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Research Article

Unveiling the wide-temperature tribological mechanisms of (MgCoNiCuZn)O high-entropy oxide: The critical role of dynamic CuO precipitation and re-dissolution

Rui Deng¹, Junhong Jia^{1,2,*}, Junjie Xi¹, Jie Yang¹, Nairu He¹, Yun Shi¹, Haichao Zhao^{3,*}

¹ College of Mechanical and Electrical Engineering, Shaanxi University of Science and Technology, Xi 'an 710021, China

² State Key Laboratory of Solid Lubrication, Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences, Lanzhou 730000, PR China

³ National Engineering Research Center for Remanufacturing, Army Academy of Armored Forces, Beijing 100072, China

Corresponding author. E-mail address: jhjia@sust.edu.cn (J. Jia), zhchebei@sina.com (H. Zhao)

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Abstract:

The rock-salt structured (MgCoNiCuZn)O high-entropy oxide (HEO) ceramics exhibit great potential for high-temperature applications, yet its tribological behavior across a wide temperature range remains to be fully deciphered. This work systematically investigated the wide-temperature tribological mechanisms of (MgCoNiCuZn)O from room temperature (RT) to 800 °C. The results indicate that the HEO's hardness and wear resistance displayed a non-monotonic dependence on temperature, while simultaneously demonstrating a reversible entropy-driven phase transition. At 400 °C, thermodynamic instability triggered CuO precipitation, which disrupts the high-entropy structure and leads to a significant degradation in hardness and increased the wear rate. However, at the elevated temperature of 800 °C, an entropy-driven re-dissolution of CuO partially restores the high-entropy structure, leading to a recovery in hardness. Concurrently, a continuous, lubricious oxide film formed on the worn surface. Density functional theory (DFT) calculations reveal that the low binding energy and high electron activity of CuO underpin its preferential precipitation and its key role in forming the Cu-rich oxide lubricating film. The synergy between phase re-stabilization and surface film formation results in excellent high-temperature wear resistance, with a minimum wear rate of approximately $0.53 \times 10^{-5} \text{ mm}^3 \cdot (\text{N} \cdot \text{m})^{-1}$ at 800 °C. This work elucidates the phase evolution and tribological mechanisms of HEO across a wide temperature range, providing valuable guidance for designing advanced wear-resistant materials for extreme environments.

Keywords: (MgCoNiCuZn)O; Friction and wear behavior; Lubrication mechanisms; DFT calculations

1 Introduction

Friction and wear constitute primary factors leading to premature failure of mechanical components. The development of high-performance wear-resistant structural materials is crucial for enhancing the operational reliability and service life of equipment [1, 2]. However, in traditional alloy design systems, the structure and properties of materials are often dominated by a single principal element. This paradigm has long confined researchers to the conventional concept of a "limited chemical space," thereby constraining breakthroughs in material performance [3, 4]. The emergence of high-entropy alloys (HEAs) has broken through this traditional design paradigm. Their multi-principal-element nature endows the material system with extremely high configurational entropy, enabling the stable formation of simple solid-solution phase structures. Consequently, HEAs exhibit outstanding comprehensive properties, including high strength, high hardness, and excellent wear resistance, opening a new pathway for designing and developing the next generation of high-performance wear-resistant materials [6-8].

Building upon the success of HEAs, the research scope of the high-entropy concept in materials science has expanded from initial alloy systems to oxide ceramic systems [9]. Rost et al. [10] pioneered the application of high-entropy design

principles to oxide ceramics, successfully developing a new class of high-entropy oxide (HEO) materials. Among HEO, the rock-salt structured (MgCoNiCuZn)O, as one of the earliest reported high-entropy oxide systems, demonstrates broad application prospects in high-temperature components and structural materials due to its simple structure, flexible compositional tunability, and excellent comprehensive properties. Song et al. [11] obtained (MgCoNiCuZn)O bulk material with a hardness of approximately 7 GPa using microwave sintering. Research by Chen et al. [12] indicates that under sintering conditions at 900 °C, (MgCoNiCuZn)O can achieve a maximum flexural strength of 323 MPa and an elastic modulus of 108 GPa. Beyond mechanical properties, the structural stability of (MgCoNiCuZn)O at elevated temperatures is of paramount importance. Lu et al. [13] experimentally revealed the reaction sequence of the oxide components in (MgCoNiCuZn)O, noting that MgO and CoO react first, while CuO participates last. Gao et al. [14] further discovered that (MgCoNiCuZn)O exhibits reversible phase transformation characteristics during heat treatment: phase separation occurs at low temperatures, and reheating to high temperatures can restore a single rock-salt phase.

With the deepening of research on high-entropy oxide materials, the rock-salt structured (MgCoNiCuZn)O has been demonstrated to exhibit excellent mechanical properties. However, its friction and wear behaviors, particularly the dynamic interplay between reversible phase transitions and the resultant lubrication mechanisms across a wide temperature range, remain elusive. Density Functional Theory (DFT) can simulate the phase structure evolution and interfacial chemical

reactions on material surfaces during high-temperature friction from atomic and electronic scales, providing a theoretical basis for understanding the high-temperature stability and wear behavior of (MgCoNiCuZn)O [15, 16]. Liu et al. [17] combined first-principles calculations with molecular dynamics simulations to investigate the interfacial bonding behavior of hydrogen-free diamond-like carbon films in nitrogen- and oxygen-containing environments, elucidating the corresponding friction and wear mechanisms. Guo et al. [18] utilized DFT calculations to reveal the regulatory role of niobium-containing oxides on the lubrication mechanisms of NiAl/Nb/Ag composite coatings and their enhancing effect on tribological performance. By analyzing the interactions and structural evolution between different metal oxides, they clarified the intrinsic connection between material structural evolution and wear models, offering new insights for the design and optimization of adaptive wear-resistant structural materials.

Current research on rock salt-structured (MgCoNiCuZn)O high-entropy oxide (HEO) has predominantly focused on its properties at ambient conditions, leaving its high-temperature tribological behavior insufficiently explored. This work systematically investigates the tribological performance evolution of (MgCoNiCuZn)O HEO across a wide temperature range from RT to 800 °C. By integrating experimental characterization with theoretical simulations, the phase evolution mechanisms of HEO are elucidated at the electronic-structure level. Furthermore, the dynamic precipitation and re-dissolution of CuO during friction processes are clarified, revealing their critical role in modulating the tribological

performance of HEO.

2 Experimental procedures

2.1 Sample preparation

The starting materials were CuO, NiO, ZnO, CoO, and MgO powders (purity > 99.9%, average particle size < 1 μm , supplied by Xinhua Metal Materials Co., Ltd.). After accurately weighing each component according to the equimolar ratio, they were placed in a planetary ball mill (from Greitman Instrument Equipment Co., Ltd.) for wet ball milling. The ball milling process was conducted at a rotational speed of 300 rpm for a total duration of 24 hours, using an intermittent operation method (30 minutes of operation followed by a 10-minute pause) to prevent overheating. The milling media consisted of zirconia jars and zirconia balls, with a ball-to-powder mass ratio set at 8:1. After ball milling, the mixed powder was placed in a vacuum drying oven and dried at 70 $^{\circ}\text{C}$ for 4 hours to obtain a homogeneous dried mixed powder. The mixed powder in a graphite die ($\Phi 30 \times 5$ mm) was then placed into a hot-pressing sintering furnace (Shanghai Chenhua Technology Co., Ltd.). The temperature was raised to 1000 $^{\circ}\text{C}$ at a ramp rate of 10 $^{\circ}\text{C}/\text{min}$ and held for 30 min under a uniaxial pressure of 35 MPa, yielding a bulk (MgCoNiCuZn)O high-entropy oxide ceramics.

