

Role of layer thickness and grain size contrast in rolling contact fatigue of coarse/fine-grained layered materials: A crystal plasticity study

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ABSTRACT

Heterogeneous layered materials combine high strength and ductility, offering improved damage tolerance under tribological loading. Among the key microstructural factors, layer thickness and grain size contrast have a critical influence on the mechanical behavior during rolling contact fatigue (RCF). A crystal plasticity finite element (CPFE) model was developed to simulate rolling contact responses in coarse-grained (CG)/fine-grained (FG) layered structures. The simulations reveal that layer thickness modulates strain localization, dislocation activity, and damage evolution in a sliding-orientation-dependent manner. FG layers serve as barriers to strain transmission and suppress damage propagation from adjacent CG layers. Furthermore, dislocation partitioning at CG/FG interfaces promotes strain delocalization and enhances RCF resistance. These findings provide mechanistic insights for optimizing layered microstructure design for advanced tribological applications.

1. Introduction

Rolling contact fatigue (RCF) arises in mechanical components subjected to repeated rolling and sliding contact. Driven by cyclic stress, it leads to surface and subsurface material removal processes (e.g., micropitting, pitting, spalling), and persists as a major reliability concern. RCF critically affects key engineering systems such as rolling bearings, gears, and railway wheels [1–4]. While both surface and subsurface crack initiation are critical in RCF, subsurface-initiated failure, driven by localized plastic deformation and stress concentration, remains a key life-limiting factor [5], particularly in high-cycle and very high-cycle fatigue scenarios [6,7], and in applications where cracks originate from internal inhomogeneous defects or inclusions [8,9]. Previous investigations have shown that nanostructured designs can

enhance the tribological performance of metallic materials, primarily due to their superior strength and hardness [10,11]. However, strength-focused design strategies alone often neglect the complex interactions between microstructural heterogeneities and damage evolution under RCF conditions. Recent studies have highlighted the critical roles of grain size distribution, crystallographic anisotropy, and interfacial constraints in determining RCF resistance, challenging the conventional paradigm that favors homogeneous microstructure optimization [12–15]. This underscores the need for advanced design approaches that can simultaneously mitigate surface wear and suppress subsurface crack initiation and propagation [16,17].

Heterogeneous layered materials, particularly those composed of alternating coarse-grained (CG) and fine-grained (FG) layers, have emerged as a promising approach to address this challenge [18–23].

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Various processing techniques have been developed to fabricate such heterogeneous layered plates [24], among which accumulative rolling bonding (ARB) stands out as a convenient and scalable method for producing layered CG/FG architectures [25]. These structures leverage layer boundaries as effective dislocation barriers and promote interlayer strain partitioning, thereby achieving superior strength-ductility synergy [26,27], extra strain hardening [28–33], and delayed fatigue crack propagation [34,35]. As a result, layered CG/FG structures offer an ideal model system for systematically investigating the tribological behavior of heterostructured materials [18].

Experimental studies [36–38] have demonstrated that layered materials exhibit superior RCF resistance compared to their homogeneous counterparts. Layer thickness is a critical yet underexplored parameter in such structures. While thinner layers promote interface-mediated strengthening, they are more susceptible to interfacial delamination. In contrast, thicker layers are easier to control during fabrication but may compromise fatigue resistance [39–41]. It should be noted that machining, running-in friction, and initial surface damage also commonly induce the formation of ultra-fine-grained or nanocrystalline layers beneath the surface of metallic materials [42–44]. Additionally, the sliding direction relative to layer boundaries induces significant friction anisotropy, which is also closely linked to layer thickness [36]. Despite these advancements, the influence of layer thickness and grain size distribution on damage accumulation in layered structures remains inadequately understood.

Classical continuum models, which neglect grain-scale plasticity and grain boundary effects, struggle to capture the localized strain gradients and fatigue crack nucleation characteristics of heterostructures [45]. Crystal plasticity finite element (CPFE) modeling offers a powerful framework to bridge this gap. By explicitly incorporating dislocation glide, crystallographic orientation effect, and intergranular stress fields, CPFE enables microstructure-sensitive predictions of fatigue damage evolution [46–50]. Recent CPFE studies on rolling, fretting, and sliding contacts have successfully captured grain size effects, texture-dependent wear behavior, and strain localization near grain boundaries [51–55]. Microstructural heterogeneity has also been linked to RCF performance via CPFE methods: Wang et al. [56] trained a machine-learning model on crystal plasticity simulations to correlate hierarchical microstructural features with fatigue resistance in martensitic steel, while Wei et al. [57] developed a numerical framework considering the effect of microstructure gradients, which reliably predicts contact fatigue life and clarifies the roles of normal load and case carburization in damage evolution. However, existing works predominantly overlooked the synergistic interactions between CG and FG layers under cyclic loading [58]. In particular, the role of layer thickness in modulating dislocation evolution, crack initiation, and damage propagation is still largely unexplored.

In this study, a dislocation-based CPFE framework is developed to investigate the RCF behavior of layered CG/FG structures, with particular focus on the effects of layer thickness (ranging from 20 to 100 μm) and sliding orientation (0° and 90° relative to the layer boundaries). Three key research questions will be addressed: (1) How does the value of layer thickness affect damage accumulation in layered CG/FG structures? (2) What are the underlying mechanisms that govern the synergistic interactions between CG layers (high ductility) and FG layers (high strength) under cyclic rolling contact? (3) How can layer thickness and grain size distribution be optimized to suppress damage development, thereby enhancing RCF resistance in heterogeneous layered materials? By linking the evolution of dislocation densities and plastic strain localization to damage accumulation, this study offers mechanistic insights for microstructural design of advanced layered materials with superior fatigue resistance, targeting applications such as aerospace bearings and biomedical implants.

This paper is organized as follows: Section 2 details the CPFE method, including parameter calibration and the setup for rolling contact simulations. Section 3 presents the effects of layer thickness and

sliding orientation on plastic strain localization, dislocation density evolution, and damage accumulation over 100 rolling contact cycles. Section 4 explores the influence of grain size on rolling contact behavior and reveals the synergistic interactions between CG and FC layers in enhancing fatigue resistance. Conclusions are summarized in Section 5.

2. Methodology

2.1. CPFE model validation and parameter calibration

The dislocation-based crystal plasticity constitutive model described in Appendix A was implemented as a user-defined material (UMAT) subroutine within the Abaqus Standard finite element software [59]. To validate the model's capability in capturing the grain size dependence of mechanical behavior, uniaxial tensile simulations were conducted on homogeneous polycrystalline copper models with different grain sizes. Experimental data reported in the literature [60] were adopted for comparison. Quasi-three-dimensional polycrystalline representative volume elements (RVEs) with average grain sizes of 12 μm and 90 μm were generated using the open-source package Neper [61]. The grain-growth morphology algorithm was employed to produce a broader grain size distribution and higher grain sphericity than standard Voronoi tessellation [62]. Both RVEs had identical dimensions of $300 \times 200 \times 5 \mu\text{m}^3$, and grain orientations were randomly assigned to reflect realistic microstructural variability, as shown in Fig. 1(a–b). The Euler angles of the grains are converted into 3×3 rotation matrices, which are then assigned as input constants of the UMAT subroutine.

The RVEs were discretized using 20-node quadratic hexahedral elements with reduced integration (C3D20R). Boundary conditions were applied by constraining the bottom, left, and back surfaces along their respective normal directions, while a true strain of $\sim 15\%$ was applied to the right surface to simulate uniaxial tensile loading, as illustrated in Fig. 1(c). The decision to limit the calibration strain below 15% is based on two considerations: (1) The maximum local plastic strain in the finite element model during rolling contact simulations is estimated to be less than 5%, so restricting the calibration window to 0–15% ensures accuracy within the strain range relevant to rolling contact while minimizing computational cost; (2) Beyond a true strain of $\sim 15\%$, plastic deformation in polycrystalline copper becomes increasingly dominated by severe strain localization and complex damage mechanisms, which are beyond the scope of the present model.

Fig. 1(d) indicates that the simulated true stress-strain curves have good agreement with experimental results, confirming the model's ability to accurately describe the grain size-dependent yield strength and strain hardening in pure copper. The calibrated constitutive parameters employed in the simulations are summarized in Table 1. Contour plots of von Mises stress in Fig. 1(e) reveal that stress concentrations mainly occur along grain boundaries. Notably, the FG model exhibits higher overall stress levels than the CG counterpart, which is attributed to the grain size effect. Some individual grains show elevated stress relative to their surroundings; these typically correspond to crystallographic orientations that are harder along the tensile direction, making slip activation more difficult. Since the FG model contains a large number of grains, it has a higher probability of including such hard-oriented grains, thereby increasing the likelihood of internal stress localization.

2.2. Rolling contact simulation

Rolling contact loading was simulated by discretely applying a Hertzian pressure profile and associated shear tractions on the surface of the polycrystalline RVE, following established procedures [52,53]. To reduce computational cost while maintaining accuracy, high-resolution crystal plasticity modeling was confined to the region in the vicinity of the contact zone. The regions located farther from the contact surface were modeled as purely elastic and meshed with coarser elements [55].

As illustrated in Fig. 2(a), each polycrystalline finite element model

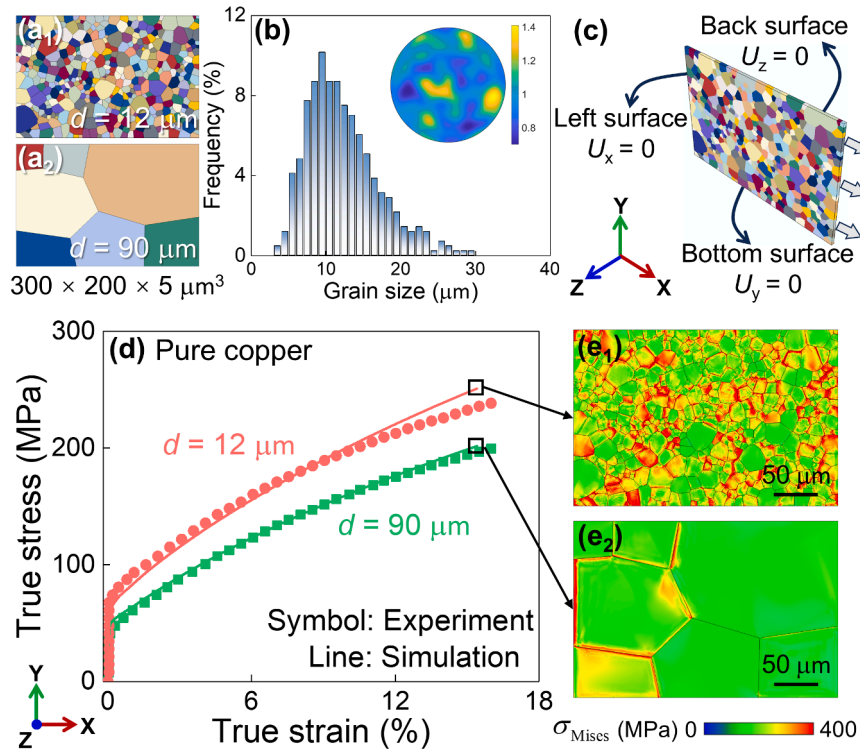


Fig. 1. Validation and parameter calibration of the crystal plasticity model through uniaxial tensile finite element simulations. (a) Microstructures of homogenous copper RVEs with the average grain sizes of 12 μm and 90 μm . (b) Grain size distribution and texture pole figure of the 12 μm RVE. (c) Boundary conditions applied in the uniaxial tensile simulations. (d) Comparison of simulated true stress-strain curves with experimental data from Ref. [60]. (e) Simulated von Mises stress distributions at a true strain of $\sim 15\%$.

