MICROSTRUCTURAL AND MECHANICAL PROPERTIES OF CUCRCOFENI HEA COATINGS ON CU SUBSTRATES: AN ATOMIC-SCALE STUDY

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Abstract

High entropy alloys (HEA) are promising candidates for protective coatings owing to their superior mechanical and tribological properties. This study employs molecular dynamics (MD) simulations to examine the nano-scratch behavior of CuCrCoFeNi HEA coatings on crystalline Cu substrates at depths of 5, 10, 15, and 20 Å. The focus is placed on microstructural evolution, deformation mechanisms, and mechanical responses. Results indicate that stacking faults (SF) appear in the Cu substrate at shallow depths (5–15 Å) but shift to concentrate within the coating at 20 Å. This transition, coupled with the FCC to HCP phase transformation, plays a central role in strain hardening, enhancing coating strength, and reducing stress transfer into the substrate. Shear strain distributions confirm that deformation becomes more continuous and localized with increasing depth, while the number of atoms with shear strain > 0.5 grows significantly, peaking at 20 Å. In terms of forces, the normal forces (F_n) always exceed the tangential forces (F_t), with F_n increasing rapidly up to 10 Å and then stabilizing, whereas F_t increases nearly linearly with depth. Correspondingly, the coefficient of friction rises from 0.08 to 0.82. These findings demonstrate the effectiveness of CuCrCoFeNi HEA coatings in absorbing deformation and protecting Cu substrates, providing a theoretical basis for the design of advanced wear-resistant coatings.

Keyword: CuCrCoFeNi HEA coatings, Cu substrate, coefficient of friction, microstructure, nano scratching.

1. INTRODUCTION

High-entropy alloys (HEAs) are advanced metallic materials composed of multiple principal elements in near-equiatomic ratios. Their unique microstructures endow them with superior properties such as high strength [1-2], corrosion resistance [3], and thermal stability, making them attractive candidates for protective coatings in harsh service environments [2],

[4]. Among these, the CuCrCoFeNi system is notable for its balanced combination of ductility, strength, and durability.

Copper (Cu) is widely used owing to its excellent ductility and conductivity, but its low hardness and limited fatigue resistance restrict its applications. Coating Cu substrates with HEAs has been shown to enhance hardness, wear resistance, and tribological performance [5-6]. In such systems, stacking faults formed within the HEA coating help redistribute stress and protect the Cu substrate. However, studies on CuCrCoFeNi coatings deposited on crystalline Cu remain limited, and the underlying wear and deformation mechanisms at the atomic scale are not yet fully understood.

The nanoscratch method is an effective tool to evaluate surface mechanical behavior, but experimental techniques face challenges in capturing atomic-scale processes. Molecular dynamics (MD) simulations overcome these limitations by enabling direct observation of dislocations, stacking faults, and phase transformations [7]. In this work, molecular dynamics (MD) simulations are employed to investigate the microstructure, deformation behavior, and mechanical response of CuCrCoFeNi HEA coatings deposited on crystalline Cu substrates under varying scratch depths, which is lacking in previous works. The outcomes of this atomistic study offer theoretical insights that can guide the design and optimization of HEA coatings for effective substrate protection.

2. METHODOLOGY

Figure 1 illustrates the molecular dynamics (MD) model employed for the nanoscratch simulation. The system consists of a crystalline Cu substrate coated with a CuCrCoFeNi high-entropy alloy (HEA), both represented with a face-centered cubic (FCC) lattice structure. The workpiece dimensions are 198 Å (x-axis), 133 Å (y-axis), and 142 Å (z-axis). The HEA coating contains five elements (Cu, Cr, Co, Fe, Ni) in equiatomic proportions (20% each). The simulation model parameters are shown in Table 1. The model is divided into four layers: the HEA coating, a Newtonian atom layer, a fixed atom layer, and a thermostat layer. To constrain boundary effects, the fixed atom layer immobilizes three atomic layers along the x- and z-directions, while the thermostat layer positioned between the fixed and Newtonian regions controls the system temperature at 300 K. The system is maintained under the NVT ensemble to ensure constant atom number, volume, and temperature.