2.2 Characterization

Phase composition of the specimens was performed using a Japanese SmartLab X-ray diffractometer (XRD) with Cu $K\alpha$ radiation ($\lambda = 0.15406$ nm). The scan rate was set at 1 $^{\circ}/\text{min}$ over a 2θ range of 20 $^{\circ}$ -80 $^{\circ}$, with operating parameters of 40 kV and

150 mA. The diffraction data of the specimens were refined using the Rietveld refinement method with GSAS-II software. The microstructure and wear morphology of the specimens was observed using a scanning electron microscope (SEM, TESCAN, Czech Republic), and the elemental composition (types and contents) was determined by energy-dispersive spectroscopy (EDS) attached to the SEM. The hardness from RT up to 800 °C was evaluated using a ZDHVZHT-30 high-temperature Vickers hardness tester under a load of 1000 g and a dwell time of 10 s, also with 10 repetitions per measurement. The density of the specimens was measured by the Archimedes water displacement method [19].

2.3 Tribological testing

To investigate the tribological performance of HEO over a wide temperature range, friction and wear tests were conducted at RT, 200 °C, 400 °C, 600 °C, and 800 °C. All wear test specimens ($\Phi 30 \times 5$ mm) were ground and polished to maintain consistent surface roughness. Both before and after the wear tests, all specimens were cleaned using ultrasonic cleaning. High-temperature wear tests were performed on an HT-1000 high-temperature friction and wear tester (Lanzhou Zhongke Kaihua). The test parameters were as follows: test duration of 30 minutes, Al_2O_3 ceramic ball (6 mm in diameter), rotation diameter of 10 mm, applied load of 10 N, motor frequency of 8.9 Hz, and rotational speed of 500 rpm. Three parallel experiments were performed. The wear rate was calculated according to Eq. 1 [20]:

$$W=V/(L \cdot F) \quad \text{Eq. 1}$$

Where W is the wear rate, ($\text{mm}^3 \cdot \text{N}^{-1} \cdot \text{m}^{-1}$), V is the wear volume (mm^3), F is the applied load (N), and L is the total sliding distance (m). The sliding distance L was calculated as: $L = 0.002 \times f \times t \times l$, where f is the motor frequency (Hz), t is the test time (s), and l is the friction stroke length (m). The wear volume (V) was measured using a DSX510 optical microscope (OLYMPUS, Japan).

2.4 DFT calculation

The crystal structures of the five constituent oxides of (MgCoNiCuZn)O were obtained from The Materials Project database. First-principles calculations based on density functional theory (DFT) were performed using the Cambridge Sequential Total Energy Package (CASTEP) module within Materials Studio software (Accelrys Inc.). During the calculations, geometric optimization was first carried out on the crystal structures of the aforementioned oxides. The final cut-off energies (E_{cut}) for the metal oxides CuO, NiO, ZnO, CoO, and MgO were all set to 710 eV, with corresponding k-point grids configured as $9 \times 9 \times 5$, $5 \times 5 \times 5$, $8 \times 8 \times 4$, $5 \times 5 \times 5$, and $5 \times 5 \times 5$, respectively. To evaluate the bonding characteristics of these metal oxides and their lubrication mechanisms during the friction process, the binding energy between the metal and oxygen atoms was calculated according to the following Eq. 2 [21]:

$$E_{\text{binding}} = E_{\text{total}} - E_{\text{slab}} - E_M \quad \text{Eq. 2}$$

Where, E_{binding} is the binding energy, E_{total} is the total energy of the optimized structure, E_{slab} is the total energy of the model after removing an individual metal atom, and E_M is the energy of an isolated metal atom.

3 Results and Discussion

3.1 Phase and Microstructure

Fig. 1 presents the XRD patterns of the mixed powders before and after sintering. The five binary metal oxides exhibit three distinct crystal structure types: MgO (PDF#45-0946), CoO (PDF#43-1004), and NiO (PDF#47-1049) possess the rock-salt phase structure, CuO (PDF#48-1548) adopts a monoclinic tenorite structure, and ZnO (PDF#36-1451) crystallizes in the hexagonal wurtzite structure [22]. As shown in Fig. 1, the characteristic diffraction peaks of the individual raw oxides remain present in the ball-milled mixed powders, indicating that the ball-milling process resulted primarily in physical mixing without inducing significant solid-state reactions or the formation of new phases. In contrast, after the sintering process, all diffraction peaks can be indexed to a single rock-salt phase structure, unequivocally demonstrating the successful formation of a complete solid solution within the HEO system.

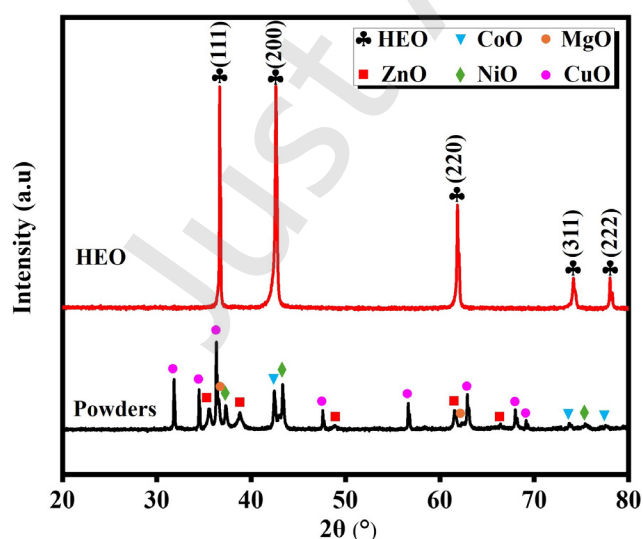


Fig. 1 XRD patterns of the specimens.

However, the monoclinic structure of CuO, with its low symmetry, differs fundamentally from the cubic rock-salt phase in terms of atomic stacking and bonding,

leading to a high interfacial strain energy and a high point defect density at the interface with the rock-salt structured matrix [23, 24]. Under the coupled local thermal and mechanical stresses generated by high-temperature friction, CuO, which has the highest structural mismatch, experiences a sharp increase in interfacial strain energy, thereby reducing its thermodynamic stability and favoring its precipitation from the HEO solid solution. Studies have indicated that even during the synthesis of certain rock-salt structured high-entropy oxides, CuO residual phases are frequently observed, corroborating the instability of CuO within HEO solid solutions [25].

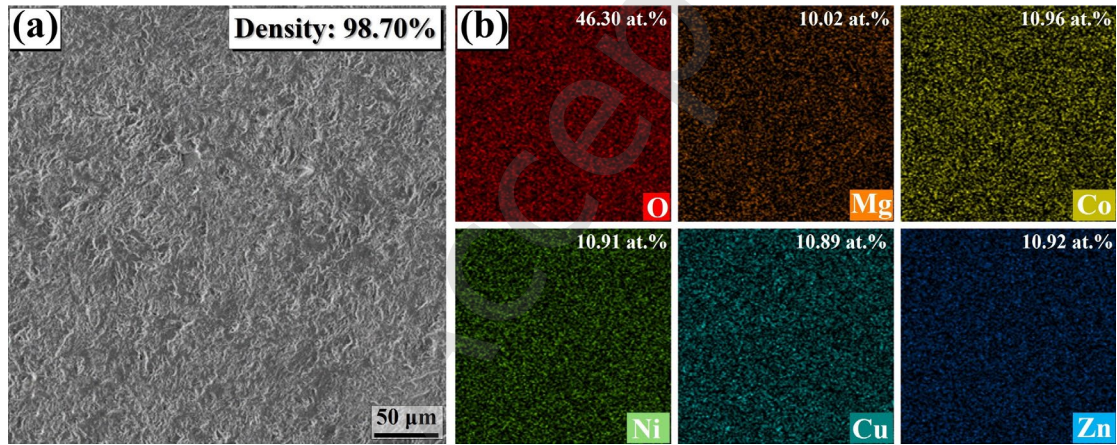


Fig. 2 Surface morphology and elemental distribution of HEO: SEM morphology; (b) Elemental distribution.