Table 1
Constitutive parameters of pure copper used in CPFE simulations.

Symbol	Description (Unit)	Value
C_{11}	Elastic constants (GPa)	168.4
C_{12}	Elastic constants (GPa)	121.4
C_{44}	Elastic constants (GPa)	75.4
ρ_{ISSD}	Initial mobile SSD density (μm^{-2})	0.03
b	Magnitude of Burgers vector (nm)	0.256
ΔH	Helmholtz energy (eV)	0.31
ΔV	Activation volume (b^3)	12.35
τ_0	Lattice friction (MPa)	10
λ	Geometric constant (-)	0.01
κ	GND arrangement factor (-)	0.6
C	Adjusting parameter for MFP (-)	200
k	Dislocation multiplication coefficient (-)	1.8
d_{anni}	Minimum annihilation distance (nm)	$3b$

is embedded in a larger isotropic elastic matrix to mitigate boundary effects, and cyclic rolling contact is applied to its top surface. The elastic matrix was assigned a Young's modulus of 144.7 GPa and a Poisson's ratio of 0.324. All polycrystalline models measured $300 \times 200 \times 5 \mu\text{m}^3$ and were constructed with random grain orientations. Guided by the experimentally observed layered CG/FG morphology in Fig. 2(a) [25], the polycrystalline models are created using the Neper package [61]. The entire domain was discretized with C3D20R elements, with a minimum element size of 2.5 μm to ensure adequate resolution for capturing intragranular deformation, as shown in Fig. 2(b). To improve computational efficiency, a graded mesh was employed in the surrounding elastic matrix, with element sizes ranging from 3 μm near the RVE to 25 μm at the outer boundaries.

Boundary conditions were carefully prescribed to ensure model stability during rolling contact loading. Except for the top surface, where the sliding regime occurs, all other surfaces were constrained as shown in Fig. 2(c). The rolling contact was simulated by imposing a sliding

normal pressure profile along the top surface, accompanied by the corresponding shear traction [51,63], as illustrated in Fig. 2(d).

Based on Hertzian contact theory [64], the contact pressure field is given by [65]:

$$p(r) = p_0 \sqrt{1 - \left(\frac{r}{a}\right)^2}, \quad (1)$$

where p_0 is the peak contact pressure, r is the radial distance from the center of the contact patch, and a denotes the Hertzian contact radius.

An angle θ is defined to describe the orientation between the indenter's moving direction and the layer boundaries, as illustrated in Fig. 2(d). In this study, two representative cases were examined: $\theta = 0^\circ$ (parallel) and 90° (perpendicular). The amplitude of the cyclic rolling contact load is also depicted in Fig. 2(d).

To emulate well-lubricated rolling contact conditions, surface shear traction was applied concurrently with the normal Hertzian pressure. The shear traction was assumed to be proportional to the local contact pressure and defined as:

$$q(r) = \mu p(r), \quad (2)$$

where μ is the coefficient of friction (COF). The shear traction is applied per unit deformed area and follows rotation, namely, the direction of the tangential force automatically adjusts to the evolving surface orientation. The parameters used to define the contact pressure and shear traction are summarized in Table 2. For simulations involving layered microstructures, the COF was fixed at 0.1 to represent mild frictional conditions [66].

3. Results

Experimental investigations have established that layer thickness plays an important role in governing the mechanical response of layered

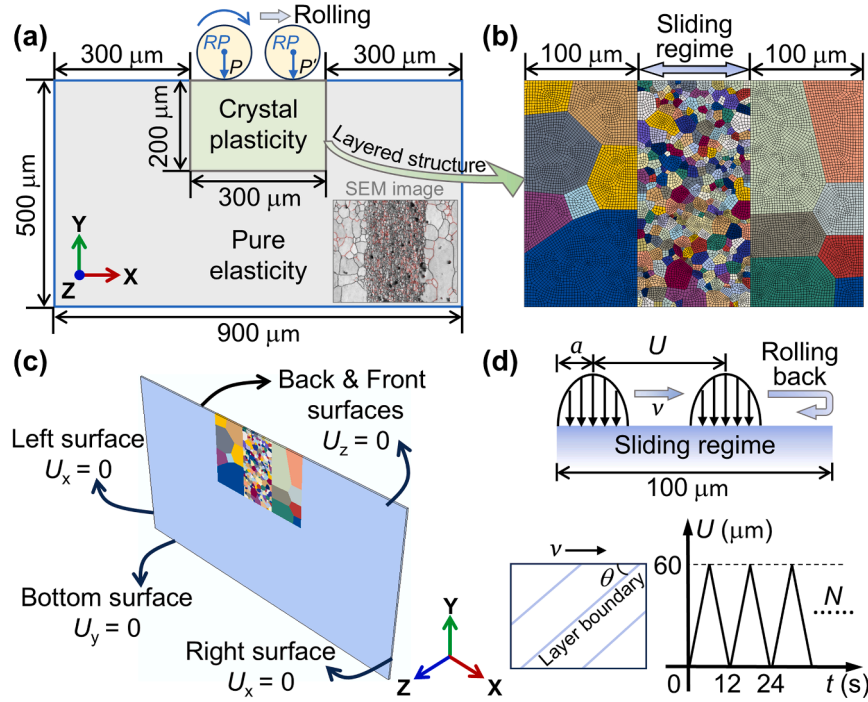


Fig. 2. Setup of the rolling contact finite element simulation. (a) Schematic and dimensions of the finite element model, consisting of a purely elastic foundation and a polycrystalline RVE; a scanning electron microscope (SEM) micrograph of the layered CG/FG material is incorporated [25]. (b) Enlarged view of the polycrystalline RVE, with different colors indicating different grain orientations. (c) Applied boundary conditions in the rolling contact simulation. (d) Schematic representation of the cyclic rolling contact loading scenario.

Table 2
Rolling contact simulation setup.

Symbol	Description (Unit)	Value
p_0	Maximum contact pressure (MPa)	150
a	Half-width (μm)	20
v	Movement speed (μm/s)	10
μ	Coefficient of friction (-)	0.1

materials by modulating interlayer interactions and enabling synergistic deformation mechanisms [27,67–69]. In the present study, a series of polycrystalline layered CG/FG models with varying layer thicknesses were constructed for finite element simulations, with particular attention paid to the orientation of sliding relative to the layer boundaries.

3.1. Effect of layer thickness under perpendicular sliding ($\theta = 90^\circ$)

For sliding perpendicular to the layer boundaries, models with layer thicknesses of 100, 50, 33, and 20 μm were constructed (Fig. 3), spanning a five-fold variation between the thickest and thinnest layers. To isolate the effect of layer thickness, the average grain sizes were held constant in every model, 8 μm in the FG layers and 55 μm in the CG layers. Although CG grains become increasingly non-equiaxed as the layer thickness decreases, it does not affect the predicted mechanical response, because the crystal plasticity constitutive model references only the assigned average grain size, and the equivalent diameter of each grain (computed from its cross-sectional area) is preserved by adjusting the number of grains accordingly. The sliding regime was defined as the central 100 μm segment of the surface, encompassing 1, 2, 3, or 5 layers depending on the specific layer thickness.

It is important to note that the mechanical response is governed not only by the absolute layer thickness but also by its size relative to the contact area. To quantify this, a ratio between the contact diameter ($2a$) and the layer thickness (T_{layer}), termed the relative contact size (S_r), was defined, ranging from 0.4 to 2 in the current models. As this ratio

increases, the contact area spans more layer boundaries, leading to enhanced interaction between CG and FG layers. This parameter enables the analysis of tribological responses across regimes ranging from single-layer-dominated deformation to multi-layer interaction behavior.

Before analyzing the full cyclic loading response, a preliminary simulation of frictionless indentation (i.e., $\text{COF} = 0$) was conducted to validate the modeling framework. The resulting pressure and shear stress contours are shown in Fig. 4. The simulated stress distributions are in good agreement with previous numerical studies [52,70,71]. Under indentation, the maximum contact pressure (i.e., most negative normal stress) is consistently located beneath the indenter, forming a pronounced stress gradient. The shear stress distribution exhibits approximate symmetry about the indenter centerline.

Fig. 5 shows the contour plots of effective plastic strain, GND density, and SSD density after 100 rolling contact cycles. The maximum plastic strain is localized within the central zone of the sliding regime, primarily in the subsurface rather than the top surface, aligning with previous experimental findings on sliding friction [72–74]. This phenomenon has been attributed to subsurface grain rotation and the formation of highly localized lattice rotation bands driven by the cyclic shear stresses [75, 76]. The overall size of the plastic deformation zone (PDZ) remains relatively consistent across all models, showing a weak layer thickness dependence. However, high-level plastic strain primarily accumulates in the CG layer due to its lower strength. In models with smaller layer thicknesses, the FG layers act as barriers that interrupt the continuity of high-strain regions within the CG layers, exhibiting pronounced strain partitioning behavior. This suggests that thinner layers enhance deformation compatibility between adjacent CG and FG layers, thereby effectively promoting strain delocalization [67].

GNDs are observed in both CG and FG layers; however, the FG layers exhibit a notably higher GND density and deeper penetration depth. This behavior is attributed to the higher grain boundary density and yield strength of the FG layers, which promote dislocation pile-up. The elevated GND density within FG layers contributes to accommodating the strain gradient at grain boundaries. In contrast, the GND distribution

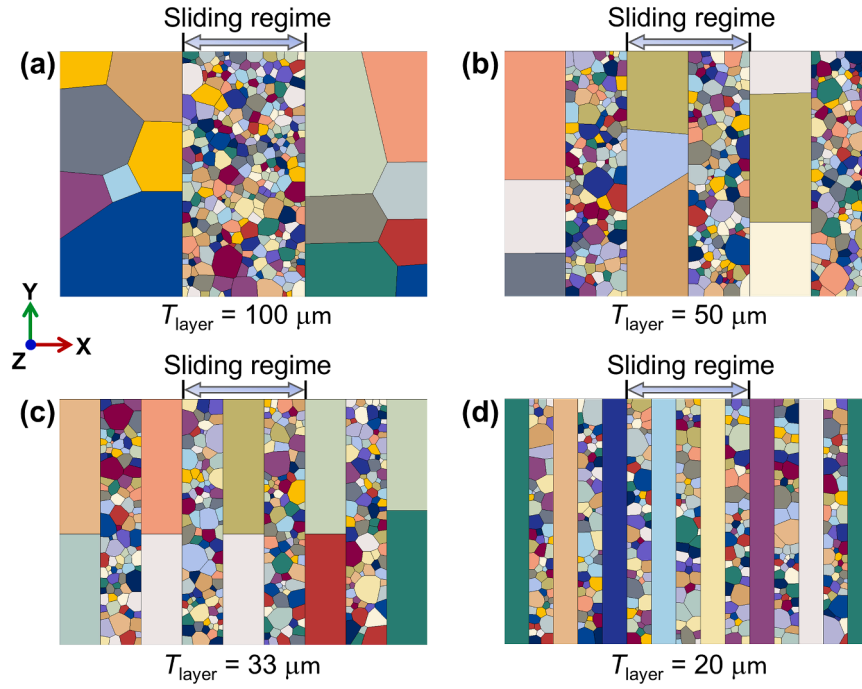


Fig. 3. Microstructural morphologies of four polycrystalline layered CG/FG models with varying layer thicknesses: (a) 100 μm , (b) 50 μm , (c) 33 μm , and (d) 20 μm .

