

Regulating particle rebound through rough surfaces

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Abstract:

High-velocity particle impact on solid surfaces is a fundamental issue in contact mechanics, tribology, and impact dynamics, prevalent in cold spraying, shot peening, and erosive wear. In these processes, particle rebound is governed by coupled normal contact and tangential friction associated with impact velocity, surface morphology, and impact angle. However, a systematic understanding of how surface roughness and impact angle regulate particle rebound and energy dissipation remains lacking, as these coupled effects induce heterogeneous stress localization and multiple dissipation mechanisms. Here, molecular dynamics simulations are used to investigate the rebound behavior of particles impacting rough surfaces. A semi-analytical model is developed for the normal restitution coefficient under head-on impact, revealing an inverse scaling with dimensionless velocity. Furthermore, the effect of surface roughness on coefficient of restitution is velocity dependent: it reduces restitution at low velocities by enhancing local plastic dissipation, but slightly increases restitution at high velocities by suppressing overall particle deformation. Under oblique impact, the deformation mode transitions from normal compression to plowing wear with increasing impact angle. These findings deepen the understanding of energy dissipation and particle deformation modes during impact and provide guidance for surface pretreatment and process optimization in surface modification technologies.

Keywords:

Surface roughness; Dynamic contact; Coefficient of restitution; Oblique impact; Plowing wear

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1. Introduction

High-velocity particle impact on solid surfaces is a fundamental issue in tribology that underpins applications such as shot peening [1], erosive wear [2], and cold spray [3]. From a tribological perspective, high-velocity particle impact involves a series of complex interfacial phenomena and undergoes coupled contact and frictional interactions, including local plastic deformation, frictional sliding, adhesion, and wear evolution [4, 5]. These interfacial responses influence not only the rebound behavior of the particle, but also the accumulation of surface damage and the development of wear morphology on the substrate [6]. Accordingly, a systematic understanding of particle rebound under high-velocity impact, especially how the coefficient of restitution depends on impact velocity, surface morphology, and incident angle, is essential for clarifying the mechanisms of erosive wear and guiding the design of wear-resistant surfaces.

Head-on impacts between particles and smooth surfaces have been extensively studied. Based on elastoplastic contact mechanics, Thornton et al. [7] developed a theoretical model for the velocity dependence of the coefficient of restitution, demonstrating that it is not a constant but follows a $-1/4$ scaling law with impact velocity, as dictated by material yielding, energy dissipation, and unloading. For micrometer-sized particles impacting at velocities from 10 m/s to beyond 1000 m/s, Yildirim et al. [8] showed numerically that increasing impact velocity drives a transition from elastoplastic to fully plastic and eventually to deeply plastic deformation, with the corresponding restitution-velocity scaling law successively changing from $-1/4$ to $-1/2$ and finally to -1 . Sun et al. [9] further directly observed the rebound of copper microparticles impacting at velocities ranging from 50 m/s to 800 m/s using the Laser-Induced Projectile Impact Test (LITIP) and reported a transition in the restitution-velocity scaling law from $-1/2$ to -1 during high-speed impact. Taken together, previous studies of normal impact have clarified the velocity dependence of the coefficient of restitution to a considerable extent. Nevertheless, most of these studies have focused on rebound from smooth surfaces, largely in the low-velocity regime, and a systematic understanding of rebound under high-velocity impact on rough surfaces remains lacking, which induces multiscale asperity contact, heterogeneous localized deformation, and multiple dissipation mechanisms.