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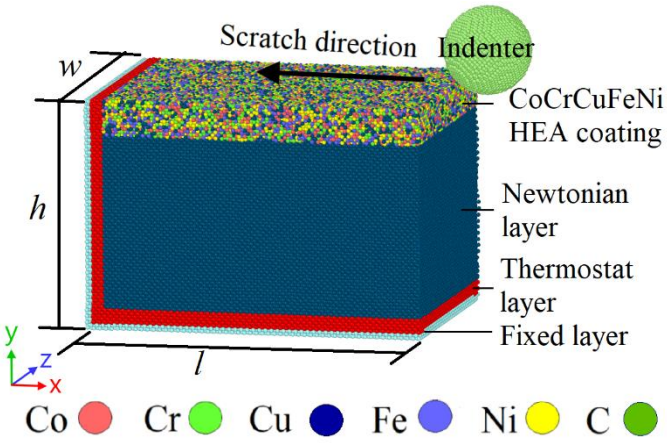

Figure 1. Mô hình cào xước lớp phủ CoCrCuFeNi trên nền Cu tinh thể

Table 1. Simulation parameters in the current research

TT	Parameter	Workpiece	Scratching tool
1	Material type	CoCrCuFeNi HEA/Cu	Diamond
2	HEA coating	$Co_{20}Cr_{20}Cu_{20}Fe_{20}Ni_{20}$	
3	Workpiece dimension	198 Å × 142 Å × 133 Å ($l \times w \times h$)	Diameter: 50 Å
4	HEA layer dimension	200 Å × 145 Å × 20 Å	

The cutting tool was represented by a rigid diamond sphere with a diameter of 50 Å, positioned 2 Å above the sample surface at the start of the simulation. The scratching process was carried out at a velocity of 200 m/s along the negative *x*-direction, with penetration depths of 5, 10, 15, and 20 Å. In MD simulations, the scratch speed is often higher than experimentally [8]. This choice is intended to reduce computational costs while still ensuring that the main goal of clarifying the deformation trends and mechanisms of the material is achieved. In cases where the cutting depth exceeds the coating thickness, the Cu substrate will be directly impacted by the abrasive grain, leading to significant damage [9] and hindering the determination of the protective role of the coating. The parameters of the scratching process are shown in Table 2. The embedded atom method (EAM) potential is adopted to describe atomic interactions within the substrate and coating, while the interaction between the diamond tip and the HEA is represented using the Lennard–Jones (LJ) potential [10]. The carbon–carbon interactions within the tool are neglected by assuming the probe to be perfectly rigid, …

The total potential energy of the system is expressed as [11]:

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$$E_i = F_\alpha\left(\sum_{i\neq j}\rho\alpha\beta\left(r_{ij}\right)\right)+\frac{1}{2}\sum_{i\neq j}\phi_{\alpha\beta}\left(r_{ij}\right) \quad (1)$$

Here, ϕ stands for a pair-potential interaction, while r_{ij} represents their interatomic distance. The term F_α corresponds to the embedding energy and indicates the local electron density. The elemental types of atoms i and j are identified by the indices α and β, respectively.

The friction coefficient μ is determined as:

$$\mu = \frac{F_t}{F_n} \quad (2)$$

Where F_t and F_n denote the tangential and normal forces, respectively, during scratching, the molecular dynamics simulations were implemented using the LAMMPS package, which provides efficient parallel computation for large-scale atomic systems [12-13]. During the simulations, atomic trajectories, structural evolution, and force data were recorded for further analysis. The visualization and qualitative interpretation of atomic configurations, dislocation evolution, and shear strain were conducted with OVITO [14], enabling a clear observation of microstructural changes during scratching. Subsequently, the quantitative data, including tangential and normal forces as well as the corresponding friction coefficients, were extracted, processed, and statistically analyzed using OriginPro to generate graphs and comparative evaluations.