Fig. 2 presents the surface morphology and corresponding elemental distribution of the sintered HEO. The SEM image in Fig. 2(a) shows a dense, uniform surface without obvious pores or cracks, indicating successful densification of the HEO material. Elemental mapping analysis in Fig. 2(b) demonstrates that the five metallic constituents--Mg, Co, Ni, Cu, and Zn--are homogeneously distributed at the micrometer scale, with no significant segregation observed. Furthermore, quantitative EDS analysis confirms that the atomic percentages of these five metallic elements are

close to the equimolar ratio, which corroborates the successful formation of a compositionally homogeneous high-entropy solid-solution structure at the atomic scale.

3.2 Hardness and Phases at High-temperature

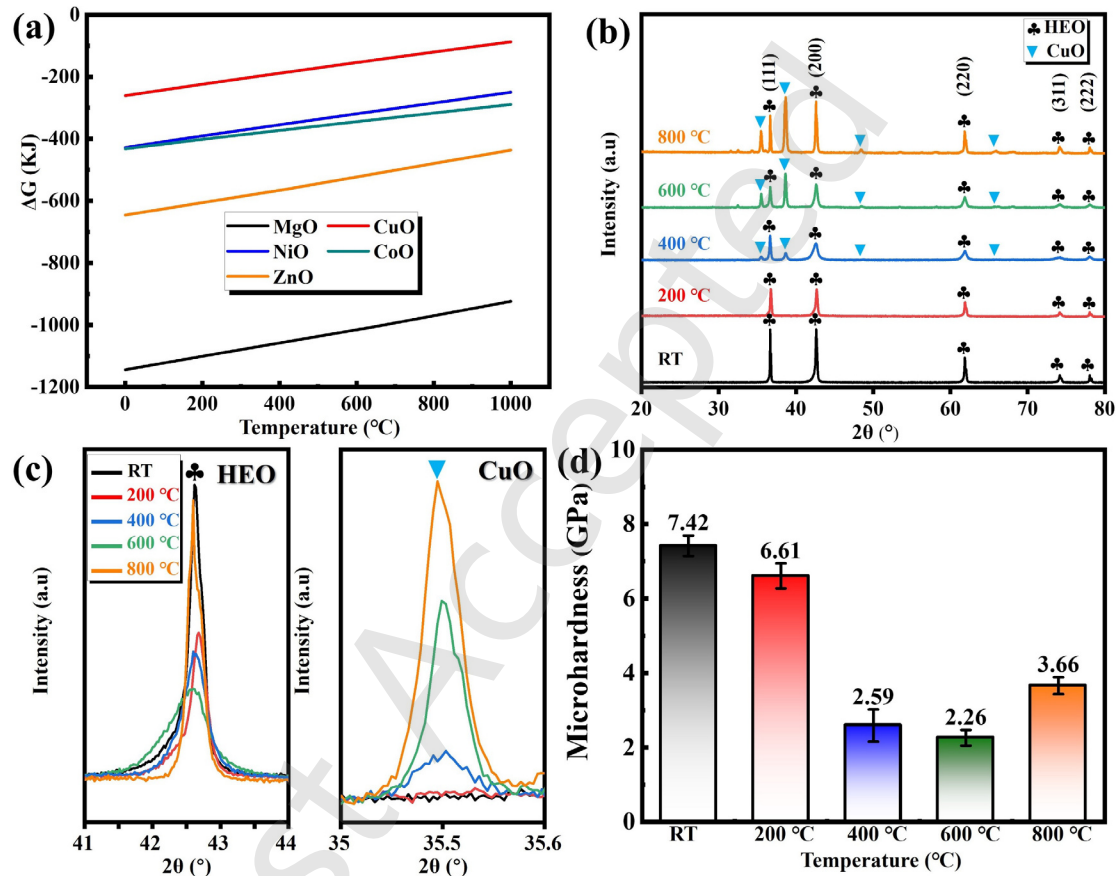


Fig. 3 Thermodynamic stability and phase evolution of the HEO: (a) Calculated Gibbs free energy of the five constituent binary oxides at different temperatures (b) In-situ XRD patterns of the HEO sample measured at different temperatures; (c) Magnified regions of the main diffraction peaks; (d) In-situ high-temperature hardness of the HEO.

(MgCoNiCuZn)O, as a prototypical entropy-stabilized oxide, exhibits a phase stability primarily governed by the competition between entropy (ΔS) and enthalpy (ΔH). Temperature variations predominantly drive phase transitions by altering the

configurational entropy of the system, which subsequently influences the properties of the HEO across a broad temperature range. Fig. 3 illustrates the evolution of phase composition and hardness of the HEO from RT to 800 °C. The thermodynamic equilibrium of the HEO system is disrupted at elevated temperatures, where differences in the Gibbs free energy among the constituent binary metal oxides become the key driver for phase separation in the HEO (Fig. 3a). Lou et al. [13] reported that within the (MgCoNiCuZn)O system, the relatively positive Gibbs free energy (ΔG) of CuO most readily meets the precipitation criterion at high temperatures. Concurrently, the relatively high positive enthalpy of Cu^{2+} further diminishes its solid-solution stability within the rock-salt matrix of the HEO. Driven by these thermodynamic factors, CuO tends to preferentially precipitate by overcoming the energy barrier through thermal activation [14, 24].

As shown in Fig. 3(d), the HEO exhibits a high room-temperature hardness of up to 7.42 GPa. This superior hardness originates from the four fundamental effects characteristic of high-entropy materials: the high-entropy effect, severe lattice distortion, sluggish diffusion, and the “cocktail effect” [10]. Notably, in the specific (MgCoNiCuZn)O system, the pronounced local Jahn-Teller distortion induced by Cu^{2+} ions further intensifies the lattice strain, which acts as a critical strengthening mechanism and contributes substantially to the overall hardness [26, 27].

As shown in Fig. 3(b), the HEO maintains a single rock-salt phase structure both at RT and 200 °C, with XRD patterns largely consistent with the as-synthesized sample, indicating excellent phase stability of the material at relatively low

temperatures. This phase stability is accompanied by only minor fluctuations in hardness (Fig. 3d), indicating that the high configurational entropy effectively counteracts the positive enthalpy of formation within this temperature range, thereby stabilizing the single-phase solid solution.

Phase separation in the HEO occurs when the temperature surpasses a critical threshold of 400 °C, at which point local unfavorable enthalpy changes override entropic stabilization [24]. The phase separation is primarily driven by Cu^{2+} ions, which exhibit a positive mixing enthalpy and a relatively low melting point. The incorporation of Cu^{2+} introduces significant Jahn-Teller distortion within the rock-salt structure lattice of the HEO [24]. To achieve a lower energy state, the system spontaneously undergoes geometric distortion, leading to substantial local lattice distortion and strain within the HEO rock-salt lattice. This contributes to a high positive enthalpy and reduces the formation energy of surrounding cation vacancies [28].

At 400 °C, the system is at a relatively low temperature where the stabilizing effect of configurational entropy is limited. Consequently, the system drives the precipitation of some Cu^{2+} ions to form the thermodynamically more stable tenorite-structured CuO, thereby reducing the local enthalpy (Fig. 3a). Although this sacrifices some configurational entropy, the overall Gibbs free energy is reduced. Despite a reduction in configurational entropy, the system's total Gibbs free energy is lowered, and the high-entropy structure is largely maintained (Fig. 3b). Nevertheless, the precipitation of CuO diminishes a crucial strengthening source: the lattice distortion

intensified by Cu^{2+} Jahn-Teller distortion is weakened, causing a pronounced drop in hardness. Moreover, the severe crystallographic mismatch between the precipitated tenorite CuO and the rock-salt matrix introduces high interfacial strain and a high density of point defects, resulting in mechanically weak interfaces and potential crack-initiation sites that further reduce the hardness [29]. The high-temperature thermal-softening process accelerates and exacerbates this degradation mechanism, resulting in a sharp decline in the hardness of the HEO to 2.59 GPa (Fig. 3d).

