Effect Of Temperature On Hardness And Elastic Modulus In Tungsten-Rhenium Alloy: Study By Dynamics Molecular

Toufik Karafi, Abdellah Tahiri, Mohamed Idiri, Brahim Boubeker

Abstract: In this work we performed a series of nanoindentations test on tungsten-rhenium (W-Re) alloys, using Molecular Dynamics simulations and Embedded Atom Method potential. We studied in first the temperature effect from 300K to 2000K on hardness and elastic modulus, we were interested later to defect mechanisms in (W-Re) alloys with a penetration rate of 3Å/ps and the Re concentration is also kept fixed as 5%Re.We found a decreased in reduced elastic modulus Er and the hardness H with the increase in temperature. The found results are in good agreement with the literature.

Index Terms: Tungsten-Rhenium alloy, nanoindentation, molecular dynamics simulations, mechanical property, temperature, defect mechanisms, hardness, elastic modulus.

1 INTRODUCTION

Nanoindentation testing is a simple method that consists principally of touching the material of interest. Among of mechanical properties are hardness, elastic modulus and defect mechanisms. It is not only used to gather information about the elastic modulus and hardness of a material [1,2] but also provides insights into cracking mechanisms [3], fracture toughness [4], strain-hardening [5], creep [6], nucleation of the defects [7]. The combination of the modern experimental testing method with the Oliver–Pharr [8] analysis has led to a widespread utilization of nanoindentation testing. Tungsten-Rhenium (W-Re) has been investigated by many research interests during the past years, because used wider applications in aerospace, electronic machine, bio-pharmaceutical, and other fields [9-14]. Molecular Dynamics (MD) is a simulation tool used to understand the properties of molecule assemblies based on their structure and microscopic interactions with each other [15-17], where Embedded Atomic Method (EAM) as an interatomic interaction potential was used [18]. In this work, we carried out a series of nanoindentations tests on W-Re alloy single crystal samples, using simulation by the method of MD with the EAM interaction potential to study the temperature effect on the mechanical behavior and the structure proprieties of W-Re alloy.

2 METHODOLOGY RESULTS AND DISCUSSIONS

2.1 interatomic potential

In MD simulation, the choice of interatomic the potential function is very important. The potential of the integrated atomic method describes the energy between the two atoms present. Energy is a sum of functions of separation between atoms and its neighbors. It was developed by Daw and Baskes (1984) [19] to study the defects of metals. The total energy ($Etot$) of a system N atom is given by:

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

Where E is the total energy of the system, $\varphi_{i,j}(r_{i,j})$ represents the pair interaction energy between an atoms i and its neighboringatom j, $f_i(r_{ij})$ is the electronic density function, and $F_i(\rho_i)$ represents an embedding function accounting for the effects of the free electrons in the metal [20].

2.2 Sample preparation

In this paper, all the simulations are carried out by using an open code LAMMPS [21] from the view of MD simulations using the EAM potential by Bonny and Bakaev [22] is used to study the structural behavior of W-5%Re alloys. The simulation model is shown in Fig.1.In MD model investigated in this study consisted of the spherical diamond indenter (30Å radius). The size of the simulation box is 200*200*200Å^3, consisting of 512191 atomsas a single crystal of the Cubic Body Center Structure (BCC).Periodic boundary conditions were used in the lateral direction (x and y) and a free surface in the indenting direction (z), using a time step of 1fs,In addition, three types of atoms are used to construct the simulation box : fixed atoms, thermostat atoms and Newtonian atoms. The lower layer of atoms in the substrate is kept fixed in space, and the layer adjacent to them is fixed at a constant temperature of 300K, The indenter velocity is set to be 3Å/ps. To visualize and analyze the MD simulation result, we is used the OVITO software [23], we are used centrosymmetry parameter (CSP) [24], Common neighbor analysis (CNA) [25],and dislocation extraction algorithm (DXA) [26] to study the Mechanisms of dislocation during the nanoindentation process.