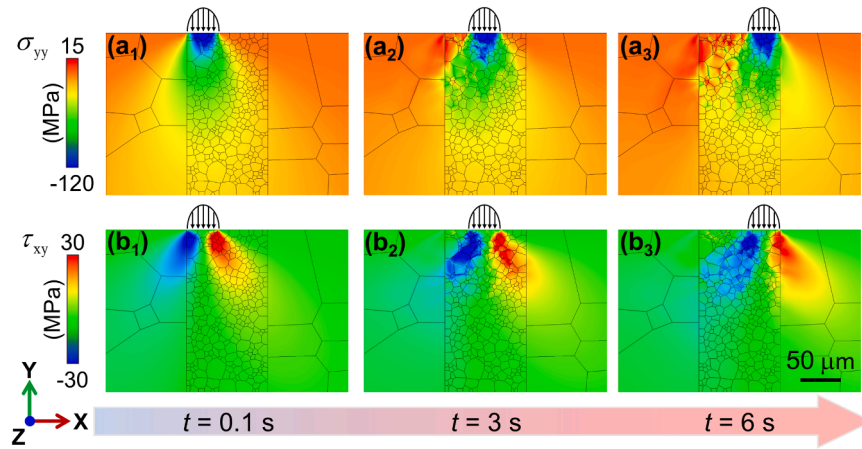


Fig. 4. Stress fields at time frames with varying contact load positions. (a) Normal stress component. (b) Shear stress component. The COF is set to zero in this simulation.

in CG layers is relatively uniform, with dislocations primarily concentrated near the contact surface or grain boundaries. As the layer thickness decreases, the GND distribution becomes more diffuse across the layered structure. The SSD distribution, closely associated with the effective plastic strain due to its dependence on dislocation glide, remains largely confined to the primary PDZ. As layer thickness decreases, the SSD density exhibits a similar partitioning behavior across the layered structure.

Fig. 6 presents the influence of layer thickness on the distribution of SED after 100 rolling contact cycles, with SED serving as a fatigue damage indicator as defined in Eq. (A11). The regions of maximum SED, indicated by white arrows in all models, consistently appear in the subsurface, in agreement with the experimental findings of Zhang et al. [36], who observed the formation of a delaminated tribolayer beneath the surface of layered Cu/CuZn materials. With decreasing layer thickness, the peak SED values are gradually reduced, and the corresponding high-SED regions become more localized, resulting in a more uniform

SED distribution within the primary PDZ. This behavior reflects improved plastic strain compatibility between adjacent layers, thereby promoting damage delocalization and enhancing fatigue performance of thinner CG/FG laminates.

To further quantify damage accumulation, Fig. 7(a) presents the evolution of peak SED as a function of rolling contact cycles for the different layered models. The results indicate that damage accumulates most rapidly within the initial ten cycles, after which the rate of increase gradually stabilizes. This trend is consistent with the experimental wear tests on layered Cu/CuZn materials reported by Zhang et al. [36], where worn surface topographies observed after 100 rolling contact cycles showed little deviation from those at the 10th cycle, indicating that the majority of damage initiates during the early stage.

Importantly, models with thinner layers exhibit a reduced rate of peak SED accumulation, suggesting that decreasing layer thickness effectively suppresses damage evolution under perpendicular sliding. This observation correlates well with the more uniform SED

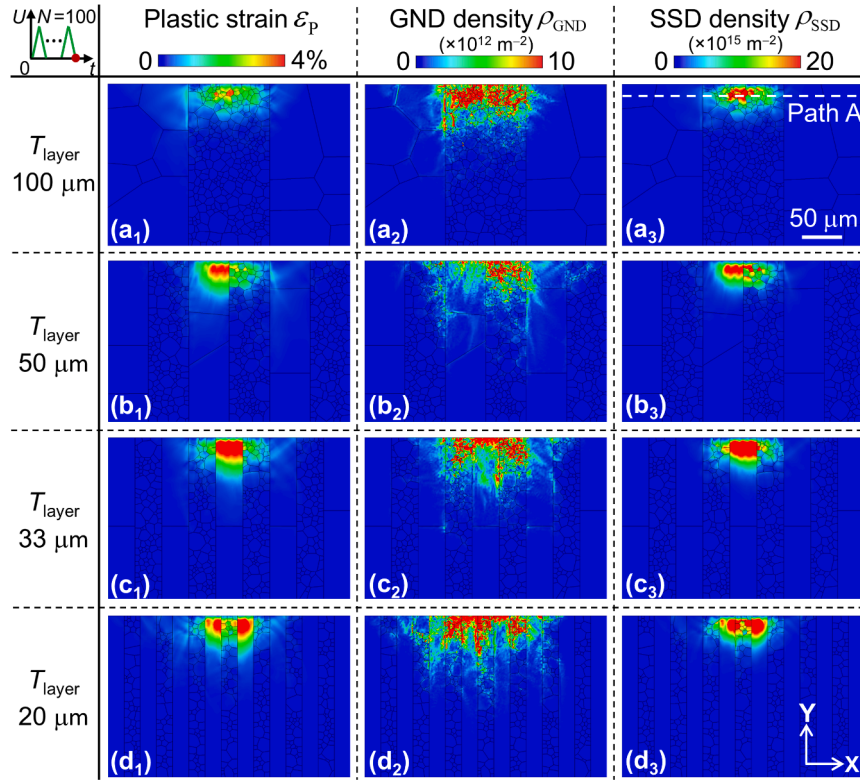


Fig. 5. Contour plots of effective plastic strain, GND density, and SSD density in the layered CG/FG models after 100 rolling contact cycles, with sliding perpendicular to the layer boundaries. The layer thicknesses are: (a) 100 μm , (b) 50 μm , (c) 33 μm , and (d) 20 μm .

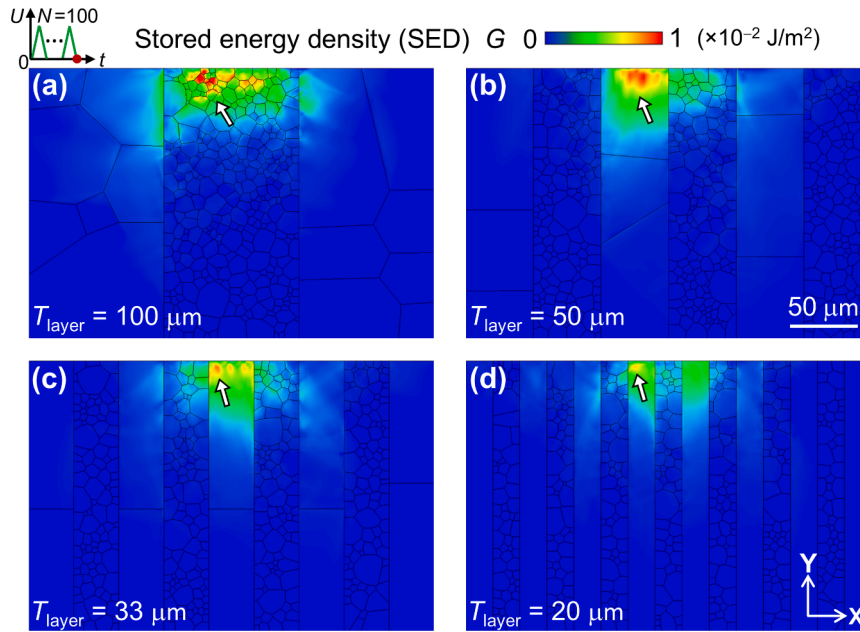


Fig. 6. Contour plots of SED at the 100th cycles for the models with layer thicknesses of (a) 100 μm , (b) 50 μm , (c) 33 μm , and (d) 20 μm .

distributions seen in Fig. 6(d), which indicate that the interlayer load sharing is enhanced in thinner-layer structures. Furthermore, Zhang et al. [36] also revealed that the wear rate decreases with reducing layer thickness when sliding is perpendicular to the layer boundaries, a finding that aligns well with the present simulation results, both supporting the notion that refined layers contribute to improved RCF resistance under this loading condition. The underlying mechanisms

responsible for this finding will be discussed in detail in Section 4.2.

In the simulations, all models initially featured perfectly smooth surfaces. With repeated sliding, surface irregularities progressively developed under the applied loading, as evidenced by the surface height profiles after 100 rolling contact cycles. The vertical displacements U_y of all surface nodes were extracted from the Abaqus field variable U , which is updated at the end of each increment. The average displacement of

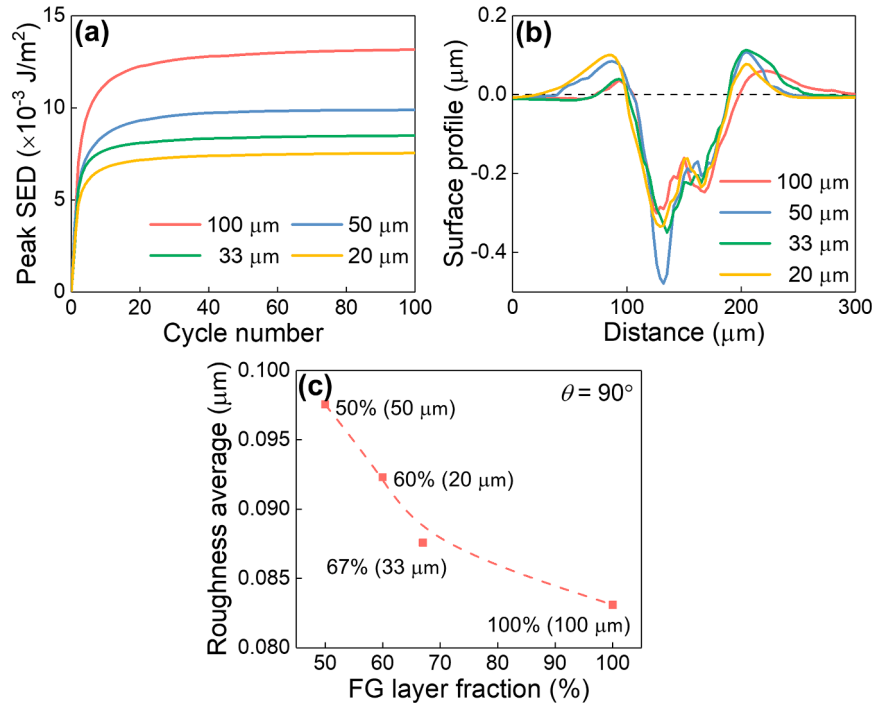


Fig. 7. Damage accumulation and surface roughness evolution after 100 rolling contact cycles with sliding perpendicular to the layer boundaries. (a) Layer thickness effect on the evolution of peak SED with increasing cycles. (b) Surface profiles after 100 cycles. (c) Correlation between surface roughness parameter (R_a) and the fraction of FG layers within the sliding regime. The corresponding layer thicknesses are also given.

nodes located at the same surface coordinate was then calculated. Plotting these average values against the surface distance reconstructs the deformed surface profile, as shown in Fig. 7(b). Notably, the surface profiles do not exhibit a straightforward dependence on layer thickness. However, as mentioned earlier, the number of layers within the sliding regime differs among models with varying layer thicknesses, resulting in different fractions of FG layers across the same contact width, specifically 100 %, 50 %, 67 %, and 60 % for the four models, respectively.