The phase separation of the HEO intensifies further at 600 °C, as indicated by a continued weakening of the rock-salt phase diffraction peaks in Fig. 3(c). This progressive phase precipitation is accompanied by a further reduction in the extent of Cu^{2+} Jahn-Teller distortion, along with more pronounced microstructural degradation and thermal softening. These combined effects lead to an additional decrease in hardness, which eventually reaches a minimum value of 2.26 GPa.

As the temperature increases to 800 °C, the continued precipitation of CuO further undermines the hardness of the HEO (Fig. S1). However, the elevated temperature simultaneously promotes atomic diffusion and mass transport between particles. Research [30] indicates that higher temperatures can effectively drive atomic diffusion and particle bonding, leading to densification of the ceramic material and thereby improving hardness to some extent [31]. Consequently, at 800 °C, despite the persistent structural weakening caused by CuO precipitation, the synergistic effect of thermally induced densification and sintering kinetics partially counteracts this detrimental influence. This results in a modest recovery of the HEO hardness,

reaching approximately 3.66 GPa.

3.3 Friction and wear behavior

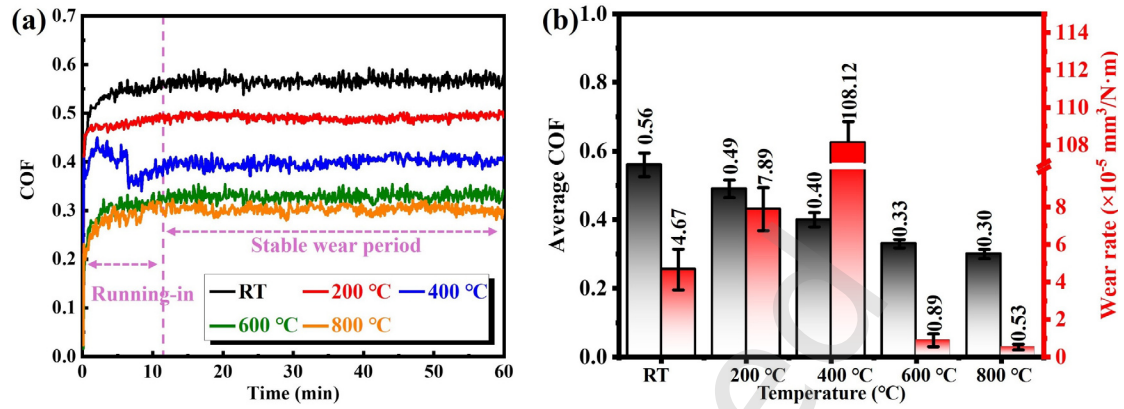


Fig. 4 Friction and wear properties of HEO across a wide temperature range: (a) Friction coefficient curves; (b) Average COF and wear rate.

The coupled effects of frictional heating and temperature-induced phase evolution govern the friction and wear behavior of the HEO. The evolution of the friction coefficient for the HEO as a function of temperature (from RT to 800 °C) is presented in Fig. 4(a). All specimens exhibited both a running-in stage and a stable wear stage. During the running-in period, the limited real contact area at the wear interface results in high localized contact stresses, leading to an unstable friction coefficient. Following approximately 12 minutes of sliding, continued mechanical loading induces work hardening in the near-surface region. This hardening reduces the friction force and, consequently, the adhesive interactions at the interface, thereby promoting a gradual stabilization of the friction coefficient [32].

The tribological behavior of the HEO evolves with increasing temperature, and the change in its wear resistance is closely associated with the precipitation and re-dissolution of CuO. As shown in Fig. 4(b), the average friction coefficient of the HEO

gradually decreases from approximately 0.56 at RT to about 0.30 at 800 °C. In contrast, the wear rate initially increases and then decreases with rising temperature, exhibiting a trend opposite to that of the hardness. At relatively low temperatures (RT and 200 °C), the HEO maintains a stable phase structure, resulting in high hardness and wear resistance. At 400 °C, the precipitation of CuO leads to the loss of the high-entropy strengthening effect, causing material softening and a sharp decline in both hardness and wear resistance; the wear rate reaches a maximum of approximately $108.12 \times 10^{-5} \text{ mm}^3 \cdot (\text{N} \cdot \text{m})^{-1}$. When the temperature rises to 600 °C, phase separation intensifies. The high-entropy effect and the hardness of the HEO are further reduced (Fig. 3). However, the accumulated CuO on the worn surface promotes the formation of a protective, lubricating oxide layer during sliding (Fig. 5h). Such oxide layers significantly influence tribological behavior [33]. A dense oxide layer effectively reduces shear stress at the interface between the wearing surface and the counterface while suppressing adhesive tendencies, thereby significantly enhancing the anti-wear capacity of the HEO [20, 34]. Consequently, the wear rate at 600 °C is significantly lowered.

At 800 °C, the wear resistance of the HEO is further enhanced. This improvement is attributed to the re-dissolution of CuO at elevated temperatures, which restores the high-entropy effect. Concurrently, a protective lubricating oxide layer forms on the worn surface. The synergistic interaction of these factors reduces the wear rate to a minimum of approximately $0.53 \times 10^{-5} \text{ mm}^3 \cdot (\text{N} \cdot \text{m})^{-1}$, demonstrating excellent anti-wear performance across a wide temperature range.

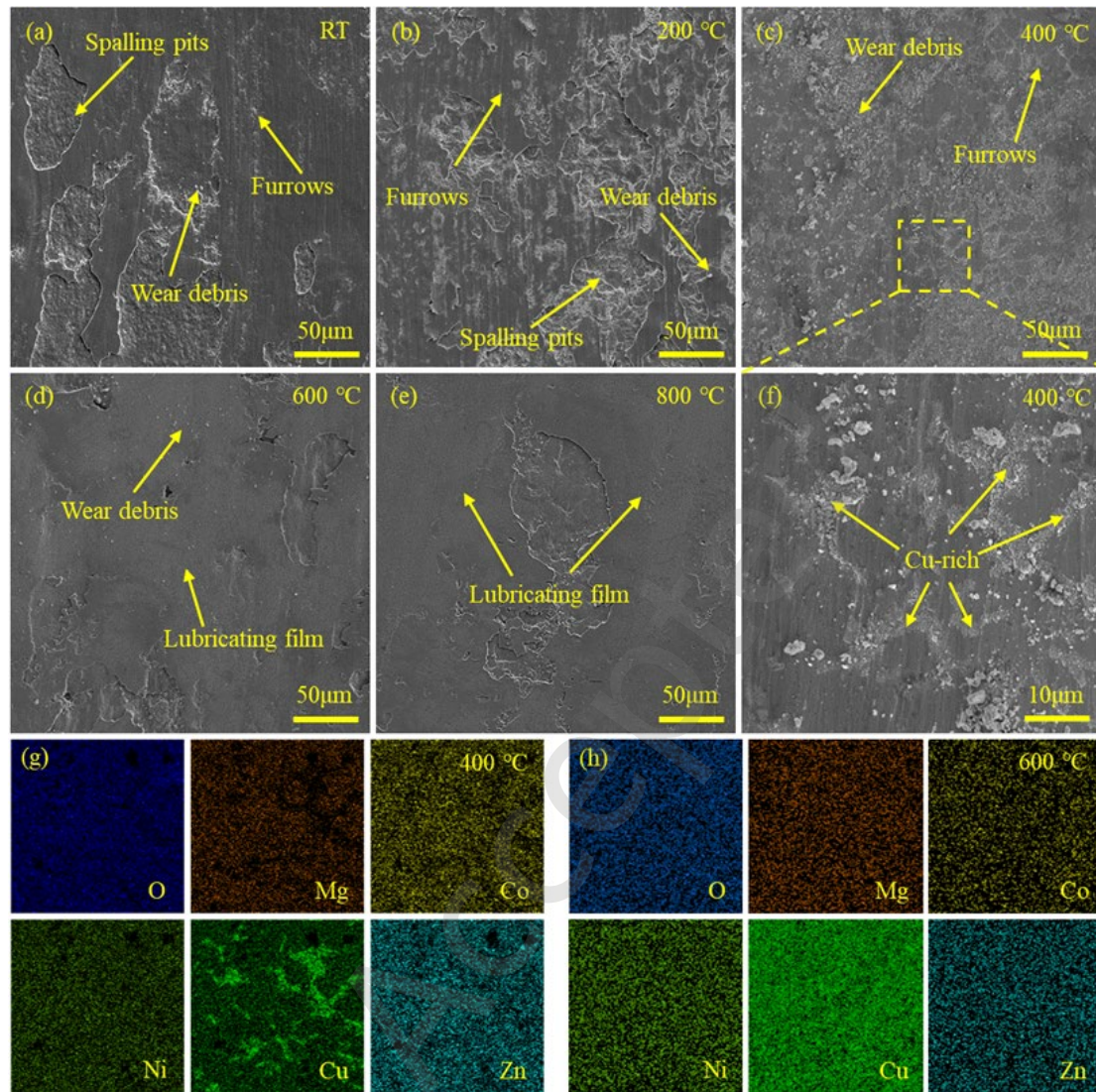


Fig.5 SEM morphologies and element distribution of the worn surfaces of the HEO at different temperatures.