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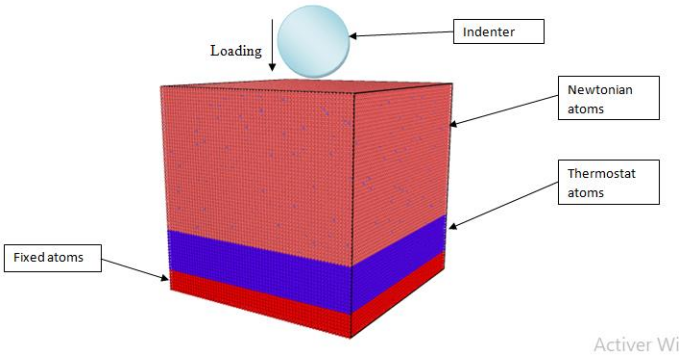

Fig. 1 Simulation model of the nanoindentation process.

3 Results and discussions

3.1 Temperature effect during nano-indentation test

The various temperatures used for the process of nano-indentation are 300K, 500K, 1000K and 2000K. Along with that the Re concentration is also kept fixed as 5%Re and loading rate as 3Å/ps for all the four temperatures.

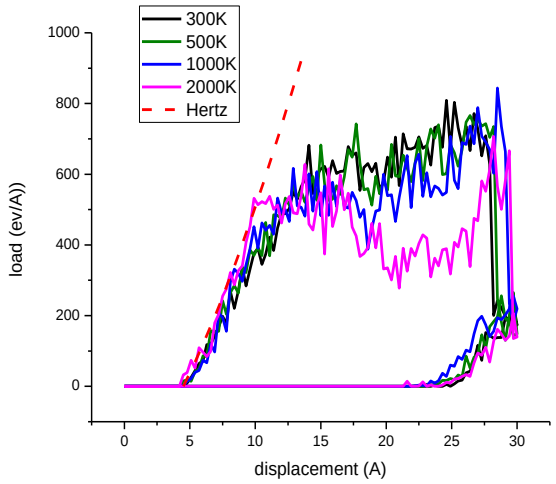

Fig.2 Load-Displacement curves of various temperatures (300K, 500K, 1000K and 2000K) at W-5%Re and 3Å/ps. Fig. 1 Simulation model of the nanoindentation process.

The indenter force was get from an average of the instantaneous indenter force over the last 100 fs before the indenter is moved down. The force in hertzian theory is given by:

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

(2)

Where R the radius of the indenter (30 Å), h is the indentation depth and Er is the reduced elastic modulus given by:

$$E_r = \frac{E}{1-\vartheta^2}$$

(3)

The hardness, H, is given by:

$$H = \frac{\mathrm{F_{max}}}{\mathrm{A}}$$

(4)

Where $\mathrm{F_{max}}$ is the maximum load and A is the projected contact area, calculated using the following equation [7]:

$$\mathrm{A} \approx 2\pi \mathrm{R h_{res}}$$

(5)

Where R is the radius of the indenter and $\mathrm{h_{res}}$ is the residual depth.

Fig. 2 shows the load-displacement curve at load rate levels of 3Å/ps at different temperatures. The table below shows the values of the results obtained after the nano-indentation test simulation for reduced elastic modulusand the hardness for various temperatures.

Table:1 reduced elastic modulus and Hardness measurements (GPa), for all temperatures T (K).

Temperatures (K)	300K	500K	1000K	2000K
Reduced elastic modulus E_r(GPa)	329.07	319.07	291.67	271.27
Hardness H(GPa)	35.44	31.24	30.5	29.7

We plotted the results of table 1 in Fig. 3 which presents the variation of the temperature vs to the reduced elastic modulus and Hardness.

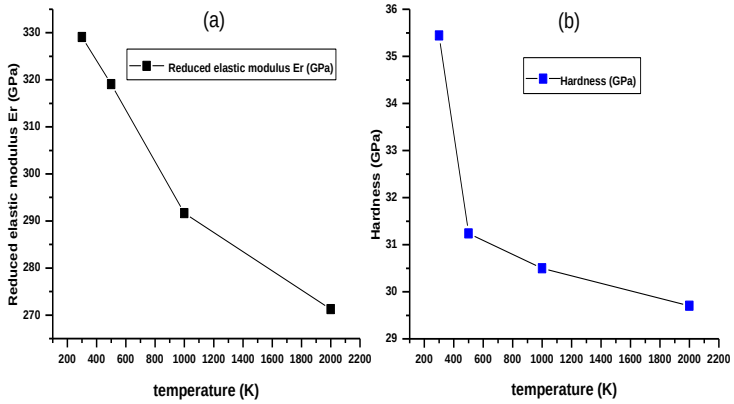

Fig.3 Mechanical properties of W-5%Re alloys at different temperature under nanoindentation test: (a) reduced elastic modulus. (b) Hardness.