Table 2. Parameters of the scratching process

Length (L)	Depth (d)	Thickness (t)	Velocity (v)	Time step	Temperature (T)	Potential
150 Å	5, 10, 15, 20 Å	20 Å	200 m/s	1 fs	300 K	EAM and LJ

3. RESULTS AND DISCUSSION

3.1. Analysis of microstructure

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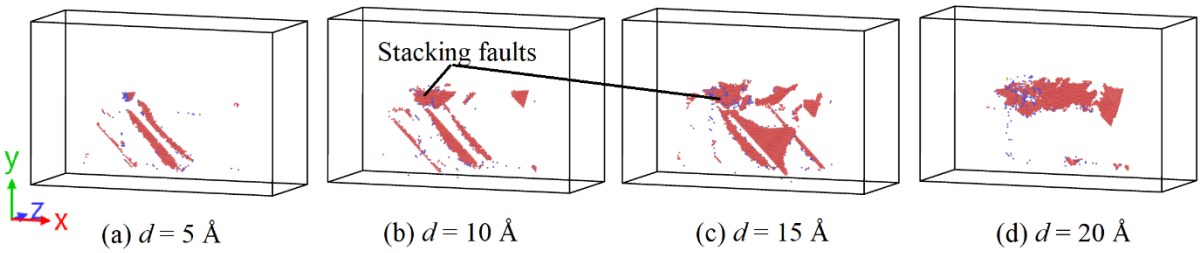

Figure 2. Stacking fault distribution in the CoCrCuFeNi HEA coating on Cu substrate after nano-scratching with scratch depths of 5, 10, 15, and 20 Å.

Figure 2 illustrates the distribution of stacking faults (SFs) in the specimen after the nano scratch process. At a scratching depth of 5 Å, only a few SFs are observed, sparsely distributed and mainly concentrated at the end of the scratch track, extending into the Cu substrate. When the depth increases to 10 Å, the SF density rises significantly and begins to propagate along the {111} slip planes; SFs are observed within the scratch groove but remain abundant in the substrate. At 15 Å, the number of SFs increases sharply, exhibiting a clearer and more continuous morphology, predominantly located within the groove. The slip planes show a tendency to connect and form larger clusters, indicating an increased density of Shockley dislocations and the dominant role of plastic slip in the FCC lattice. At a depth of 20 Å, SFs become dense and are primarily distributed within the coating, especially around the scratch groove. This behavior can be explained as follows: at shallow depths, the small contact area leads to stress concentration that is easily transmitted into the Cu substrate. In contrast, when the scratching depth equals the coating thickness, the stress is predominantly concentrated within the HEA layer, resulting in strong local deformation that absorbs most of the energy and reduces its transmission into the Cu substrate.

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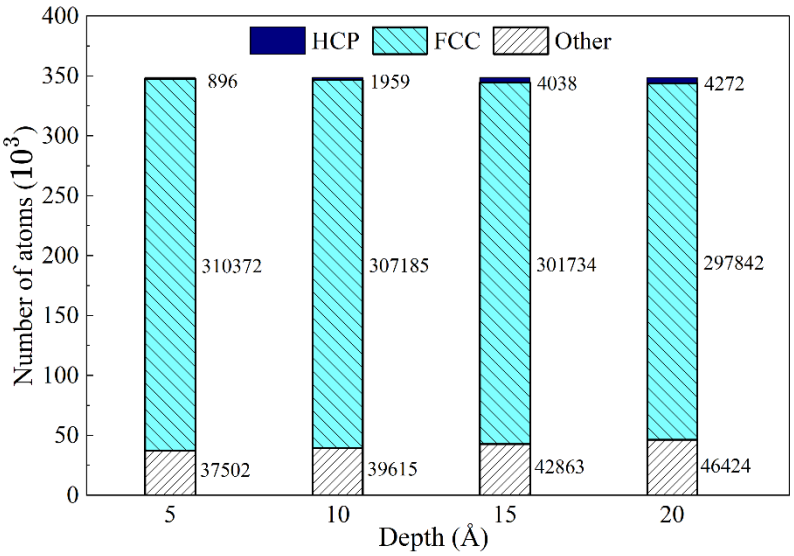

Figure 3. The number of atoms with FCC, HCP, and other structures in CuCrCoFeNi HEA coatings on Cu substrates under nano-scratching at depths of 5, 10, 15, and 20 Å.