Table 1 Element distribution on the worn surfaces of the HEO at different wear temperatures

(at.%)

	O	Mg	Co	Ni	Cu	Zn
RT	46.33	10.42	10.95	10.84	10.59	10.87
200 °C	46.97	10.18	10.65	10.73	10.58	10.89
400 °C	46.54	8.84	9.32	9.57	16.14	9.59
600 °C	46.91	4.98	5.51	5.33	31.91	5.36
800 °C	46.08	3.92	3.62	3.55	39.39	3.44

Fig. 5 presents the SEM morphologies and corresponding elemental distribution maps of the worn surfaces of the HEO at different wear temperatures. At RT and 200 °C, the worn surfaces exhibit minor wear debris, shallow grooves, and localized spalling pits, indicating that the dominant wear mechanisms are mild abrasive wear and fatigue wear. The fatigue spalling primarily originates from the cyclic accumulation and release of shear stress in the subsurface layer during the friction process [35]. Concurrently, the elemental distribution in Table 1 reveals that the five metal elements maintain a near-equiatomic ratio distribution. This further confirms that the HEO retains a homogeneous, high-entropy solid-solution structure at lower temperatures, consistent with its high hardness and superior wear resistance [36, 37].

Fig. 5(c) illustrates the worn surface of the HEO at 400 °C, which is extensively covered by wear debris. This debris acts as abrasive particles during the sliding process, leading to the formation of deep grooves and severe material spallation, which consequently results in a significant increase in the wear rate. The corresponding phase transformation at this temperature is primarily driven by the thermodynamic instability of the HEO system, which promotes the precipitation of CuO from the rock-salt matrix. This precipitation disrupts the high-entropy solid-solution structure and diminishes the associated strengthening effects, such as high configurational entropy and severe lattice distortion, ultimately causing a notable deterioration in both hardness and wear resistance [11]. Furthermore, localized SEM images and elemental distribution maps in Fig. 5(f) and (g) confirm that the coarse wear debris consists mainly of agglomerated Cu-rich particles.

As the temperature further increased to 600 °C and 800 °C (Fig. 5d-e), the smooth and continuous Cu-enriched oxide layers gradually formed on the worn surfaces, as evidenced in Fig. 5(h). During the wear process, the HEO debris undergoes oxidation and sintering, a process that intensifies with increasing temperature. Moreover, differences in the Gibbs free energy of formation among the constituent binary metal oxides lead to selective oxidation of the HEO debris. The relatively less negative Gibbs free energy of CuO indicates its higher thermodynamic instability, making it more susceptible to oxidation under higher temperature (Fig.3a). Concurrently, the dynamically precipitated CuO from the HEO matrix selectively migrates and enriches the worn surface, further promoting the formation of a dense Cu-rich oxide lubricating film. Ultimately, a continuous surface film predominantly composed of CuO is formed. Consequently, the elemental distribution on the worn surface, as presented in Table 1, demonstrates a significant enrichment of Cu content at elevated temperatures (600°C and 800°C), while the contents of other metallic elements (Mg, Co, Ni, Zn) decrease correspondingly. Accordingly, the stronger CuO diffraction peaks in Fig. 3(b) stem from the diffusion of Cu to the surface and subsequent Cu-rich oxide lubricating film formation rather than further precipitation. While the entropy-driven re-dissolution of CuO partially restores the substrate hardness (Fig. 3d), the primary contribution to wear reduction stems from the formation of a superior oxide layer. As evidenced in Fig. 5(e) and 5(h), the oxide layer at 800 °C is significantly more continuous, compact, and glassy-like compared to the relatively particulate and heterogeneous layer observed at 600 °C. At 800 °C, the

synergistic effect of thermal densification and oxide sintering in the material partially restored its hardness. Coupled with the formation of a friction-reducing oxide layer enabled by surface Cu enrichment, this synergy markedly improves the high-temperature wear performance.

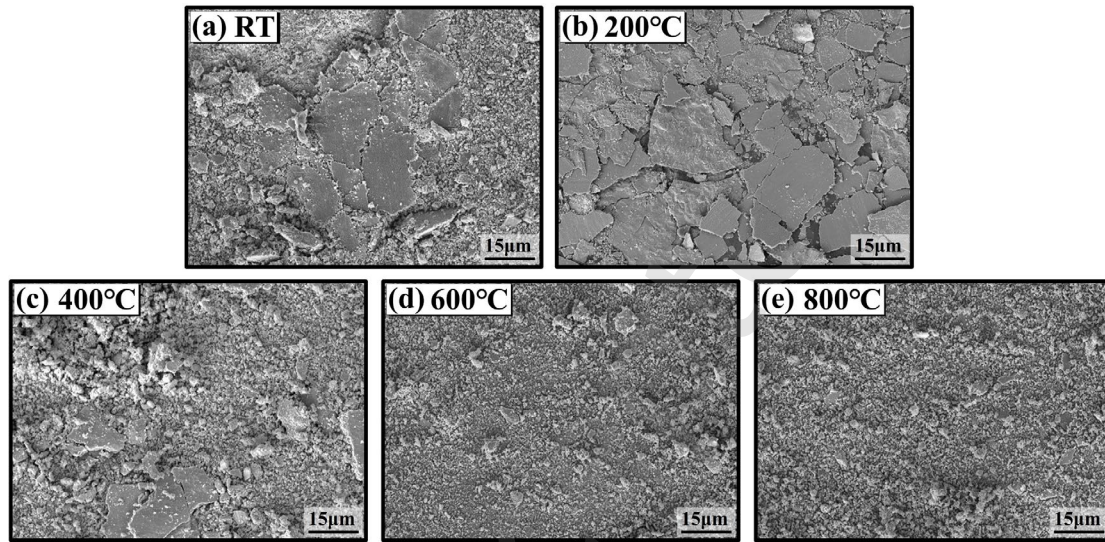


Fig. 6 SEM morphologies of the wear debris at different temperatures.

Fig. 6 presents the morphology of wear debris generated from the HEO at different temperatures. At RT, the debris primarily consists of large, flake-like delamination particles, accompanied by a minor fraction of fine fragments, indicating abrasive wear and fatigue spalling. This observation is consistent with the grooves and spalling features observed on the corresponding worn surface (Fig. 6a). At 200 °C, the proportion of flake-like delamination debris increases significantly, suggesting an aggravated fatigue delamination wear mechanism. This morphological change correlates well with the elevated wear rate observed at this temperature (Fig. 6b).

Fig. 6(c) reveals a notable transition in the morphology of wear debris at 400 °C. The amount of debris increases substantially, comprising both fine granular particles

and large spalled fragments. The fine debris suggests severe abrasive wear, while the large spalled sheets are associated with material delamination due to abrasive impact. These observations are consistent with the heavily debris-covered worn surface at 400 °C shown in Fig. 5, collectively demonstrating that the hardness degradation induced by CuO precipitation aggravates abrasive wear mechanisms, leading to a sharp rise in the wear rate.