To quantitatively assess the relationship between the change of surface roughness and the FG layer fraction, a representative surface roughness parameter is required. Numerous metrics have been developed to characterize surface roughness. Over 20 such parameters have been evaluated in terms of their correlation with slip resistance [77,78]. Among them, the center-line average (CLA) of surface heights, also known as roughness average (R_a), is one of the most widely adopted. R_a is defined as the arithmetic average of the absolute deviations of the surface height y_i from the mean line over a specified length [78], typically reported in micrometers

$$R_a = \frac{1}{n} \sum_{i=1}^n |y_i|, \quad (3)$$

where n is the number of discrete data points sampled along the profile. Lower R_a values indicate reduced variation between peaks and valleys on the surface, corresponding to a smoother surface. Although the nominal pressure distribution remains constant throughout the simulation, the actual shear traction continuously adjusts to the evolving surface topography and thereby intrinsically captures the effects of roughness development over successive rolling contact cycles.

As illustrated in Fig. 7(c), a higher FG layer fraction generally results in lower surface roughness after cyclic rolling contact. The overall trend suggests that increased proportions of high-strength FG layers enhance surface stability. Therefore, under sliding perpendicular to the layer boundaries, the FG layer fraction within the sliding regime plays a dominant role in governing the evolution of surface roughness.

3.2. Effect of layer thickness under parallel sliding ($\theta = 0^\circ$)

This section examines the effect of layer thickness under loading conditions where the sliding direction is parallel to the layer boundaries. As shown in Fig. 8, four layered models were constructed with layer thicknesses of 100 μm , 50 μm , 33 μm , and 20 μm , consistent with the cases studied under perpendicular sliding, which correspond to 2, 4, 6, and 10 layers, respectively. The average grain sizes of the FG and CG layers were kept constant across all models at 8 μm and 55 μm , respectively.

In each model, the topmost layer subjected to rolling contact was composed of FG material to ensure consistent contact conditions. Since the contact area is located on the surface of only one layer, the relative contact size (S_d) is then defined as the ratio between the contact diameter ($2a$) and the average grain size (d) of the contact layer. This value is calculated to be 5 across all current models. The sliding regime extended over a central zone of 100 μm along the surface of the layered structure. All other boundary conditions and parameters were kept identical to those employed in the perpendicular sliding simulations.

The contour plots of effective plastic strain, GND density, and SED after 100 rolling contact cycles are shown in Fig. 9. Consistent with the observations in Fig. 5, plastic strain is primarily localized within the subsurface region. However, the extent of the PDZ increases as the layer thickness decreases. For instance, in the model with a layer thickness of 100 μm (Fig. 9(a₁)), the maximum depth of plastic deformation is ~46 μm , whereas in the 20 μm -thick model (Fig. 9(d₁)), this depth extends to ~70 μm . This result indicates that a reduced layer thickness promotes deeper subsurface plastic deformation under parallel sliding conditions.

GNDs are mainly concentrated in the topmost FG layer in all cases. Interestingly, in the model with a 20 μm layer thickness, significant GND accumulation is additionally located within the CG layers near the subsurface region (Fig. 9(d₂)), revealing a more inhomogeneous plastic deformation behavior. Moreover, SED localization becomes more prominent with decreasing layer thickness. The maximum SED is observed in the subsurface CG layer, as highlighted by the red region in Fig. 9(d₃), revealing that thinner layers exacerbate damage

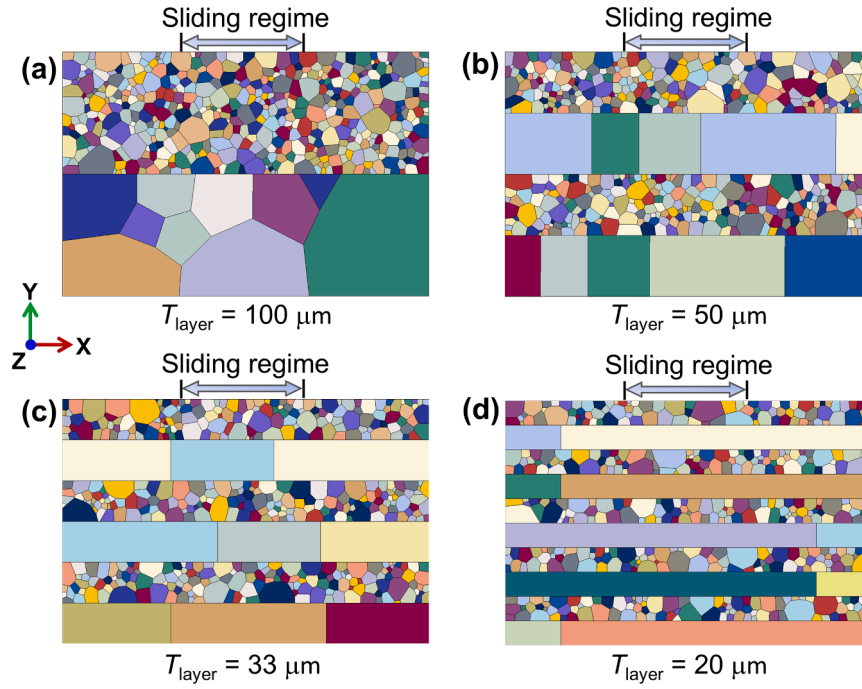


Fig. 8. Microstructural morphologies of four polycrystalline layered CG/FG models with varying layer thicknesses: (a) 100 μm , (b) 50 μm , (c) 33 μm , and (d) 20 μm .

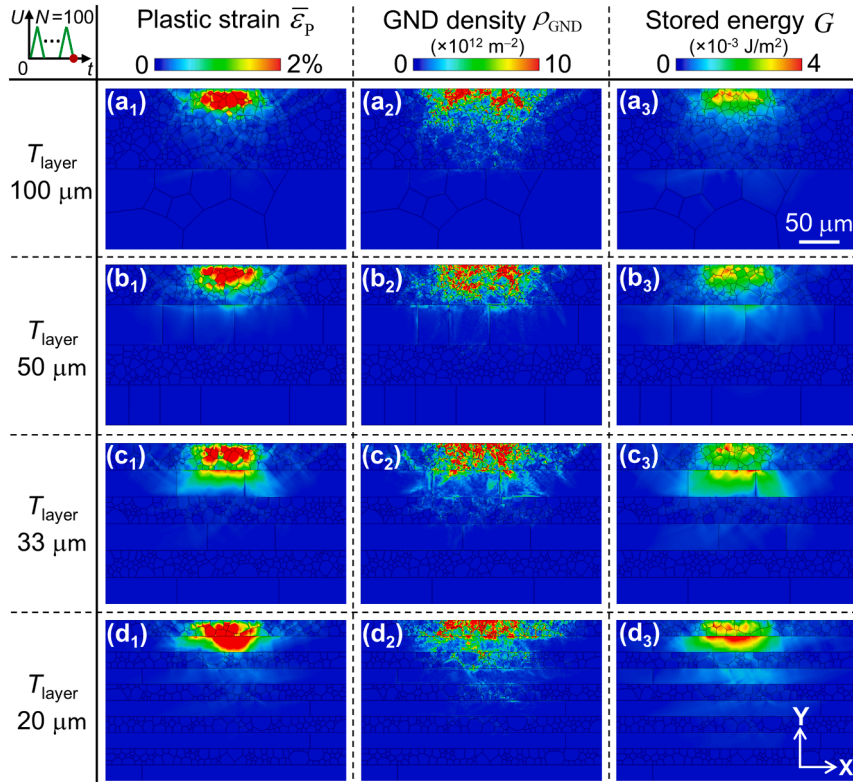


Fig. 9. Contour plots of effective plastic strain, GND density, and SED in the layered models after 100 rolling contact cycles, with sliding parallel to the layer boundaries. The layer thicknesses are: (a) 100 μm , (b) 50 μm , (c) 33 μm , and (d) 20 μm .

accumulation under the parallel sliding condition.

Fig. 10(a) illustrates the evolution of SED over 100 rolling contact cycles, indicating that damage accumulates more rapidly in models with thinner layers. Additionally, the surface profiles, as shown in Fig. 10(b), exhibit increasingly pronounced deviations as layer thickness decreases,

showing a greater degree of surface roughness change. To quantitatively assess the surface degradation, the surface roughness average R_a was calculated for all four models, as shown in Fig. 10(c). The results indicate that models with thicker layers exhibit lower R_a values after repeated rolling contact, implying improved resistance to surface

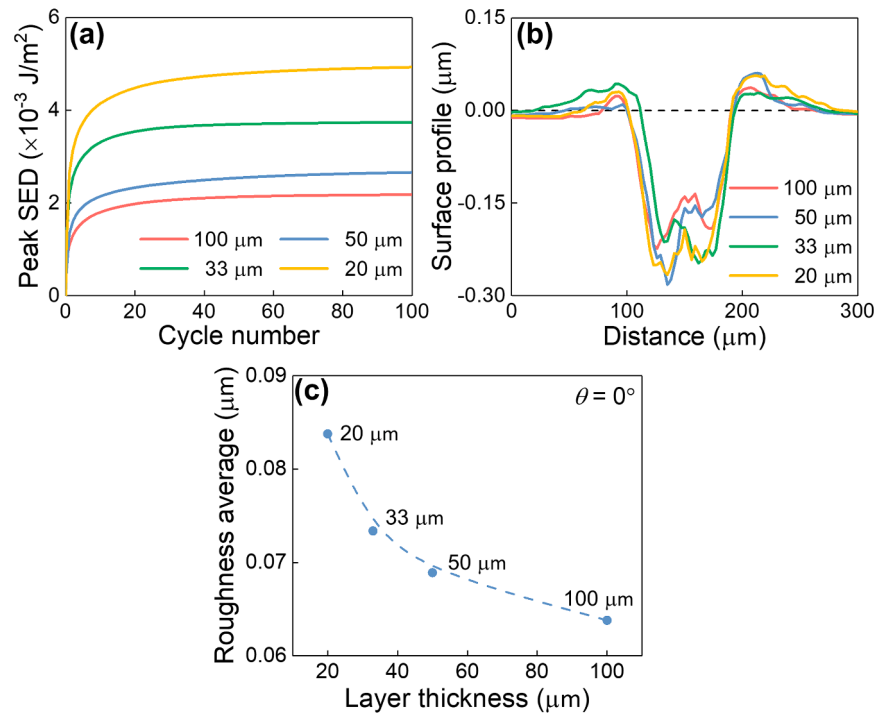


Fig. 10. Evolution of damage and surface roughness under sliding parallel to the layer boundaries. (a) Effect of layer thickness on the evolution of peak SED over 100 rolling contact cycles. (b) Surface profiles after 100 cycles. (c) Correlation between surface roughness parameter (R_a) and layer thickness for parallel sliding ($\theta = 0^\circ$).

roughening.