From Fig.3 and table 1.we can see that the reduced elastic modulus and hardness decrease with the increased temperature. This was because of thermal softening. The indentation thermal softening occurred as a result of the material dislocation propagation that easily slips at high temperature or high kinetic energy. However, the interaction binding energy of the work piece decreases when the temperature increases, and thus resulting in the decrease of material hardness from the microscale level. The Lebedev et al. [27] microscale experimental investigation explains this phenomenon where the elastic modulus decreased when the temperature rose in sub-microcrystalline copper. The increase in temperatures causes the force-displacement curves to fluctuate as a result of the vibration of atoms and the nucleation of voids at the depth of indentation within the

substrate.

3.2 Mechanisms of phase transformation during nanoindentation process

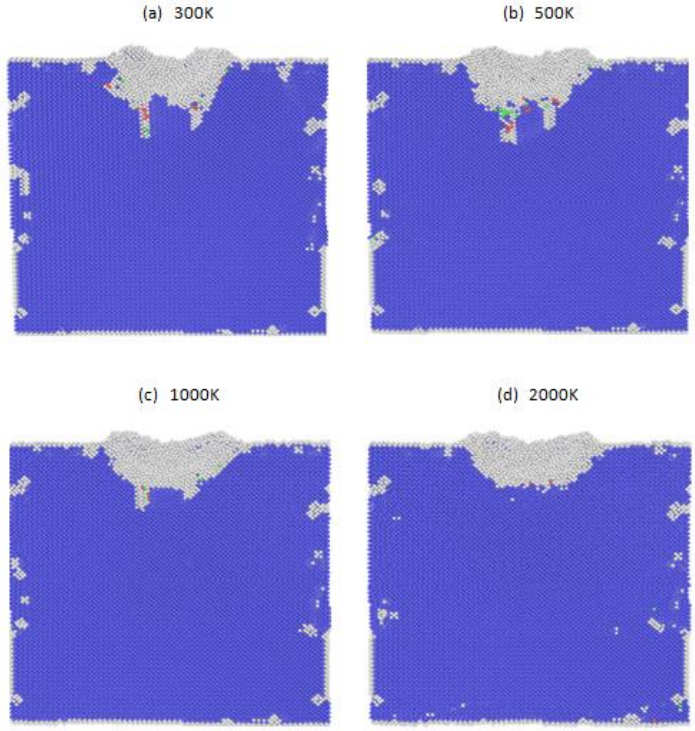

Fig.4 Deformation behaviour of the specimen at the maximum indentation depth at different temperatures: (a) 300K, (b) 500K, (c) 1000K, (d) 2000K.

Fig.4 displays the deformation behavior of the specimen at the maximum indentation depth at different temperatures. Atoms are colored by green, red and gray to denote their belongings in FCC, HCP and disordered structure [28].

3.3 Mechanisms of dislocation during nanoindentation process

Fig.5.shows the dislocation network formed at the maximum indentation depth of 30Å for the (a) 300K, (b) 500K, (c) 1000K and (d) 2000K.Two major types of dislocations with Burgers vectors b = 1/2 ⟨111⟩ (green colour) and b = ⟨100⟩ (pink colour) were revealed. The results are presented in Fig. 4 and Fig. 7(a) showing: we observe in the range 300K and 500K an increase in the dislocation lines and in the range 500K and 2000K a decrease in the dislocation lines. This agrees with earlier works [29].