However, real engineering surfaces are rarely smooth and typically exhibit multiscale roughness, arising from the combined effects of asperities, local slopes, and random geometric fluctuations [10, 11]. Rough surfaces alter the contact-stress distribution and contact deformation mode, and introduce extra microscopic plastic dissipation [12]; accordingly, the rebound behavior of particles under high-velocity impact on rough surfaces cannot be directly extrapolated from smooth surface models. Li et al. [13] experimentally showed that increased roughness typically intensifies friction and local plastic dissipation under elastoplastic contact deformation, leading to an overall reduction in the normal

coefficient of restitution. Sandeep et al. [14] further demonstrated that the coefficient of restitution decreases with increasing roughness of either the particle or the substrate, owing to local additional asperity-scale plastic deformation and the associated energy loss. Based on a numerical model of rough elastoplastic contact, Ghanbarzadeh et al. [15] similarly showed that surface roughness generally reduces the coefficient of restitution, with its influence diminishing only when the indentation depth substantially exceeds the characteristic roughness scale. Conversely, the influence of surface roughness on energy dissipation does not necessarily follow a monotonic trend. Wang et al. [16] showed through finite element analysis that rough surfaces can alter the contact mode in a manner that reduces total viscoelastic dissipation, and may even yield a higher coefficient of restitution than smooth surfaces during low-velocity viscoelastic collisions. To summarize, these studies suggest that rough surfaces alter the mechanisms of energy dissipation in particle impact through their effects on the contact-stress distribution and deformation mode. However, current studies of normal impacts on rough surfaces remain largely confined to the low-velocity regime, and the effects of roughness under high-velocity impact, together with their microscopic mechanisms, have yet to be systematically clarified. In addition, the role of surface roughness in governing energy dissipation under oblique impact remains poorly understood. Under oblique impact, the problem becomes even more complex because tangential motion couples with normal contact, giving rise to shear-induced energy dissipation and transitions from normal compression to plowing-dominated deformation. Therefore, under oblique impact, surface roughness modulates not only the normal rebound but also the tangential contact response associated with interfacial sliding and plowing.

Furthermore, oblique impact rather than normal impact is the prevailing collision scenario in practical processes such as particle erosion and wall impingement [17]. In oblique impact, the particle experiences normal compression and tangential sliding simultaneously. The incident angle determines not only the normal component of velocity, but also the extent of tangential friction, scratching, and plowing, and thus makes the rebound response inherently more complex [18, 19]. Through combined experimental and numerical analyses, Altmeyen et al. [20] demonstrated the deformation mode becomes increasingly dominated by asperity plasticity, asperity erosion, and rolling-sliding mechanisms on rough surfaces at relatively large oblique-impact angles. Transitions in particle deformation mode, in turn, lead to corresponding changes in the coefficient of restitution. Through finite element and semi-analytical analyses, Wu et al. [21] further pointed out that the normal coefficient of restitution increases with the rising incident angle. Xie et al. [22] also demonstrated experimentally that the normal coefficient of restitution varies significantly with normal velocity under different incident-angle conditions. Liu et al. [23] developed an oblique-impact model applicable from the elastic regime to the plastic regime, in which the coefficient of restitution is

explicitly linked to incident angle, impact velocity, and material properties. Despite these efforts, current studies of oblique impact still rely predominantly on smooth surfaces and low-velocity regime, and there remains a clear lack of investigation into high-velocity oblique impact on rough surfaces, especially with respect to how incident angle and surface roughness jointly regulate particle rebound. On the one hand, roughness alters local contact interactions and strengthens tangential impediment to particle motion [24]; on the other hand, increasing incident angle may trigger a transition in the particle deformation mode [25]. In real processes, including cold spraying and erosive wear, particle rebound occurs on rough surfaces and frequently under oblique impact. This makes the impact response fundamentally different from head-on impact on smooth surfaces. Thus, elucidating the coupled effects of impact angle and roughness on energy dissipation and deformation transitions, remains a critical issue.

In this study, the rebound behavior of particles under high-velocity impact is systematically investigated through theoretical analysis and molecular dynamics (MD) simulations, with particular emphasis on the power-law evolution of the coefficient of restitution with impact velocity, the effect of surface roughness on energy dissipation, and the mechanism governing deformation mode transitions in oblique impact. The study establishes a unified scaling law for the coefficient of restitution of different materials at a given dimensionless velocity, clarifies the underlying mechanism by which roughness enhances plastic dissipation at low velocities but suppresses it at high velocities, and determines the conditions for deformation-mode transition under oblique impact. The remainder of this paper is organized as follows. Section 2 describes the model and methodology, Section 3 presents the results and discussion, Section 4 validates the key findings with copper and Section 5 summarizes the main conclusions.