4. Discussion

The preceding sections established a CPFE framework to investigate the rolling contact behavior of layered CG/FG structures with varying layer thicknesses and sliding orientations. The simulation results

revealed distinct deformation responses between the CG and FG layers, highlighting the role of layer thickness in governing damage accumulation and surface degradation. Building on these insights, this section aims to provide mechanistic interpretations and practical implications of the findings, with a particular focus on addressing the three central questions outlined in the introduction.

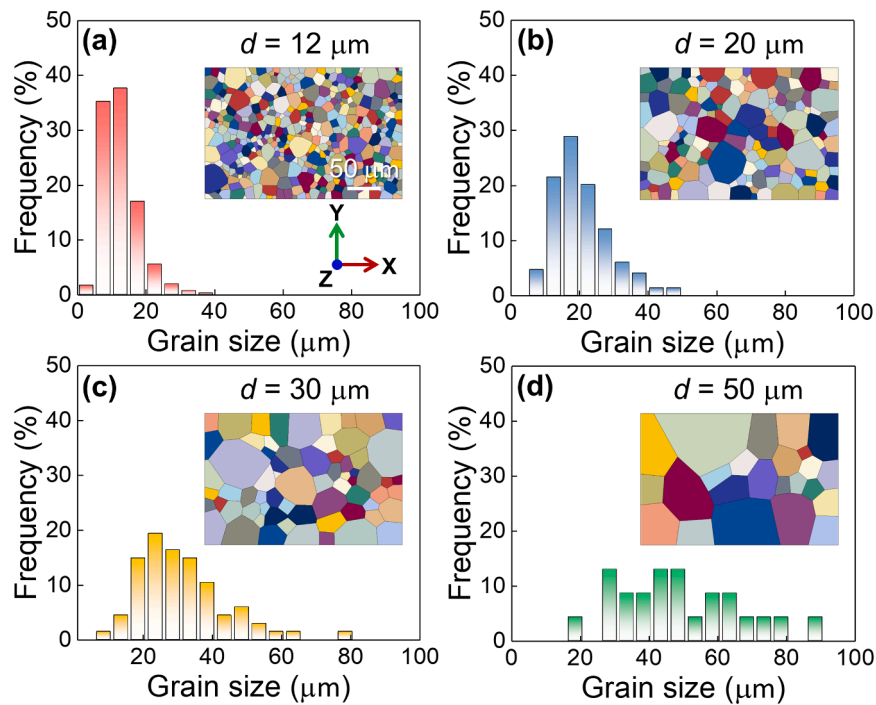


Fig. 11. Microstructural morphologies and grain size distributions of four homogeneous polycrystalline RVEs. The average grain sizes are: (a) 12 μm , (b) 20 μm , (c) 30 μm , and (d) 50 μm , respectively.

4.1. Grain size effect on tribological behavior

A defining characteristic of the layered CG/FG structure is the significant grain size disparity between adjacent layers, which gives rise to notable contrasts in mechanical responses. To elucidate the deformation mechanisms governing such layered structures under rolling contact conditions, it is essential to first evaluate the influence of grain size on tribological behavior.

Previous studies have established certain trends in this regard. Zhang et al. [79] demonstrated that reducing grain size enhances fretting fatigue resistance using CPFE simulations. Li et al. [80] experimentally verified that finer grains improve the wear resistance of Inconel 600 alloys. Conversely, Shanthi et al. [81] observed that, despite variations in mechanical properties, the wear behavior remained largely insensitive to grain size differences. Ashton et al. [82] conducted CPFE modeling and emphasized that reliable fretting fatigue predictions must consider the interplay between slip length scale, grain size, and contact width.

To investigate the grain size effect under rolling contact conditions, four homogeneous polycrystalline copper RVEs were constructed with average grain sizes of 12 μm , 20 μm , 30 μm , and 50 μm , as shown in Fig. 11. The largest grain size was approximately four times the smallest. Simulations were carried out under COFs of 0, 0.1, 0.2, and 0.3, resulting in a total of 12 simulation cases. For simplification, only a single cycle was simulated in each case.

Contour plots of effective plastic strain and GND density at the end of this cycle are shown in Fig. 12 and Fig. 13, respectively. As shown in Fig. 12, a distinct subsurface PDZ develops beneath the contact region in all models. For a given COF, models with larger average grain sizes exhibit more pronounced plastic deformation, as indicated by the enlarged red regions (high plastic strain). This trend reflects a reduction in RCF resistance with increasing grain size, consistent with the Hall-Petch relationship, which describes the inverse dependence of yield strength on grain size.

Notably, although the magnitude of plastic strain increases with grain size, the depth of the PDZ remains relatively constant across all cases. For a fixed grain size, increasing the COF leads to higher plastic strain levels due to the elevated shear stresses applied to the surface. While plastic strain remains primarily localized in the subsurface region,

a COF of 0.3 induces substantial strain accumulation near the contact surface, indicating a transition to more severe sliding-induced plastic deformation at high friction levels.

As shown in Fig. 13, for a given COF, GND accumulation becomes more significant as grain size decreases, accompanied by an expansion in the spatial extent of GND generation. GNDs are predominantly concentrated beneath the contact surface, particularly along grain boundaries, reflecting significant deformation incompatibility and high plastic strain gradients. This behavior arises from the increased grain boundary density and more intricate grain misorientation in FG models, which demand higher GND densities to accommodate the resulting plastic strain heterogeneity. Moreover, for a fixed grain size, increasing the COF significantly amplifies GND accumulation, underscoring the critical role of friction-induced shear stresses in promoting deformation incompatibility and strain gradient.

Based on the results shown in Figs. 12–13, the average effective plastic strain and GND density versus the relative contact size (S_d) for all 12 cases were quantified within a defined region of interest (ROI), as illustrated in Fig. 14(a). The ROI extends $5a$ along the X-axis and $4a$ along the Y-axis, where a denotes the half-width of the indenter. The results reveal that both increasing grain size (decreasing relative contact size) and COF lead to higher plastic strain accumulation within the ROI. Furthermore, GND density is consistently greater in FG models (larger relative contact size) across all COF levels, whereas in CG models (smaller relative contact size), variation in COF exerts a comparatively weaker influence on GND accumulation.

Fig. 14(b) displays the post-sliding surface profiles for cases under COFs of 0 and 0.3. Larger COF values produce more obvious variation in surface alteration, a trend observed across all grain sizes. To further quantify this effect, Fig. 14(c) compares the surface roughness average R_a . At a fixed COF, R_a increases with grain size, indicating reduced surface roughening resistance in CG materials. This observation aligns well with experimental findings in the rolling contact tests of pure copper foils with varying grain sizes [83].

The above results highlight the distinct mechanical responses of CG and FG materials under rolling contact conditions. FG structures exhibit a high density of GNDs and enhanced resistance to plastic deformation, yet are prone to stress concentration, which may accelerate damage initiation. Conversely, CG structures accommodate greater plastic

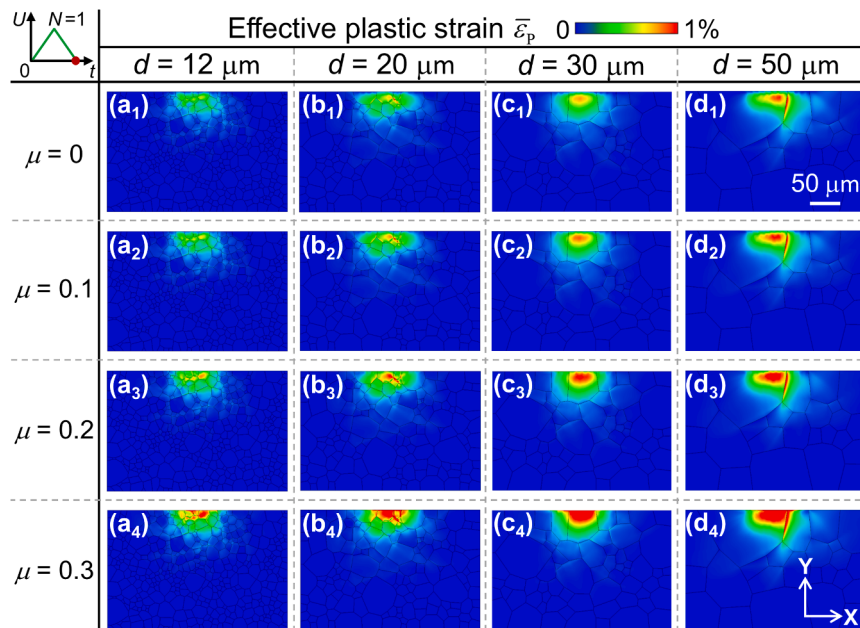


Fig. 12. Contour plots of effective plastic strain in homogenous RVEs with varying grain sizes after one-cycle rolling contact under different COFs. The average grain sizes are: (a) 12 μm , (b) 20 μm , (c) 30 μm , and (d) 50 μm . COFs used are 0, 0.1, 0.2, and 0.3.

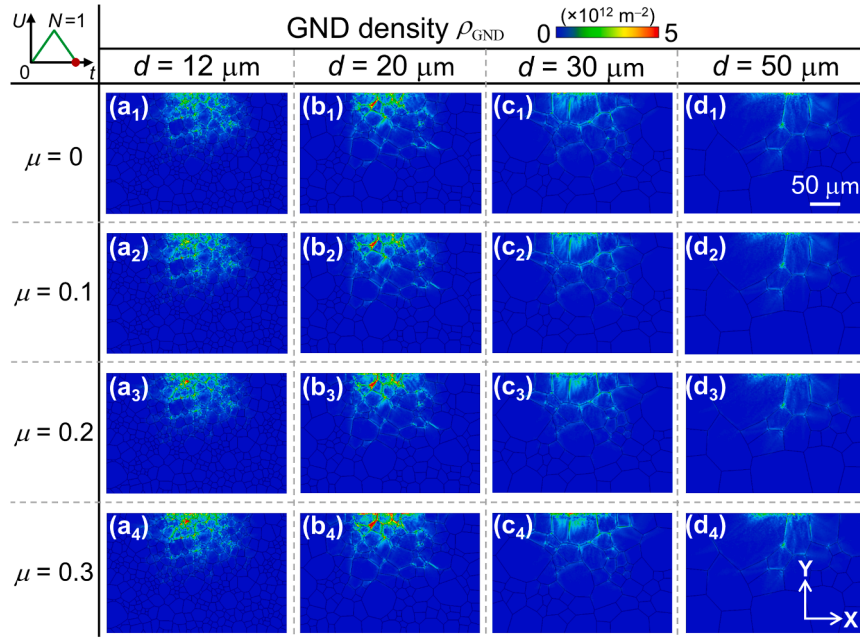


Fig. 13. Contour plots of GND density in homogenous RVEs with varying grain sizes after one-cycle rolling contact under different COFs. The average grain sizes are: (a) 12 μm , (b) 20 μm , (c) 30 μm , and (d) 50 μm . COFs used are 0, 0.1, 0.2, and 0.3.