Fig. 6(d-e) reveals that at elevated temperatures of 600 °C and 800 °C, the wear debris consists almost entirely of fine particles, with flake-like debris largely disappearing. Such uniform and fine debris is more prone to undergo oxidation and sintering on the worn surface, thereby promoting the formation of a smooth, dense, and Cu-enriched continuous lubricating film (Fig. 5d-e). Serving as an effective physical barrier layer, this lubricating film significantly reduces the direct contact area between friction pairs, suppresses adhesive wear, and lowers interfacial shear stress. Furthermore, its dense structure impedes the rapid diffusion of oxygen into the substrate, mitigating material loss caused by cyclic oxidation [20]. Consequently, the dominant wear mechanism shifts from the abrasive wear and fatigue spalling observed below 400 °C to mild abrasive wear and oxidative wear at high temperatures. The protective oxide layer formed during oxidative wear significantly reduces the HEO's wear rate. Therefore, the synergy between the partial re-dissolution of CuO, which restores the HEO's hardness, and the formation of a Cu-enriched lubricating film on the worn surface collectively facilitates the transition in wear mechanisms and enhances wear resistance.

3.4 Raman and XPS analysis

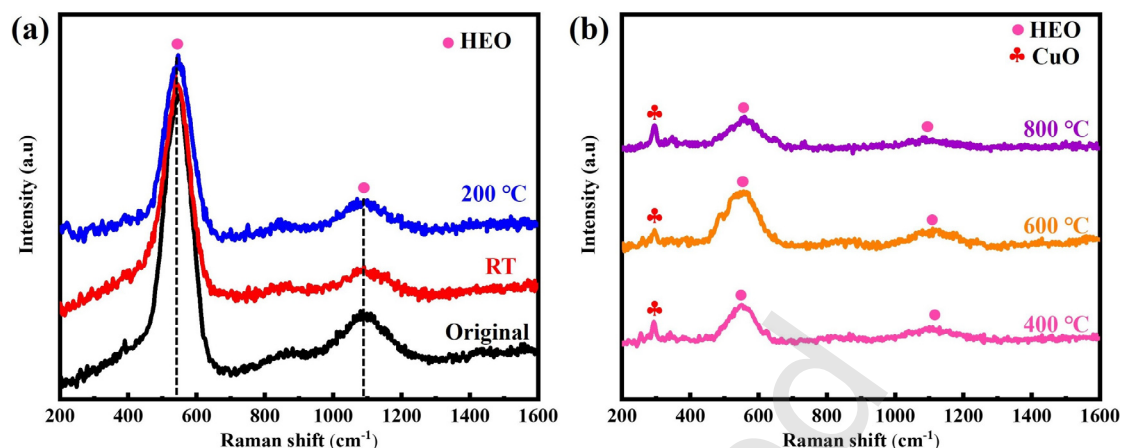


Fig. 7 Raman spectra of worn surfaces of HEO at different test temperatures.

Fig. 7 presents the Raman spectra of the worn surfaces of the HEO at different temperatures. At RT and 200 °C, only the characteristic peaks of the HEO rock-salt phase are detected both on the pristine surface and within the wear track, further confirming the excellent phase stability and tribochemical resistance of the material at relatively low temperatures (Fig. 7a).

As the wear temperature rises to 400 °C and 600 °C (Fig. 7b), significant changes occur in the phase structure of the worn surface. The intensity of the characteristic peaks for the HEO rock-salt phase gradually weakens. In contrast, distinct characteristic peaks of tenorite-structured CuO emerge. These observations are consistent with the XRD results shown in Fig. 3.

When the temperature is further increased to 800 °C, the intensity of the CuO characteristic peaks increases significantly (Fig. 7b). This enhancement is unlikely due to an aggravation of phase separation. However, it is more likely related to thermodynamic processes at the friction interface. Under high-temperature wear conditions, the mechano-alloying effect of wear debris and severe plastic deformation

may facilitate the formation of coarse CuO particles. Simultaneously, the continuously exposed fresh surfaces and the frictional heat generated during sliding accelerate the selective oxidation of Cu, leading to the formation of a tribo-oxidation layer enriched with nano- or microcrystalline CuO on the worn surface. The dense, continuous Cu-enriched oxide layer results in a notable increase in the Raman signal intensity.

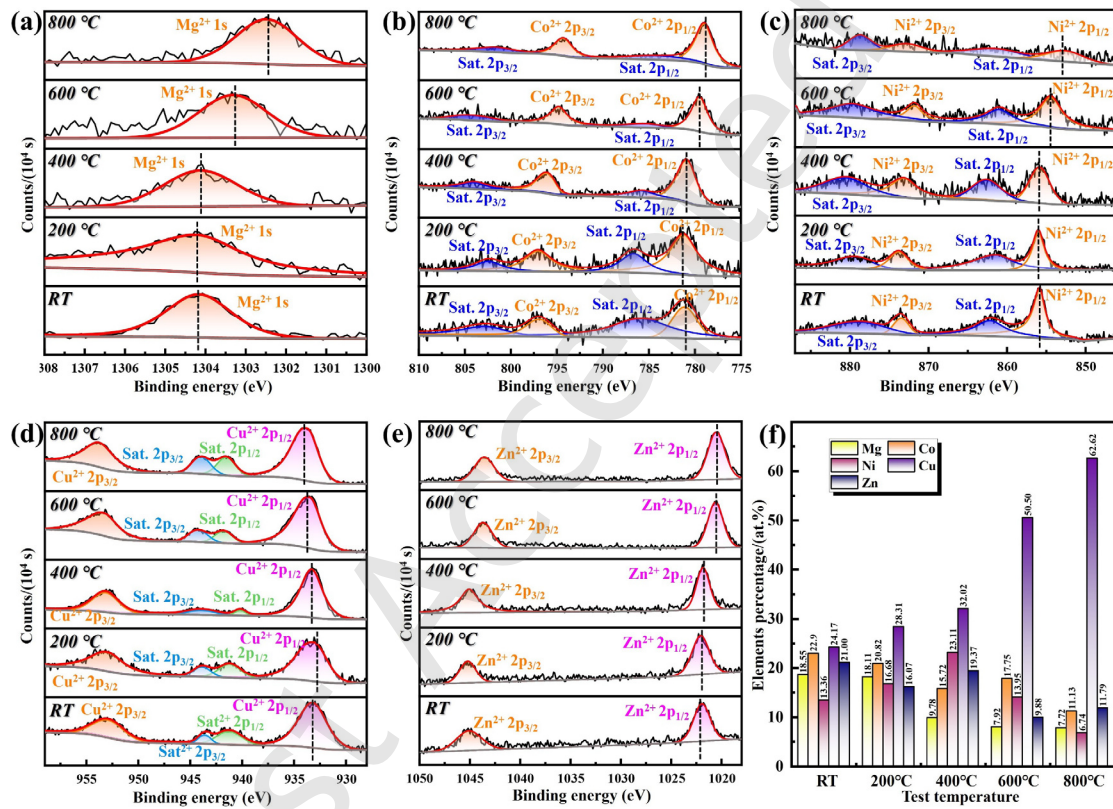


Fig. 8 XPS spectra of the worn surface at different temperature: (a) Mg; (b) Co; (c) Ni; (d) Cu; (e) Zn; (f) Element percentage.

XPS analysis further confirmed the evolution of surface chemistry during high-temperature wear. XPS analysis further elucidates the evolution of surface chemistry during high-temperature wear. High-resolution spectra of Mg, Co, Ni, Cu, and Zn were fitted based on established references [20, 38-41], as presented in Fig. 8(a-e). A comparison of the same core energy levels for the same element at different

temperatures reveals that increasing the temperature does not alter the valence states of the elements, but it does significantly affect the positions of their binding energies.