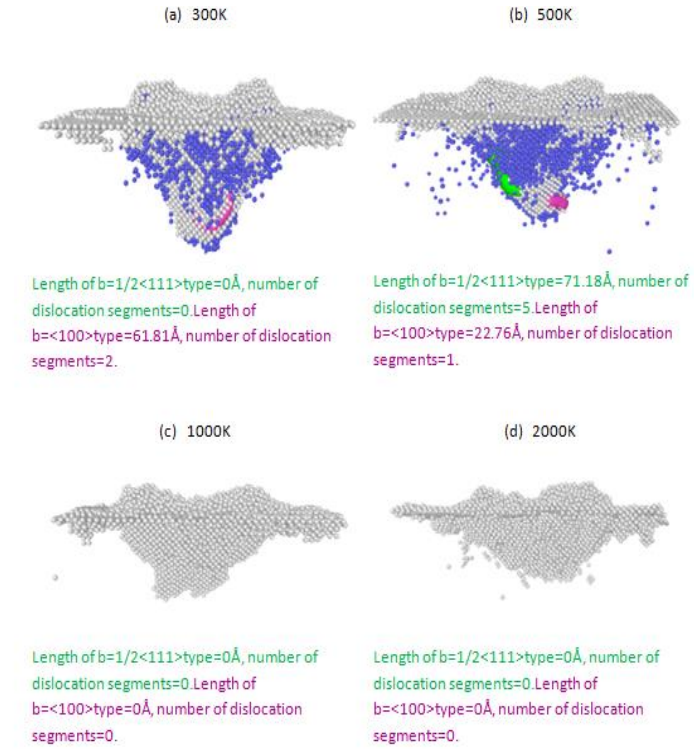

Fig.5 Snapshots in the XY planes obtained from DXA processing shows plastic deformation zone, crystal defects and free surfaces comparing sample defects created for: (a) 300K, (b) 500K, (c) 1000K, (d) 2000K at a penetration depth of 30Å. Dislocations with b = 1/2 ⟨111⟩ are shown in green and b = ⟨100⟩ are shown in pink.

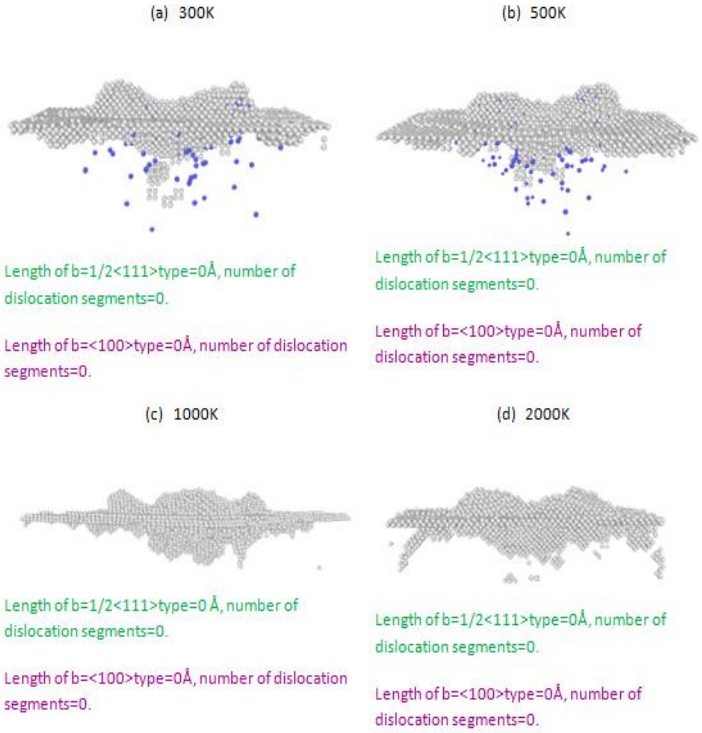

Fig.6 Snapshots in the XY planes obtained from DXA processing shows plastic deformation zone, crystal defects and free surfaces comparing sample defects created for: (a) 300K, (b) 500K, (c) 1000K, (d) 2000K at a unloading. Dislocations with b = 1/2 ⟨111⟩ are shown in green and b = ⟨100⟩ are shown in pink.