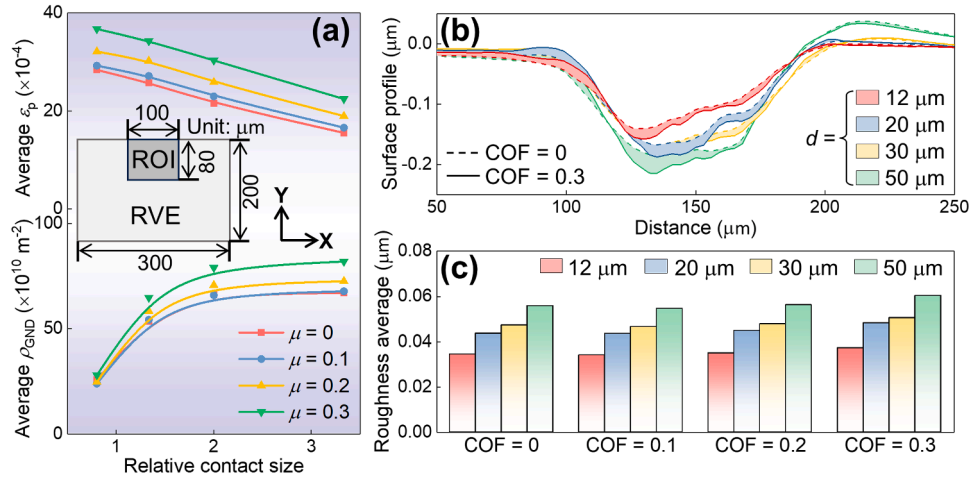


Fig. 14. Grain size effects on plastic strain, GND density, and surface roughness in homogeneous RVEs under rolling contact. (a) Evolutions of average effective plastic strain and GND density with increasing relative contact size (S_d). (b) Surface profiles under COFs of 0 and 0.3. (c) Surface roughness average (R_a) after one-cycle rolling contact.

deformation, but this comes at the cost of increased surface roughness evolution. Therefore, in layered CG/FG structures, a comprehensive understanding of the synergistic interactions and complementary mechanical attributes of the constituent layers is essential for optimizing tribological performance. The following section provides an in-depth analysis of the underlying mechanism.

4.2. Synergistic interaction between CG and FG layers

The mechanical response of CG and FG layers during deformation is governed by dislocation-mediated interactions both within and across the layers. Under tensile loading, plastic strain gradients near the CG/FG layer boundaries promote the generation of GNDs in the CG layers, leading to the development of long-range internal stresses, manifesting as back stresses in CG layers and forward stresses in adjacent FG layers [84]. This internal stress redistribution facilitates hetero-zone

interactions [85,86], which significantly affects strain partitioning throughout the layered structure [87]. A similar dislocation partitioning mechanism is activated under rolling contact conditions.

Fig. 15 presents the distributions of SSDs and GNDs along the path A in Fig. 5(a₃) for the layered CG/FG structures. A distinct dislocation partitioning phenomenon is observed, characterized by the preferential segregation of dislocation types across the layers: SSDs concentrate predominantly in the CG layers, while GND density accumulates in the FG layers. This distribution arises from the higher grain boundary density in the FG layers, which facilitates GND generation, as previously discussed in Section 4.1. In contrast, the higher yield strength of the FG layers limits their plastic strain capacity, leading to reduced SSD formation.

This dislocation partitioning behavior promotes strain delocalization and enhances interlayer compatibility, thereby suppressing localized damage under cyclic loading. According to Eq. (A11), the SED depends

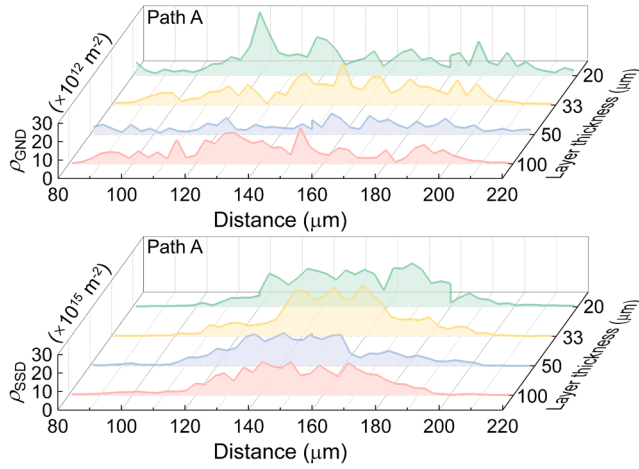


Fig. 15. Along-path distributions of GND and SSD densities after 100 rolling contact cycles in layered CG/FG models with varying layer thicknesses under sliding perpendicular to the layer boundaries. The layer thicknesses are 100 μm , 50 μm , 33 μm , and 20 μm . The path A is indicated by the white dashed line in Fig. 5(a₃).

on both GND and SSD densities; thus, the observed dislocation partitioning delays SED localization and retards damage evolution. Moreover, the presence of coherent layer boundaries fosters coordinated deformation between CG and FG layers, thereby reducing severe strain localization and hindering the formation of brittle tribolayers [36].

Overall, this mechanism underscores the critical role of microstructural heterogeneity in accommodating plastic strain and improving RCF resistance. The synergistic interaction between CG and FG layers significantly contributes to enhanced damage tolerance under cyclic rolling contact conditions.

4.3. Microstructure design for improving RCF damage resistance

The above simulation results provide practical guidelines for selecting an appropriate layer thickness to optimize damage resistance. Fig. 16(a) compares the peak SED after 100 rolling contact cycles as a function of layer thickness for both sliding orientations, showing that the effect of layer thickness is strongly orientation-dependent. When sliding is parallel to the layer boundaries ($\theta = 0^\circ$), thinner layers accelerate damage evolution. Notably, as shown in Fig. 9, subsurface CG layers promote severe plastic strain localization and rapid damage accumulation, thereby increasing the risk of premature failure. Consequently, a thicker top-surface FG layer is beneficial for improving RCF resistance in the parallel sliding configuration. Conversely, when sliding is perpendicular to the layer boundaries ($\theta = 90^\circ$), damage

accumulation accelerates with increasing layer thickness, whereas thinner layers promote deformation compatibility and suppress SED localization. In this orientation, reducing the layer thickness enhances the synergistic interaction between FG and CG layers, thereby improving strain accommodation and overall RCF durability. At identical layer thicknesses ranging from 20 to 100 μm , parallel sliding results in a lower peak SED in the layered CG/FG structure compared to perpendicular sliding.

Fig. 16(b) reveals an inverse relationship between the relative contact size (S_t) and the peak SED under perpendicular sliding. As S_t increases, a large number of CG and FG layers are engaged within the contact region, promoting more extensive interlayer interaction. This enhanced synergistic effect improves resistance to damage accumulation by facilitating better plastic strain compatibility across layers.

Moreover, previous experimental studies have demonstrated that the superior tribological properties of layered heterostructures primarily arise from strain delocalization facilitated by layer boundaries [36]. However, the mechanism of strain delocalization and its controlling factors remain unclear. Numerical simulations offer a precise way to capture the evolution of strain distribution and damage in different layered architectures, thereby providing insight into the governing mechanisms.

Among the various microstructural parameters, the grain size ratio, defined as the ratio of the average grain size in the CG layer to that in the FG layer, plays a pivotal role in dictating the mechanical contrast between adjacent layers. Therefore, tuning the grain size disparity offers a viable strategy for optimizing the synergistic deformation behavior between CG and FG layers.

To elucidate this effect, a series of three-layered FG/CG/FG models with varying grain size ratios were constructed, as illustrated in Fig. 17. While it is experimentally challenging to vary grain size ratios by adjusting only a part of layers and keeping the others constant, such control is readily achievable in computational modeling. The grain size in the CG layer was fixed at 100 μm , while that of the FG layers was varied (10 μm , 20 μm , and 50 μm), corresponding to grain size ratios of 10, 5, and 2, respectively. All layers consisted of equiaxed grains with relatively uniform size distributions to minimize intra-layer grain size variation. The CG layer comprised two grains with identical crystallographic orientations across all models, and the sliding regime was configured to fully encompass the surface of the CG layer. Under these conditions, any variation in the mechanical response of the CG layer can be solely attributed to changes in the FG layers. All other simulation parameters remained consistent with those described in Section 2.2.

Fig. 18(a-c) shows the contour plots of effective plastic strain, GND density, and SED after 100 rolling contact cycles. Although plastic deformation is predominantly localized within the CG layer, the PDZ extends into the adjacent FG layers. This cross-layer-boundary deformation becomes increasingly pronounced as the grain size ratio decreases from 10 to 2. In the CG layer, GNDs are primarily generated near

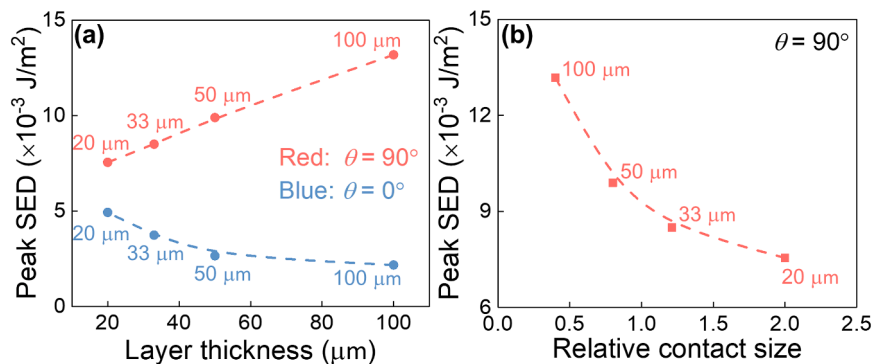


Fig. 16. Peak SED after 100 rolling contact cycles for both sliding orientations. (a) Variation with increasing layer thickness. (b) Variation with increasing relative contact size (S_t).

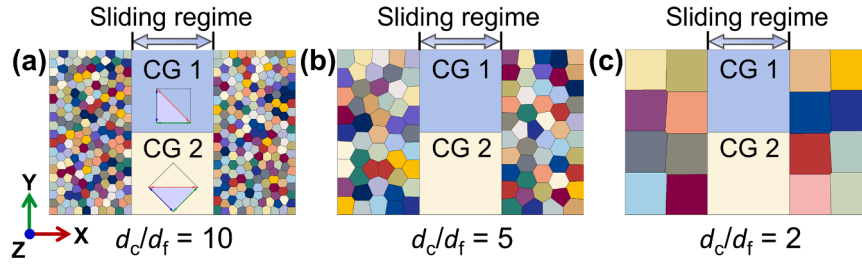


Fig. 17. Microstructural morphologies of three polycrystalline layered CG/FG models with varying grain size ratios. The grain size ratios are: (a) 10, (b) 5, and (c) 2. The Euler angles for grains in the CG layer are fixed at CG 1 ($0^\circ, 0^\circ, 0^\circ$) and CG 2 ($45^\circ, 0^\circ, 0^\circ$).