Specifically, the core-level spectra confirm the presence of Mg^{2+} (Mg 1s, 1304.1 eV), Co^{2+} (Co 2p_{3/2}, 796.9 eV; Co 2p_{1/2}, 781.2 eV), Ni^{2+} (Ni 2p_{3/2}, 873.6 eV; Ni 2p_{1/2}, 855.9 eV), and Cu^{2+} (Cu 2p_{3/2}, 953.2 eV; Cu 2p_{1/2}, 933.3 eV), corresponding to MgO, CoO, NiO, and CuO, respectively. At RT and 200 °C, the binding energies and atomic concentrations of these elements show negligible variation, indicating chemical stability and the absence of severe oxidative wear, which aligns with the SEM morphologies observations in Fig. 5.

However, as the temperature rises above 400 °C, a divergent trend emerges. The binding energies of Mg, Co, Ni, and Zn shift progressively toward lower values, whereas that of Cu shifts toward higher values. This phenomenon is attributed to the formation of a dense, Cu-rich oxide lubricious oxide overlayer at elevated temperatures. This behavior indicates that a dense layer of Cu-rich oxide gradually formed on the worn surface at high temperatures, effectively shielding the underlying high-entropy matrix and preventing it from being directly detected.

3.5 DFT analysis

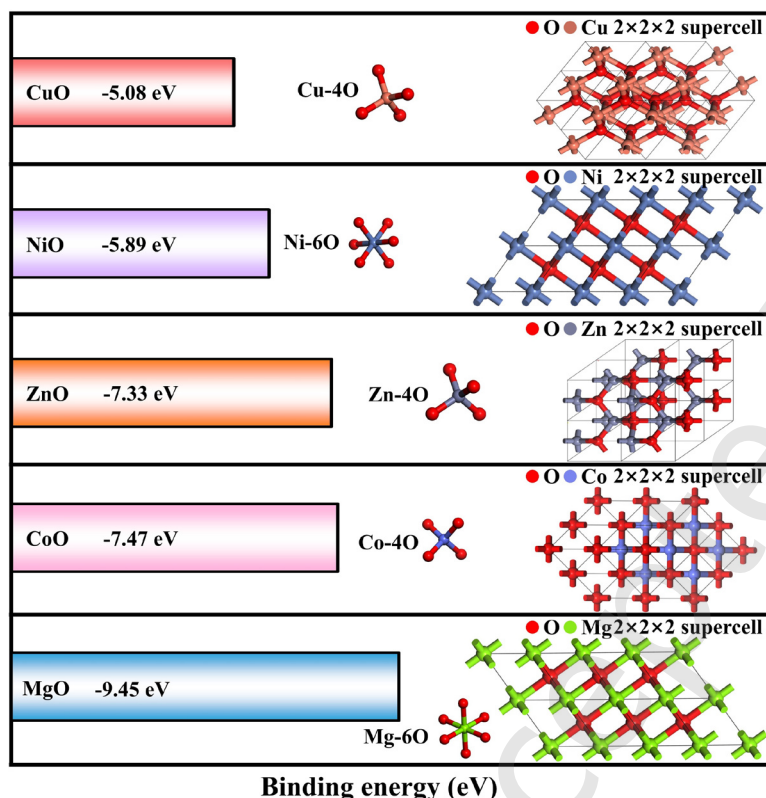


Fig.9 Binding energy of five composition oxides in HEO.

The crystal structures of the five constituent oxides of the HEO--CuO, NiO, ZnO, CoO, and MgO--were geometrically optimized using first-principles calculations, as illustrated in Fig. 9. The optimized structures confirm the presence of only a single type of metal-oxygen bond in each oxide. To evaluate the relative stability of each oxide within the HEO matrix, the binding energy was calculated by removing an individual metal atom to break the corresponding metal-oxygen bond [21, 42]. Among the oxides studied, CuO exhibits the lowest Cu-O binding energy (approximately -5.08 eV), indicating that breaking and reforming Cu-O bonds requires the least energy. This result suggests, from a bond-energy perspective, that CuO has a greater tendency to migrate and precipitate within the HEO system.

Thermodynamic considerations further support the propensity for CuO precipitation. As shown in Fig. 3(a), the relative order of Gibbs free energy among the five constituent oxides is $\text{CuO} > \text{NiO} > \text{ZnO} > \text{CoO} > \text{MgO}$. This trend aligns with the binding energy sequence: a lower binding energy corresponds to a more positive Gibbs free energy, implying lower thermodynamic stability of the oxide within the solid solution. When the temperature increases, the structural stability of the HEO system is perturbed. Consequently, the system tends to precipitate the thermodynamically less stable CuO phase to minimize the overall energy.

Furthermore, the CuO precipitated in the HEO during high-temperature friction possesses a relatively low binding energy. Under shear stress, this facilitates fracture and promotes the formation of a dense, continuous lubricating oxide layer at elevated temperatures (Fig. 5) [20, 43]. Research indicates that such an oxide layer effectively isolates direct contact between the friction pairs, thereby significantly reducing friction [44]. Simultaneously, the dense layer acts as a barrier against high-temperature oxidation by preventing fresh metal surfaces from exposure to air, consequently enhancing oxidation and wear resistance. This observation aligns well with the superior tribological performance of HEO at high temperatures (Fig. 4) [45]. Hence, beyond its thermodynamically driven preferential precipitation, CuO contributes to improved high-temperature friction performance via its low binding energy and propensity for fracture, which collectively promote the formation of a protective Cu-rich oxide lubricating film.

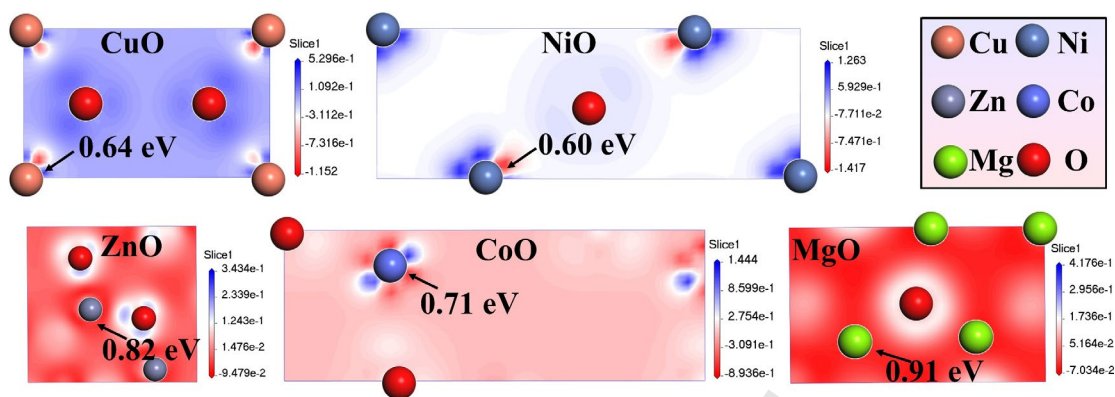


Fig.10 Difference charge density of five composition oxides in HEO.

The bonding characteristics of the constituent oxides in the HEO are closely linked to their electron density distributions. Fig. 10 displays the differential charge density analysis of the five component oxides, where blue and red regions indicate electron accumulation and depletion, respectively. In agreement with the binding energy data in Fig. 9, CuO and NiO, which have lower binding energies, exhibit prominent blue regions in their differential charge density maps, reflecting a strong tendency to gain electrons. Notably, CuO exhibits a deeper blue hue, indicating a greater degree of electron enrichment, consistent with its relatively low binding energy. In contrast, ZnO, CoO, and MgO exhibit predominantly red regions in their differential charge density profiles, suggesting a pronounced electron-donating propensity. Among these, MgO displays the lightest color intensity, corresponding to the strongest ability to lose electrons.