2. Model description and methodology

2.1 Particle collision model

Molecular dynamics (MD) simulations were performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [26] to examine particle rebound during high-speed impact. The model consisted of a deformable particle impacting with a fixed rigid substrate, as schematically illustrated in Fig. 1. A rigid substrate was adopted to decouple the complexity associated with substrate deformation, thereby highlighting the role of rough surface morphology in modulating contact deformation and rebound behavior. To clearly visualize the rotational motion of the particle during impact, the spherical particle is partitioned into upper and lower hemispheres distinguished by contrasting colors. The simulation parameters are summarized in Table 1. The particle radius was $40r_0$, while the substrate had in-plane dimensions of $200r_0 \times 200r_0$. The thickness of the smooth surface was $5r_0$ along the z direction. For rough surfaces, the thickness was increased from $10r_0$

to $60r_0$, depending on the surface roughness. Both the particle and the substrate were initialized as defect-free face-centered cubic (FCC) crystals. The crystallographic directions $[100]$, $[010]$, and $[001]$ were aligned with the x , y , and z axes, respectively. Periodic boundary conditions were imposed in the two in-plane directions, whereas a shrink-wrapped boundary condition was applied along the out-of-plane z direction. Before impact, the system was first relaxed by energy minimization and then equilibrated in the NVT ensemble using a Langevin thermostat. The target temperature was $0.005\varepsilon/k_B$, where ε is the reduced energy unit and k_B is the Boltzmann constant. The equilibration time was $50t_0$, and the integration time step was $0.0025t_0$, with t_0 denoting the reduced time unit. After equilibration, the particle was assigned an initial velocity v_i along the z direction toward the rigid substrate. The impact velocity ranged from $0.1r_0/t_0$ to $2.0r_0/t_0$. The collision was simulated in an NVE ensemble to conserve total energy and accurately capture the natural dissipation mechanisms until the particle rebound.

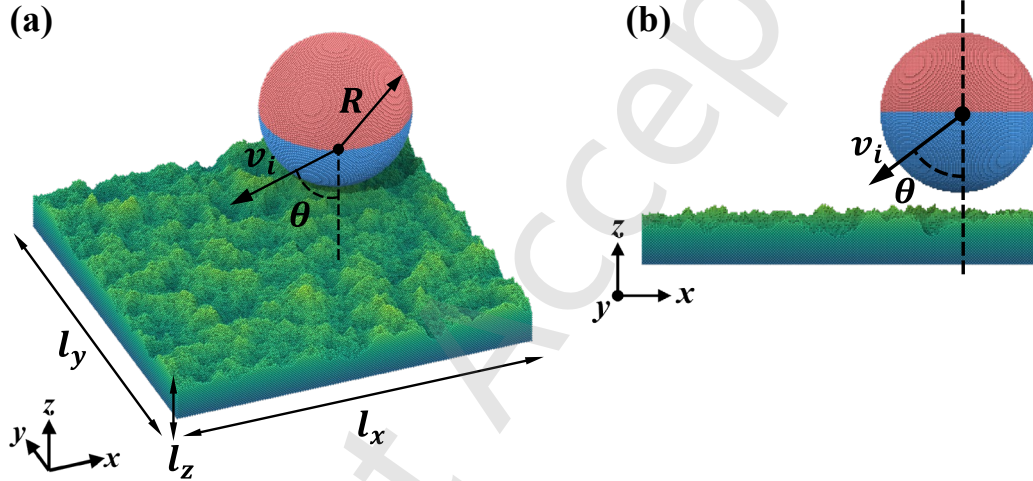


Fig. 1. Geometrical model of particle impact on rough surface: (a) 3D geometrical model; (b) 2D view defining impact angle θ .