Figure 3 presents the number of atomic structures (FCC, HCP, and others) in the coating–substrate system at different scratching depths. The results indicate that FCC atoms dominate the overall structure; however, their number decreases progressively from 310,372 at 5 Å to 297,842 at 20 Å. In contrast, the number of HCP atoms, which represent stacking faults, increases significantly with scratching depth, rising from only 896 atoms at 5 Å to 4,272 atoms at 20 Å. A similar upward trend is observed in the category Other, reflecting highly distorted atomic environments near the groove and the coating–substrate interface. This structural evolution is consistent with the well-established deformation mechanism of FCC materials, in which perfect dislocations tend to dissociate into Shockley partials, leaving behind local HCP stacking sequences [15]: 1/2 [110] = 1/6 [112] + 1/6 [112] + Stacking faults. The increase in HCP atoms with depth confirms the greater extent of plastic deformation and stacking fault accumulation as the applied stress intensifies. These findings are in good agreement with the observations in Figure 2, where SFs evolve from being sparse and localized at shallow depths to forming dense, continuous networks along {111} slip planes and around the scratch groove at higher depths. This correspondence highlights the critical role of the FCC to HCP transformation through stacking fault formation in accommodating plastic deformation in CoCrCuFeNi HEA coatings under nano scratching.

3.2 Mechanical properties and deformation mechanisms

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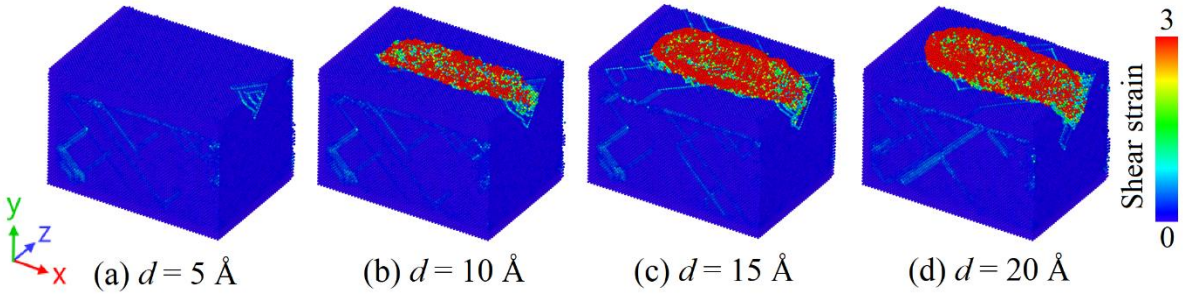

Figure 4. The distribution of shear strain in CoCrCuFeNi HEA coatings on Cu substrates after nano-scratching at depths of 5, 10, 15, and 20 Å.

Figure 4 shows the shear strain distribution in the CoCrCuFeNi HEA coating on Cu substrate at different scratch depths, in which the color scale shows the shear strain level. At a depth of 5 Å, only a few small localized deformation zones appear, indicating that the stress is not large enough to trigger significant plastic deformation. From 10 to 20 Å, the shear strain is mainly concentrated in the scratch groove and around the tool, reflecting the location of maximum shear stress. However, the extent and intensity are clearly different: at 10 Å, the deformation zone is limited and localized; at 15 Å, the deformation zone is expanded, continuous and spreads in the z direction, indicating the simultaneous activation of multiple {111} slip systems; up to 20 Å, the strain is concentrated in the coating and the material tends to extrude to the surface, while the strain transfer to the substrate is significantly reduced.

This difference is closely related to the microstructural transition from FCC to HCP through the formation of a stacking fault. The increase in the number of HCP atoms with scratch depth not only reflects the higher shear deformation zone but also leads to hardening due to the stacking fault, which increases the material's hardness. As the hardness increases, the deformation tends to be more concentrated and localized, instead of spreading deep into the Cu substrate. This result is consistent with previous studies [16], confirming the role of the transformation process from FCC to HCP in controlling the plastic deformation mechanism and enhancing the wear resistance of HEA coatings.