A comparative analysis of the charge states of metal atoms in CuO and MgO further reveals a strong correlation between the oxides' electron-transfer tendencies and the effective charge carried by their constituent metal ions. Within the HEO matrix, the Mg atom exhibits the highest positive charge (+0.91 e), which is indicative

of pronounced ionic bonding character in MgO and a highly localized charge distribution around the oxygen anions. This strong ionic interaction contributes to its enhanced bonding stability. In contrast, the Cu atom in CuO possesses a relatively moderate positive charge, and the electrons involved in the Cu-O bond are more delocalized, resulting in a correspondingly weaker bond energy. The lower charge localization and the consequently reduced diffusion energy barrier rationalize the propensity of CuO to undergo bond breaking or structural reconstruction within the HEO lattice, as well as its tendency to migrate to the surface under high-temperature frictional conditions preferentially. The differential charge density analysis corroborates that CuO exhibits a greater degree of electron enrichment, consistent with its lower binding energy and greater tendency to migrate and precipitate.

As shown in Fig. 11, the density of states (DOS) spectra of the five-component oxides show that CuO has a relatively high electron density near the Fermi level, suggesting a large number of electronically active states per unit energy and a high electron mobility. This delocalized electronic feature, consistent with the weak electron localization in Cu-O bonds, further explains CuO's tendency to undergo diffusion and structural reorganization at elevated temperatures. Therefore, CuO not only precipitates preferentially in the HEO system due to its low bond energy and high charge density but also readily forms a continuous, dense, and lubricating surface oxide film during friction, thereby significantly improving the high-temperature tribological performance of the HEO.

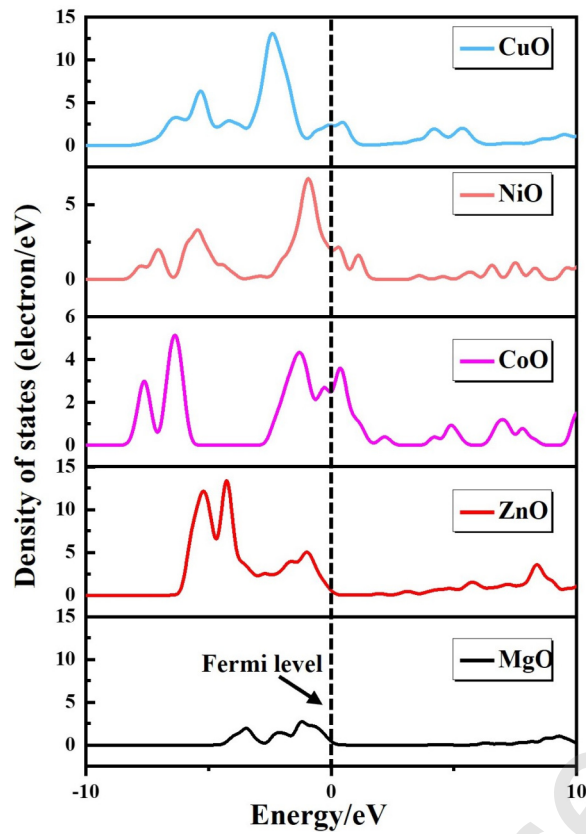


Fig. 11 Density of states analysis of five component oxides in HEO.

3.6 Wear mechanisms

The wear mechanisms of the HEO at different temperatures are summarized in Fig. 12. At RT, the worn surface exhibits only minor shallow grooves and spalling pits, indicating that the dominant wear mechanisms are mild abrasive wear and fatigue-induced delamination. As the temperature increases to 200 °C, the grooves become more pronounced and numerous, accompanied by a noticeable increase in lamellar debris, suggesting an aggravation of both abrasive and fatigue-driven spalling mechanisms. This morphological evolution correlates well with the rising wear rate observed in this temperature range.

When the temperature reaches 400 °C, thermodynamic instability within the HEO system promotes the precipitation of CuO from the rock-salt matrix, disrupting

the high-entropy solid-solution structure and leading to a significant reduction in material hardness. The worn surface is characterized by extensive debris accumulation, deep grooves, and large-scale spalling caused by abrasive impact. Under these conditions, severe abrasive wear and impact-induced spalling become the predominant wear mechanisms, resulting in a sharp increase in the wear rate.

Although the re-dissolution of CuO at 800°C restores the single-phase high-entropy structure and recovers substrate hardness, the wear reduction is not strictly dependent on mechanical strength alone. Instead, the morphological evolution of the oxide layer is the determining factor. Concurrently, Cu species diffuse toward the surface and participate in the formation of a continuous, dense lubricating film. This film exhibits easy shear, which significantly improves interfacial friction. As a result, the wear mechanism transitions to mild abrasive wear and oxidative wear, leading to a substantial decrease in the wear rate at high temperatures.

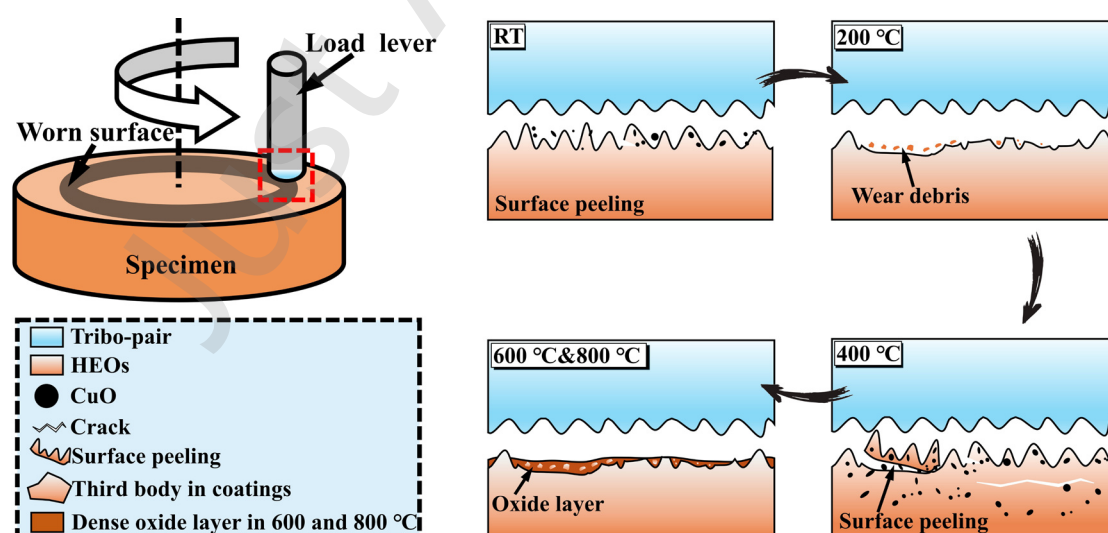


Fig 12 Schematic diagram of wear mechanisms in HEO at different temperatures.

4 Conclusions

In this paper, the tribological behavior and underlying mechanisms of rock salt-structured (MgCoNiCuZn)O high-entropy oxide ceramics across a wide temperature range (RT to 800 °C) were systematically investigated. The phase evolution, mechanical properties, wear mechanisms, and the role of in-situ formed oxides were explored by combining experimental characterization with density functional theory calculations. The main conclusions are as follows:

- 1) The phase stability of HEO at elevated temperatures is governed by the competition between enthalpy and entropy. At a relatively low temperature (400 °C), unfavorable local enthalpy changes drive the precipitation of CuO--which exhibits a lower melting point and a more positive enthalpy--thereby disrupting the high-entropy solid-solution effect and resulting in a sharp decline in hardness and wear resistance.
- 2) At 800 °C, the entropy-stabilizing effect promotes the re-dissolution of partial CuO into the matrix, contributing to the recovery of hardness. Meanwhile, the remaining CuO facilitates the formation of a Cu-rich oxide lubricating film under shear-cyclic loading, which substantially reduces wear.
- 3) DFT calculations confirm that CuO possesses the lowest metal-oxygen binding energy (approximately -5.08 eV) and a relatively high charge density among the five constituent oxides in the HEO. These characteristics lead to its strong tendency to precipitate and endow the HEO with excellent

lubricating capability at elevated temperatures.

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this work.

Data Availability

Data will be made available on request.

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