Table 1 Simulation parameters for particle impact.

Parameters (units)	Values
Particle radius (r_0)	40
Substrate size (r_0)	$l_x = l_y = 200, l_z = 4 \sim 100$
Total number of atoms in the model	1520552~2641338
Impact velocity (r_0/t_0)	0.1~2.0
Time step (t_0)	0.0025
Temperature (ε/k_B)	0.005
Relative surface roughness, R_a/R	0.025~0.275

To explore the rebound behavior of particles with different mechanical properties, we employed

the modified Morse potential [27] to model interatomic interactions within particles and substrates. The modified Morse potential is given as follows:

$$\frac{E(r)}{\varepsilon_0} = \begin{cases} e^{-2\alpha_0(r-r_0)} - 2e^{-\alpha_0(r-r_0)} & r < 1.1r_0 \\ a_3r^3 + a_2r^2 + a_1r^1 + a_0 & 1.1r_0 \leq r < r_c \\ 0 & r_c \leq r \end{cases} \quad (1)$$

In this potential, $E(r)$ represents the interaction energy between two atoms separated by a distance r . The potential well depth was set to $\varepsilon_0 = 1.0$, and r_0 was taken as the reduced length unit corresponding to the equilibrium atomic spacing. The bond stiffness was governed by α_0 , which was set to $7.3r_0^{-1}$. To preserve the elastic response up to a strain of 10%, the interaction was truncated at $1.1r_0$. The cutoff radius r_c controlled the long-range tail of the potential. Polynomial coefficients $a_0 \sim a_3$ were introduced to guarantee continuity of both the potential energy and the interatomic force. These parameter values were adopted from validated literature data [27], and the modified Morse potential has been widely used in atomistic simulations of tribological contact and particle collision [28-30]. To isolate the effects of plastic dissipation and surface roughness, particle-substrate interfacial interactions were configured as non-adhesive, thereby eliminating the influence of interfacial adhesion and separation on the particle impact and rebound behavior. For the analysis of microstructural evolution, dislocation microstructure during impact was quantified using the dislocation extraction algorithm (DXA) [31]. The dislocation density was calculated by normalizing the total dislocation line length by the particle volume. Atomic configurations, dislocation networks, microstructural evolution, and particle motion were visualized using OVITO [32].

2.2 Creation of rough surface

Self-affine rough surfaces were generated using a power spectral density (PSD) method [33]. This approach characterizes surface topography not only through height statistics, but also through the wavelength distribution of asperities, thereby providing a more realistic description of rough surfaces than purely random height assignment. In the PSD framework, the surface is treated as a spatial stochastic height field. A target PSD function is prescribed, and the corresponding surface profile is reconstructed by inverse fast Fourier transform (IFFT) [34]. The generated rough surfaces followed a Gaussian height distribution and were statistically isotropic in the x and y directions.

A set of surfaces with prescribed roughness amplitudes was constructed using the power spectral density (PSD), as illustrated in Fig. 2. In this approach, a self-affine rough surface is defined by five parameters [34]. The lower and upper wavelength limits, $L_{\min}$ and $L_{\max}$, specify the spectral window of the PSD function, whereas the cutoff wavelength L_{cut} determines the transition within this wavelength range. These three wavelength parameters collectively control the spatial distribution and density of surface asperities. The Hurst exponent, H , characterizes the fractal nature of the

surface topography and ranges from 0 to 1. The roughness amplitude is quantified by R_a , which is defined as the standard deviation of the surface height and primarily controls the vertical scale of asperities. In the present study, R_a was varied from $3r_0$ to $11r_0$ to examine the role of surface roughness in particle rebound. Also, particle impact on a perfectly smooth surface was considered for comparison. All other PSD parameters are set as follows, with $H = 0.8$, $L_{\max} = 200r_0$, $L_{\min} = \sqrt{2}r_0$ (lattice constant), and $L_{\text{cut}} = 10\pi r_0$. The selected PSD parameters were calibrated against experimentally measured surface profiles [35]. The Hurst exponent $H = 0.8$ is consistent with Persson contact theory [36] and is representative of typical engineering surfaces [37].