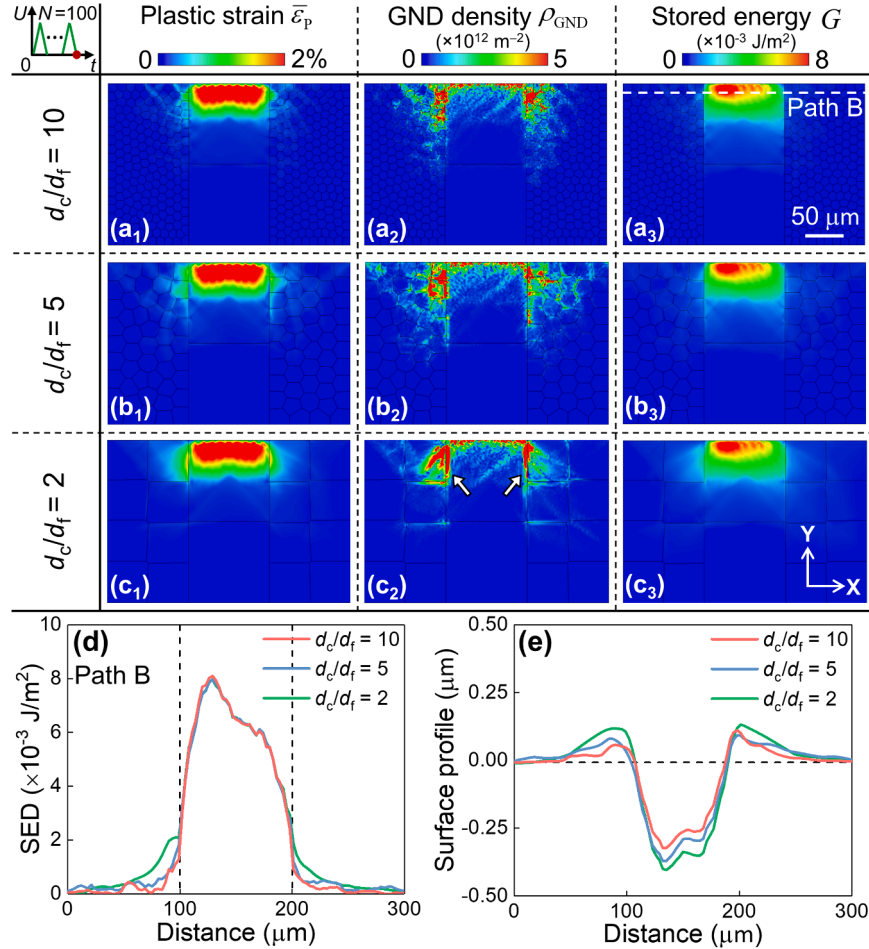


Fig. 18. Influence of grain size ratio on damage accumulation and surface alteration in layered models after 100 rolling contact cycles. Contour plots of (a) Effective plastic strain, (b) GND density, and (c) SED. (d) SED distribution along the path B marked by the white dashed line in (a₃). (e) Surface profiles after 100 cycles.

the surface, while in the FG layers, they are concentrated near the layer boundaries. Although the grain size ratio has limited influence on GND accumulation at the contact surface, a lower grain size ratio results in a marked increase in GND density at the layer boundaries, as indicated by the white arrows in Fig. 18(c₂). This phenomenon reflects an intensified plastic strain gradient, which may accelerate damage evolution under cyclic loading [88].

Under uniaxial tensile loading, reducing the grain size ratio typically diminishes the mechanical mismatch between layers, thereby alleviating strain incompatibility and reducing GND accumulation at layer boundaries [62,89,90]. However, this trend is reversed under rolling contact conditions, where the multiaxial stress state (comprising both normal and tangential components) interacts with the layer boundaries in a fundamentally different manner. The mechanistic basis for this

contrasting behavior will be further elaborated later in this paper.

Fig. 18(a₃-c₃) reveal that, while the SED distribution within the CG layer remains largely unchanged across the models, the SED within the FG layers increases significantly with decreasing grain size ratio. Consistent with the GND distributions, the SED in the FG layers is concentrated near the layer boundaries. Fig. 18(d) quantifies the SED distribution along the path B shown in Fig. 18(a₃). The overlapping SED profiles in the CG layer suggest that the grain size change of the surrounding FG layers has a negligible effect on damage accumulation in the middle CG layer. In contrast, the FG layers exhibit a progressively broader damage-affected zone near the layer boundary as the grain size ratio decreases. This trend indicates that reducing the FG layer's grain size enhances its ability to constrain the damage originating from the CG layer within the sliding regime. The distinguishing feature of these three

models is the grain size ratio between layers. Fig. 18(d) indicates that a higher ratio enhances the resistance to the damage propagation from the CG layer to the FG layer. Furthermore, as shown in Fig. 18(e), higher grain size ratios correspond to reduced surface roughness changes after 100 cycles, reflecting improved surface roughness resistance under repeated rolling contact loading.

To further elucidate the mechanism of plastic strain transfer from the CG layer to the adjacent FG layer, contour plots of effective plastic strain were extracted at the 1st, 5th, and 100th rolling contact cycles for grain size ratios of 10 and 2, as shown in Fig. 19. The corresponding strain distributions along the predefined path (the path C in Fig. 19(a₁, b₁)) are plotted in Fig. 19(a₄, b₄). After the first cycle, a PDZ emerges within the CG layer in both cases; however, the extent of the PDZ is significantly larger for the lower grain size ratio. Notably, in the case of grain size ratio 2 (Fig. 19(b₁)), plastic strain is already evident in the FG layers near the layer boundaries, even before the CG layer's PDZ reaches the boundaries. This early activation of plasticity at the layer boundaries induces plastic strain gradients, promoting GND accumulation, consistent with the observations in Fig. 18(c₂).

With continued cyclic loading, the PDZ in the CG layer progressively grows and eventually penetrates into the adjacent FG layers. After 100 cycles, the extent of PDZ within the FG layers is also significantly larger for the lower grain size ratio. At a grain size ratio of 10, the PDZ in the CG layer remains relatively confined, indicating a constraining effect imposed by the surrounding high-strength FG layers (Fig. 19(a)). In contrast, for the grain size ratio of 2, the PDZ expands into the FG layers, suggesting that a reduced grain size ratio facilitates plastic strain transmission and damage propagation across the layer boundaries, which is harmful to the RCF resistance in layered structures.

The dislocation activity and damage evolution during cyclic rolling

contact are primarily governed by shear stress [53]. To clarify why the SED profiles in the CG layer remain nearly invariant across different grain size ratios, shear stress contour plots were analyzed at a representative moment during the 100th cycle (just before the indenter reaches the left boundary of the CG layer), as shown in Fig. 20 (a₁–c₁). The magnified view of the upper grain within the CG layer is given in Fig. 20 (a₂–c₂) for detailed comparison. In all three models, peak shear stresses are localized near the edges of the contact zone. While the FG layers exhibit distinct shear stress distributions due to changes in grain size and orientations, the shear stress fields within the CG layer are nearly identical across all studied cases. For a quantitative comparison, Fig. 20 (d) presents shear stress profiles along the path D in the coarse grain (5 μm below the surface, see Fig. 20(a₂)). The three models display nearly identical shear stress distributions, indicating that the local stress state in the CG layer is largely unaffected by the grain size of the adjacent FG layers. This behavior explains the minimal variation in SED distribution within the CG layer across different grain size ratios, as observed earlier in Fig. 18(d).

5. Conclusion

This study systematically investigated the cyclic rolling contact behavior of heterogeneous layered materials composed of CG and FG layers using CPFE simulations. The simulations successfully capture the experimentally observed friction anisotropy with respect to the sliding orientation [36]. Result analysis elucidated the reason for the influence of layer thickness on damage accumulation during rolling contact, highlighting the combined effect of layer thickness and sliding direction on RCF stability, and the critical role of dislocation partitioning. This mechanism facilitates synergistic interactions between CG and FG

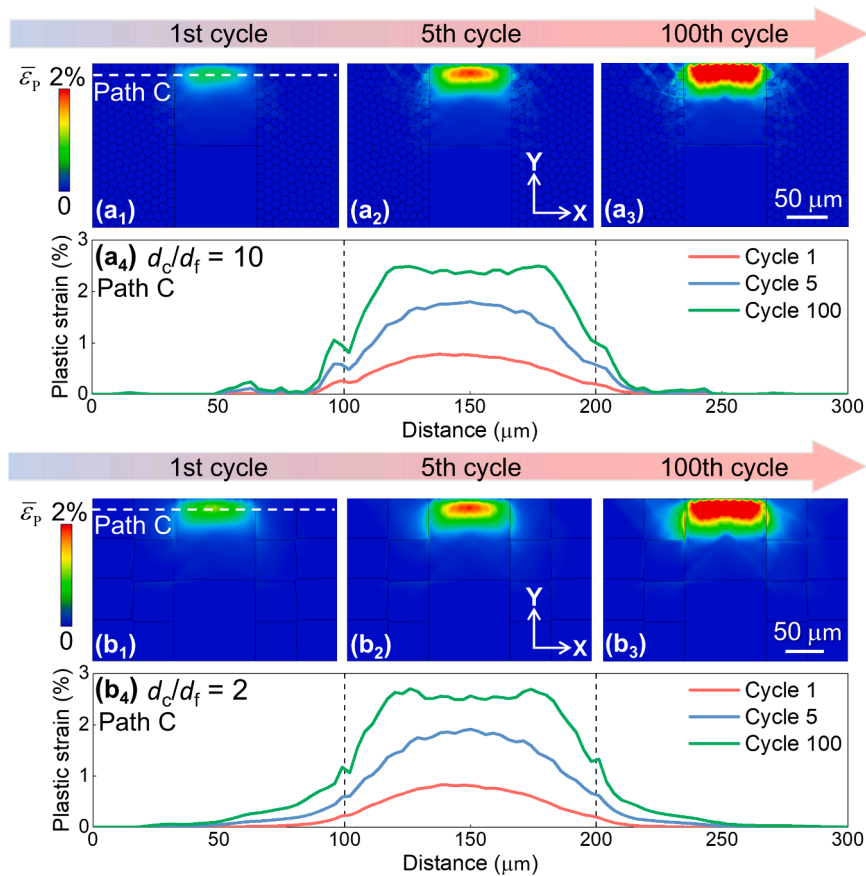


Fig. 19. Temporal evolution of effective plastic strain in layered models with different grain size ratios after the 1st, 5th, and 100th rolling contact cycles. Grain size ratios: (a) 10 and (b) 2.

