following formula [24, 29]:

$$\rho_{disl} = \frac{L}{2\pi R_{plast}^3 / 3 - 2\pi R^3 / 3} \quad (5)$$

where, L represents the total length of the dislocation, R denotes the maximum depth of the indentation, while R_{plast} represents the radius of the plastic material.

Table 4. The total length of dislocation, number segments of dislocation and type of dislocation, were determined at 30Å across all %Re

%Re	0%	5%	10%	25%
Total length of dislocation (Å)	41.35	61.81	95.12	114.49
Number Segments of dislocation	2	2	4	5
Type of dislocation	*b*=1/2<111> and *b*=<100>	*b*=1/2<111> and *b*=<100>	*b*=1/2<111> and *b*=<100>	*b*=1/2<111> and *b*=<100>

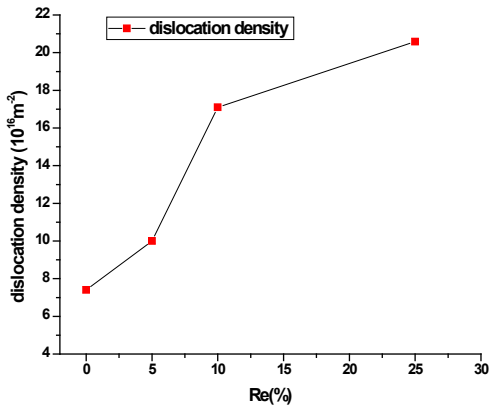

Figure 4. Relationship between Dislocation Density and Re Addition

Figure 3 shows the snapshots the dislocation network that formed at the maximum indentation depth of h=30Å for different %Re: 0%, 5%, 10%, and 25%. The details of these dislocations have been summarized and are presented in Table 4. The results of our analysis have revealed the existence of two primary categories of dislocations characterized by Burgers vectors of b = 1/2 ⟨111⟩ (represented by green) and b = ⟨100⟩ (represented by pink). It is interesting to note that these types of dislocations are similar to those observed in other BCC metals such as single crystalline Mo [23], Fe biocrystal [24], and Nano twinned Ta [25].

By examining the total lengths and numbers of dislocations present in the samples, we were able to observe a significant increase in the latter with the addition of Re, as shown in Table 4. This finding shows that the presence of Re in (W) causes the density of dislocations to increase as shown in Figure 4. Overall, the addition of Re to W can have a significant impact on dislocation behavior and the mechanical properties of the alloy. These findings have important implications for the development of new W-Re alloys with tailored mechanical properties for specific applications.

4. CONCLUSIONS

Our study employed MD simulation and EAM potential to investigate how the mechanical properties of W-Re alloys are affected by varying %Re via nanoindentation testing has allowed for the discovery of important information about dislocation mechanisms during nanoindentation. The results obtained from this simulation have led to the following conclusions:

- Using molecular dynamics (MD) to model the nanoindentation of W-Re alloy enables predicting deformation mechanisms and calculating mechanical properties with high accuracy. Additionally, this technique provides detailed information about the microstructure of the alloy, which is often difficult to obtain with other experimental methods. It also allows establishing a correlation between the mechanical behavior during deformation and the microscopic arrangement of atoms in the alloy.
- The first important conclusion of this study is that the addition of %Re to W results in a decrease in hardness, reduced elastic modulus, and yield strength. This is due to the fact that the addition of Re disturbs the ideal crystalline structure of W, leading to a reduction in the material's strength.
- In addition, this study found two different forms of dislocations with the Burgers vectors b = 1/2 ⟨111⟩ and b = ⟨100⟩.
- Moreover, the findings of this study indicate that dislocation density, Number Segments of dislocation and total length of dislocation increase upon adding Re to W.

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