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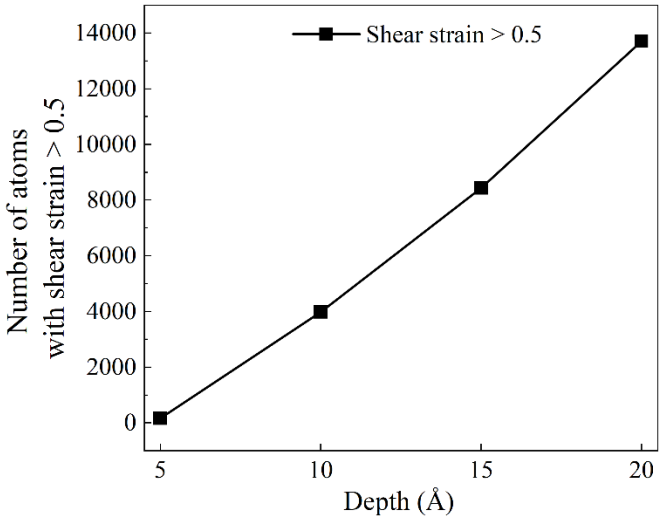

Figure 5. The number of atoms with shear strain > 0.5 in CoCrCuFeNi HEA coatings on Cu substrates after nano-scratching at depths of 5, 10, 15, and 20 Å.

Figure 5 shows the number of atoms with shear strain greater than 0.5 at different scratch depths. The results show that the number of atoms with strong strain increases almost linearly as the scratch depth increases from 5 to 20 Å. At a depth of 5 Å, only 163 atoms have shear strain > 0.5. When the depth reaches 10 and 15 Å, the number of atoms with considerable shear strain increases rapidly, reaching about 3980 and 8430, respectively, consistent with the expansion and continuity of the deformation zone in Figure 4. Especially at 20 Å, the number of atoms exceeding the shear strain threshold of 0.5 reaches a maximum (~13700), indicating that the HEA coating is strongly deformed and absorbs most of the applied energy, instead of transmitting it to the Cu substrate. This quantitative increase reinforces the intuitive observation from Figure 4 that not only the extent but also the magnitude of deformation increases markedly with scratch depth.

The scratch force and coefficient of friction are key indicators for evaluating the deformation mechanisms and wear resistance of coating–substrate systems. Figure 6 shows the variation of average tangential force (F_t) and normal force (F_n) with scratching depth, while Figure 7 presents the corresponding coefficient of friction (μ). Both F_t and F_n increase with depth, although F_n consistently exceeds F_t across all conditions, which is typical for scratching processes. Specifically, F_n increases rapidly from about 27.6 nN at 5 Å to nearly 76 nN at 10 Å, then rises slowly, reaching nearly 100 nN at 20 Å. In contrast, F_t increases nearly linearly from about 1.82 nN at 5 Å to about 75 nN at 20 Å, reflecting the steady increase in sliding and

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material removal. The fact that F_n is always larger than F_t suggests that the normal component dominates the concavity and maintains a stable depth of cut, while F_t mainly contributes to chip formation and friction dissipation. The increasing trends of F_n and F_t are in good agreement with the results observed in Figures 4 and 5.

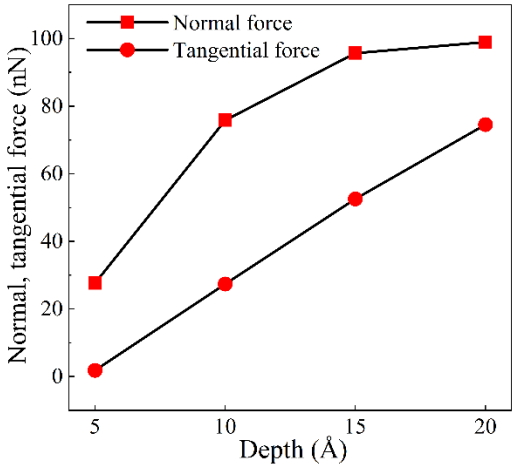

Figure 6. The average normal and tangential forces in CoCrCuFeNi HEA coatings on Cu substrates during nano scratching at depths of 5, 10, 15, and 20 Å.