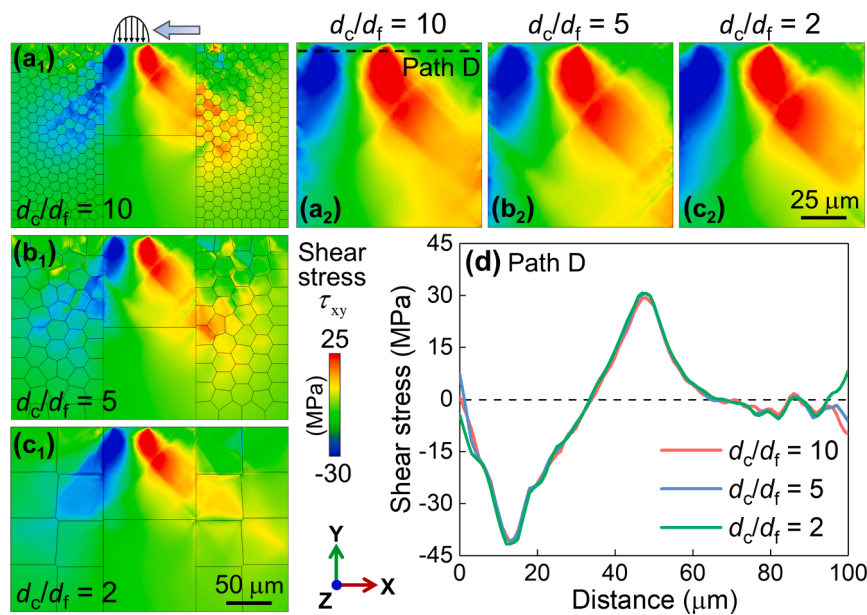


Fig. 20. Shear stress distribution in layered models with varying grain size ratios. Contour plots of shear stress for grain size ratios of (a) 10, (b) 5, and (c) 2. (d) Shear stress along the path D marked by the black dashed line in (a₂).

layers, contributing to enhanced damage resistance and superior tribological performance of the layered heterostructures. The main conclusions are summarized as follows:

- (1) Grain size exerts a significant influence on the rolling contact response of polycrystalline materials. Under identical loading conditions, decreasing grain size (i.e., increasing relative contact size) results in reduced plastic strain, higher GND density, and less surface roughening. This grain size effect leads to the dislocation partitioning in layered CG/FG structures under perpendicular sliding ($\theta = 90^\circ$): SSDs tend to localize within the CG layers, whereas GNDs predominantly accumulate in the FG layers. This behavior promotes SED delocalization.
- (2) The influence of layer thickness on damage evolution is highly dependent on the angle (θ) between the sliding direction and the layer boundaries. When $\theta = 90^\circ$ (perpendicular sliding), reducing the layer thickness significantly suppresses damage accumulation. In contrast, when $\theta = 0^\circ$ (parallel sliding), thinner layers accelerate damage evolution due to intensified plastic strain localization. For a given layer thickness considered in this study, parallel sliding yields a lower peak SED in the layered CG/FG structure compared to perpendicular sliding.
- (3) A higher grain size ratio increases mechanical mismatch between adjacent layers, which effectively hinders the transmission of plastic strain from the CG layer to FG layer, and retards damage propagation across the CG/FG interfaces. Moreover, a higher grain size ratio contributes to reduced surface roughening under cyclic loading. Therefore, selecting an appropriate grain size contrast is beneficial for mitigating the damage propagation and surface degradation.

These findings emphasize the critical role of microstructural design in optimizing the tribological performance of metallic materials. The mechanistic insights provide guidance for the development of RCF-resistant heterogeneous layered structures.

Statement of originality

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which has been published previously, by the current authors or by others, of which the source is not explicitly cited in the paper.. I would like to declare on behalf of my co-authors that the work described was original research that has not been published previously and is not under consideration for publication elsewhere, in whole or in part.

CRediT authorship contribution statement

Xiaochong Lu: Writing – original draft, Visualization, Software, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Xikai Yu:** Methodology, Investigation, Formal analysis. **Zixu Guo:** Writing – review & editing, Visualization, Formal analysis. **Xiaohua Zhang:** Visualization, Validation, Investigation. **Guglielmo Vastola:** Writing – review & editing, Validation. **Daniele Dini:** Writing – review & editing, Supervision, Resources, Project administration, Conceptualization. **Yilun Xu:** Writing – review & editing, Validation, Methodology, Investigation, Formal analysis, Conceptualization. **Yong-Wei Zhang:** Writing – review & editing, Validation, Supervision, Project administration.

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 paper.

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Appendix A. Crystal plasticity constitutive model

In this study, a dislocation-based CPFE framework is employed for constitutive modeling. Grain size effects are incorporated to capture the differences in slip resistance and dislocation evolution between coarse and fine grains. A brief summary is provided here, with full details available in [91].

The slip shear rate $\dot{\gamma}^\alpha$ per slip system is governed by thermally activated dislocation motion overcoming pinning obstacles [91]:

$$\dot{\gamma}^\alpha = \rho_{\text{ISSD}} b^2 \nu_D \exp\left(-\frac{\Delta H}{k_B T}\right) \sinh\left[\frac{\Delta V}{k_B T} \left(|\tau_{\text{eff}}^\alpha| - \tau_c^\alpha\right)\right] \text{sgn}(\tau_{\text{eff}}^\alpha), \quad (\text{A1})$$

where ρ_{ISSD} is the initial density of mobile statistically stored dislocations (SSDs), b is the magnitude of the Burgers vector, $\nu_D = 10^{11} \text{ s}^{-1}$ is the Debye frequency describing dislocation escape attempts at obstacles, ΔH and ΔV are the Helmholtz energy and activation volume, $k_B = 1.38 \times 10^{-23} \text{ J/K}$ is the Boltzmann constant, T is the temperature in Kelvin, τ_{eff}^α is the effective shear stress acting as the driving force for dislocation slip [92]:

$$\tau_{\text{eff}}^\alpha = \tau^\alpha - \tau_b^\alpha, \quad (\text{A2})$$

where τ^α is the resolved shear stress, τ_b^α is the back stress raised by GND pile-ups:

$$\tau_b^\alpha = \kappa G b L^\alpha \rho_{\text{GND}}^\alpha, \quad (\text{A3})$$

where $\kappa = 0-1$ is the factor describing the arrangement of geometrically necessary dislocations (GNDs); G is the shear modulus, which can be estimated from the single-crystal elastic constants using the Voigt scheme [93]:

$$G = \frac{C_{11} - C_{12} + 3C_{44}}{5}. \quad (\text{A4})$$

These elastic constants are defined as material parameters in the UMAT subroutine and are used to construct the elastic matrix of the face-centered cubic (FCC) lattice structure during the simulation [94]:

$$\mathbf{C}_{\text{FCC}} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ & C_{11} & C_{12} & 0 & 0 & 0 \\ & & C_{11} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & & & & C_{44} & 0 \\ & & & & & C_{44} \end{bmatrix}. \quad (\text{A5})$$

The mean free path (MFP) L^α between the dislocations is influenced by the average grain size d and the current dislocation densities [95]:

$$\frac{1}{L^\alpha} = \frac{C}{d} + \sqrt{\rho_{\text{SSD}}^\alpha + \rho_{\text{GND}}^\alpha}, \quad (\text{A6})$$

where C is an adjusting parameter, ρ_{SSD}^α and ρ_{GND}^α are the densities of SSDs and GNDs, respectively.

τ_c^α in Eq. (A1) is the critical resolved shear stress (CRSS) for dislocation slip. For incorporating the grain size effect, the classical Taylor's hardening relation is extended according to Ref. [95]:

$$\tau_c^\alpha = \tau_0 + \frac{\lambda G b}{L^\alpha} = \tau_0 + \lambda G b \left(\frac{C}{d} + \sqrt{\rho_{\text{SSD}}^\alpha + \rho_{\text{GND}}^\alpha} \right), \quad (\text{A7})$$

where τ_0 is the lattice friction, λ is a geometric constant.

The evolution of SSD density is governed by the Kocks-Mecking law [92,96]:

$$\dot{\rho}_{\text{SSD}}^\alpha = \left(\frac{k}{L^\alpha} - 2d_{\text{anni}} \rho_{\text{SSD}}^\alpha \right) \frac{|\dot{\gamma}^\alpha|}{b}, \quad (\text{A8})$$

where k is the coefficient controlling dislocation multiplication, d_{anni} is the minimum annihilation distance for two dislocations with opposite signs.

The GND density is derived from the Nye tensor, which captures the lattice curvature due to heterogeneous plasticity and is computed as the curl of the plastic deformation gradient tensor $\mathbf{F}_p$:

$$\mathbf{\Lambda} = \text{curl}(\mathbf{F}_p) = \sum_{\alpha=1}^N (\rho_{\text{GS}}^\alpha \mathbf{b} \mathbf{s}^\alpha \otimes \mathbf{s}^\alpha + \rho_{\text{Gen}}^\alpha \mathbf{b} \mathbf{s}^\alpha \otimes \mathbf{t}^\alpha + \rho_{\text{Gen}}^\alpha \mathbf{b} \mathbf{s}^\alpha \otimes \mathbf{n}^\alpha), \quad (\text{A9})$$

where $N = 12$ is the total number of slip systems in the FCC lattice, ρ_{GS}^α is the screw component of GNDs with line vector along the slip direction ($\mathbf{s}^\alpha$), ρ_{Gen}^α and ρ_{Gen}^α are the edge GND densities in the normal ($\mathbf{n}^\alpha$) and tangential ($\mathbf{t}^\alpha = \mathbf{s}^\alpha \times \mathbf{n}^\alpha$) direction, respectively. The L_2 norm is employed as the sum of squares of various GND densities to solve the minimization problem [97–99]. Then the scalar GND density is expressed by [98]

$$\rho_{\text{GND}} = \sqrt{\sum_{a=1}^N [(\rho_{\text{Gs}}^a)^2 + (\rho_{\text{Get}}^a)^2 + (\rho_{\text{Gen}}^a)^2]}. \quad (\text{A10})$$

Moreover, stored energy density (SED) is employed as the damage indicator because it captures the energetic consequences of heterogeneous slip and dislocation interactions at the crystallographic scale [100], which are critical for the nucleation and growth of short cracks in microstructure-sensitive fatigue [101]. Unlike traditional stress- or strain-based criteria that overlook lattice curvature effects, SED directly reflects the energy stored by GNDs, particularly near grain boundaries where sharp strain gradients develop [102,103]. In the layered CG/FG structures studied here, SED provides a physically meaningful and spatially resolved measure of damage propensity, making it a more suitable metric than conventional fatigue indicators [104]. The damage indicator SED is defined by [100]

$$G = \int \frac{\xi |\boldsymbol{\sigma} : d\mathbf{e}_p|}{\sqrt{\rho_{\text{SSD}} + \rho_{\text{GND}}}}, \quad (\text{A11})$$

where ξ represents the fraction of plastic work stored in dislocation structures, typically estimated as 0.05 [105]. SED has been used to identify crack initiation at the microscale under both monotonic [106] and cyclic loading conditions [107,108]. This metric has proven effective in capturing microstructure-sensitive crack nucleation and short crack propagation behavior [109].

In this study, grain orientations are specified by Euler angles and subsequently converted into rotation matrices for use within the UMAT subroutine. The Euler angles follow the Z-X-Z rotation sequence, yielding the rotation matrix given by [110]:

$$\mathbf{R}(\varphi_1, \theta, \varphi_2) = \begin{bmatrix} \cos\varphi_1 \cos\varphi_2 - \sin\varphi_1 \sin\varphi_2 \cos\theta & \sin\varphi_1 \cos\varphi_2 + \cos\varphi_1 \sin\varphi_2 \cos\theta & \sin\varphi_2 \sin\theta \\ -\cos\varphi_1 \sin\varphi_2 - \sin\varphi_1 \cos\varphi_2 \cos\theta & -\sin\varphi_1 \sin\varphi_2 + \cos\varphi_1 \cos\varphi_2 \cos\theta & \cos\varphi_2 \sin\theta \\ \sin\varphi_1 \sin\theta & -\cos\varphi_1 \sin\theta & \cos\theta \end{bmatrix}. \quad (\text{A12})$$

The novelty and significance of the present CPFE study can be summarized in two points. (i) The crystal plasticity formulation explicitly incorporates both grain size effect and back stress hardening, and is applied to the tribological response of layered heterostructures. (ii) The effects of grain-level microstructural features within the CG and FG layers on rolling contact behavior are quantified, and the underlying deformation mechanisms are identified.

Data availability

Data will be made available upon reasonable requests addressed to the corresponding authors.

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