Fig.6. shows the dislocation network formed at the unloading indentation for the (a) 300K, (b) 500K, (c) 1000K, (d) 2000K, we observed a decrease in the total dislocation length up to 0 for all temperatures; these are also highlighted in Fig. 7(b).

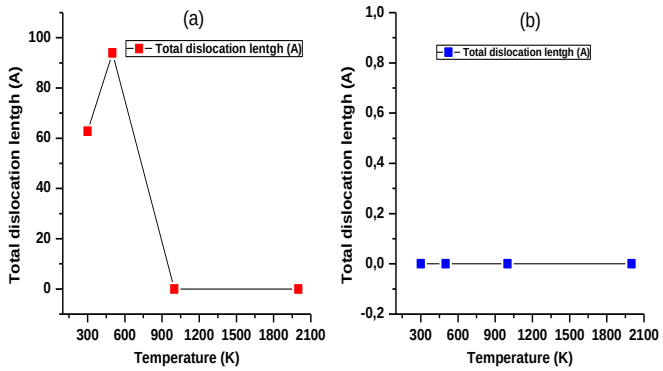

Fig.7 Total dislocation length as a function of concentration of Re at: (a) the loading indentation and (b) the unloading indentation.

4 CONCLUSION

In this study, MD simulation was used to study the temperature effect by nanoindentation test on the of W-5%Re alloys. The study of the mechanical properties of W-5%Re alloys and the Mechanisms of dislocation during nanoindentation made it possible to draw the following conclusions:

1) The Reduced elastic modulus and the hardness of the W-5%Re alloy decreased with increasing temperature.

2) The total length of the dislocation in the case of loading indentation increase in the range 300K and 500K and in the range 500K and 2000K a decrease of the total length of the dislocation.

3) The total length of the dislocation in the case of unloading indentation decrease up to 0 for all temperatures.

REFERENCES

[1] A.C. Fischer-Cripps, Nanoindentation, Mechanical Engineering Series, 2nd edition, Springer, New York, 2004.

[2] R. Armstrong, W. Elban, S. Walley, Int. J. Mod.Phys. B 27 (08) (2013).

[3] E. Weppelmann, M. Wittling, M.V. Swain, D. Munz, Indentation cracking of brittle thin films on brittle substrates, in: R.C. Bradt, D.P.H. Hasselman, D. Munz, M. Sakai, V.Y. Shevchenko (Eds.), Fracture Mechanics of Ceramics, Springer, Boston, MA, USA, 1996, pp. 475–486.

[4] A.A. Volinsky, J.B. Vella, W.W. Gerberich, Thin Solid Films 429 (1–2) (2003) 201–210.

[5] B. Yang, L. Riester, T. Nieh, Scr. Mater. 54 (7) (2006) 1277–1280.

[6] P.M. Sargent, M.F. Ashby, Mater. Sci. Technol. 8 (7) (1992) 594–601.

[7] A. Bendavid, P. Martin, H. Takikawa, Thin Solid Films 360 (1–2) (2000) 241–249.

[8] W.C. Oliver, G.M. Pharr, J. Mater. Res. 7 (06) (1992) 1564–1583.

[9] Tian, B., Yu, Q., Zhang, Z., Du, Z., Ren, W., Shi, P., & Jiang, Z. (2018).Effect of magnetron sputtering parameters on adhesion properties of tungsten-rhenium thin film thermocouples. Ceramics International. doi:10.1016/j.ceramint.2018.08.334.

[10] Tian, B., Zhang, Z., Shi, P., Zheng, C., Yu, Q., Jing, W., & Jiang, Z. (2017). Tungsten-rhenium thin film thermocouples for SiC-based ceramic matrix composites.Review of Scientific Instruments, 88(1), 015007. doi:10.1063/1.4973967

[11] T. Palacios, J. Reiser, J. Hoffmann, M. Rieth, A. Hoffmann, J. Pastor, Microstructural and mechanical characterization of an nealed tungsten (W)and potassium-doped tungsten foils, Int. J. Refract. Met. H. 48 (2015) 145–149.

[12] J. Kappacher, A. Leitner, D. Kiener, et al. / Materials and Design 189 (2020) 108499,Thermally activated deformation mechanisms and solid solution softening in W-Re alloys investigated via high temperature nanoindentation.