The coefficient of friction is presented in Figure 7, increasing from 0.08 at 5 Å to 0.82 at 20 Å. At shallow depths, the indenter primarily slides on the surface, resulting in a very low friction level. As the depth increases, the contact area between the indenter and the material expands, while the formation of stacking faults within the coating enhances its hardness and impedes sliding motion. This leads to a marked increase in the coefficient of friction. At 20 Å, where the scratch depth coincides with the coating thickness, the coefficient reaches its maximum value. This trend highlights the combined influence of contact geometry and microstructural evolution on the frictional performance of the HEA coating.

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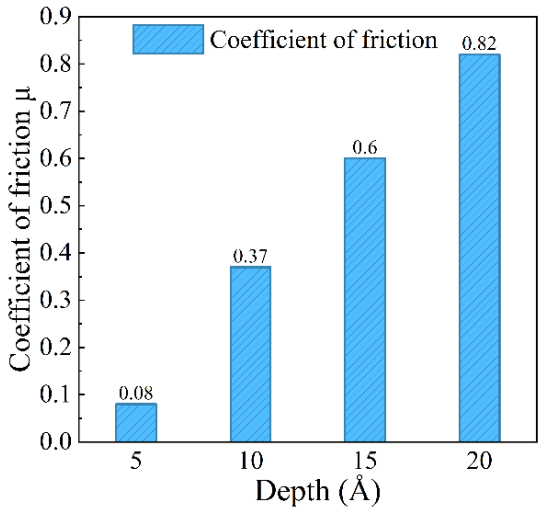

Figure 7. The coefficient of friction (μ) in CoCrCuFeNi HEA coatings on Cu substrates after nano scratching at depths of 5, 10, 15, and 20 Å.

3.3 Comparison of the friction coefficient of CoCrCuFeNi HEA coating after scratching

The results in Table 3 show that the coefficient of friction of FeNiCrCoCu coating on Cu substrate (Li et al. [9]) is about 0.95, which is higher than in other studies because the sample is only fixed at the bottom surface. Meanwhile, Trinh et al. [3] reported values of 0.80–0.91 for CuCrCoFeNi coating on Cu substrate when changing the composition ratio, indicating improved wear resistance. This study went further by investigating the scratch depth in the range of 5–20 Å, recording the coefficient of friction ranging from 0.08 to 0.82. The results confirm the protective role of CuCrCoFeNi coating and demonstrate its stability in a wider range of scratching conditions.

Table 3

An analysis of the friction coefficient is presented in various reports.

Material	μ	T (K)	v (m/s)	d (Å)	Method	Ref.
FeNiCrCoCu coating on Cu	0.95	300	200	20	MD simulation	Li J et al. [9]
CuCrCoFeNi HEA coating on Cu	0.8-0.91	300	200	20	MD simulation	Trinh et al. [3]
CuCrCoFeNi HEA coating on Cu	0.08-0.82	300	200	5-20	MD simulation	This study

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3. CONCLUSIONS

This study used molecular dynamics simulations to analyze the microstructure and mechanical properties of CuCrCoFeNi HEA coatings on crystalline Cu substrates with varying scratch depth. The results showed that stacking faults formed in the Cu substrate at a depth of 5–15 Å, but shifted to be concentrated mainly in the coating when the depth reached 20 Å. The appearance of stacking faults from the FCC to HCP phase transition played a key role in the strengthening mechanism, contributing to increased hardness and limiting stress transfer to the substrate. Regarding the dynamic properties, the normal force was always larger than the tangential force; while the tangential force increased nearly linearly with depth, the normal force increased rapidly from 5 Å to 10 Å and tended to increase slowly at about 10–20 Å. The coefficient of friction increased steadily from 0.08 to 0.82 with scratch depth. These results confirm the effective strain absorption ability of the HEA coating, thereby protecting the Cu substrate from damage during scratching.

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