[13] AbdellahTahiri, Mohamed Idiri, BrahimBoubeker (2020), Mechanicals Behaviors of Tungsten-Rhenium Alloy Single Crystals from 77K to 300K - Atomic Simulation Study. International Journal of Engineering Research in Africa, 177-181

[14] Chen-hao QIAN, et al/Trans, Microstructure and hardness of W−25Re alloy processed by high-pressure torsion, Nonferrous Met. Soc. China 27(2017) 2622−2629.

[15] H.A. Wu, X.X. Wang, X.G. Ni, Acta. Meta.Sin. 38 (2002) 1219–1222.

[16] Gupta, Tibra Das, et al. “Temperature and Strain Rate Dependent Mechanical Properties of a Square Nickel Plate with Different Shaped Central Cracks: A Molecular Dynamics Study.” Journal of Nano Research, vol. 55, Trans Tech Publications, Ltd., Nov. 2018, pp. 32–41. Crossref, doi:10.4028/www.scientific.net/jnanor.55.32.

[17] Zhang, Yan, et al. “Study of Processability of Cu/Ni Bilayers Using Molecular Dynamics Simulations.” Journal of Nano Research, vol. 52, Trans Tech Publications, Ltd., May 2018, pp. 43–53. Crossref, doi:10.4028/www.scientific.net/jnanor.52.43.

[18] G. Bonny, A. Bakaev,.D.Terentyev, and Yu. A. Mastrikov, Interatomic potential to study plastic deformation in tungsten-rhenium alloys, J. Appl. Phys. 121, 165107 (2017).

[19] F. F. Abraham, R. Walkup, H. Gao, M. Duchaineau, T. D. D. L. Rubia, and M. Seager,—Simulating materials failure by using up to one billion atoms and the world’s fastestcomputer: Work-hardening,‖ Proc. Natl. Acad. Sci., vol. 99, no. 9, pp. 5783–5787, Apr.2002.

[20] Finnis M. Interatomic Forces in Condensed Matter. Oxford University Press 2003;129-186

[21] S. Plimpton, Fast parallel algorithms for short-range molecular dynamics, J. Comput. Phys. 117 (1995) 1–19. doi:10.1006/jcph.1995.1039.

[22] G. Bonny, A. Bakaev,.D.Terentyev, and Yu. A. Mastrikov, Interatomic potential to study
plastic deformation in tungsten-rhenium alloys, J. Appl. Phys. 121, 165107 (2017).

[23] A. Stukowski, Visualization and analysis of atomistic simulation data with OVITO--the Open Visualization Tool, Model. Simul.Mater.Sci.Eng. 18 (2009) 15012.

[24] C.L. Kelchner, S.J. Plimpton, J.C. Hamilton, Dislocation nucleation and defect structure during surface indentation, Phys. Rev. B. 58 (1998) 11085.

[25] J.D. Honeycutt, H.C. Andersen, Molecular dynamics study of melting and freezing of small Lennard-Jones clusters, J. Phys. Chem. 91 (1987) 4950–4963.
[26] A. Stukowski, K. Albe, Extracting dislocations and non-dislocation crystal defects from atomistic simulation data, Model. Simul.Mater.Sci. Eng. 18 (2010) 85001.
[27]Lebedev, A.B.; Burenkov, Y.A.; Romanov, A.E.; Kopylov, V.I.; Filonenko, V.P.; Gryaznov, V.G. Softening of the elastic modulus in submicrocrystalline copper. Mater.Sci. Eng. A 1995, 203, 165–170.
[28] J. Li, Q.H. Fang, Y.W. Liu, L.C. Zhang, A molecular dynamics investigation into the mechanisms of subsurface damage and material removal of monocrystalline copper subjected to nanoscale high speed grinding, Appl. Surf. Sci. 303 (2014) 331–343.
[29]T.M. Pollock and R.D. Field, Dislocations and High-Temperature Plastic Deformation of Superalloy Single Crystals, Dislocations in SolidsVolume 11, 2002, Pages 547-618.