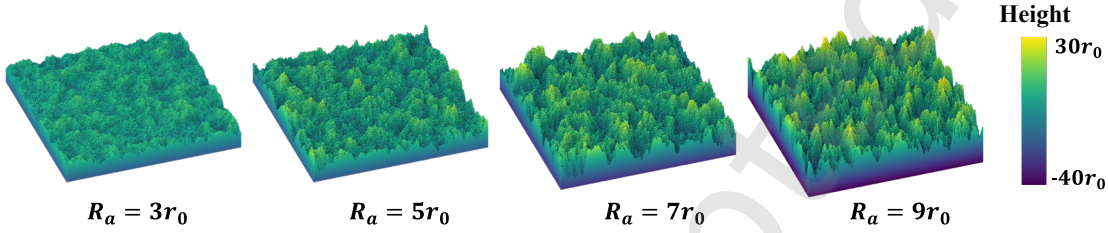


Fig. 2. The self-affine randomly rough surfaces for different root-mean-square roughness of R_a .

3. Results and discussion

This section systematically investigates particle rebound behavior and energy dissipation mechanisms during impact. We establish a unified power-law scaling for restitution coefficient on smooth surfaces, reveal the velocity-dependent dual role of surface roughness, and identify an incident angle dependent deformation mode transition in oblique impacts. These findings are validated by MD simulations of model materials and real copper.

3.1 Unified scaling laws for particle rebound under normal impact on smooth surfaces

In this section, we first examine the variation of the coefficient of restitution for normal head-on impacts between the particle and a smooth rigid surface. The coefficient of restitution is a key parameter of particle rebound during impact, defined as the ratio between the rebound and incident velocities $e = v_r/v_i$, and it provides a direct measure of impact-induced energy dissipation. As shown in Fig. 3(a), for different materials considered, the coefficient of restitution decreases monotonically with increasing dimensionless velocity under high-velocity impact, indicating that plastic dissipation is progressively enhanced as the incident kinetic energy increases. Based on the MD results for different plastic Morse materials, we find that the normal coefficient of restitution e_n , follows an inverse power-law scaling with the dimensionless velocity. Moreover, both the MD results and the published experimental data [38] for different materials, including copper, aluminum, zinc, and nickel, indicate that this scaling law is reasonably universal for dimensionless velocities ranging from 0.1 to 1.4.

To rationalize this scaling behavior, a semi-analytical model for the coefficient of restitution is developed based on the energy balance during particle rebound. During the impact, the incident kinetic energy is partitioned into plastic dissipation and recoverable elastic strain energy. Here, stress-wave propagation is naturally captured by the MD simulations, but its associated energy loss is not treated as an independent dominant dissipation mechanism in model because plastic dissipation dominates under high-velocity impact. For example, for a steel sphere impacting a mild-steel block at approximately 70 m/s, only about 3% of the initial kinetic energy was attributed to stress-wave radiation, whereas plastic deformation dominated the energy dissipation [39]. The rebound kinetic energy originates from the elastic recovery energy stored in the particle during unloading [7]. This recoverable elastic energy is mainly concentrated in an effective elastic deformation zone adjacent to the contact region. The effective volume responsible for storing the recoverable elastic energy inside the particle is denoted as V_{eff} . In regions of high contact stress undergoing severe plastic deformation induced by high-velocity impact, the elastic strain approaches its upper-bound scaling, $\varepsilon_e \sim \sigma_y/E^*$. Then, the recoverable elastic-zone thickness h_e near the particle contact region scales as:

$$h_e \sim \varepsilon_e R \sim \frac{\sigma_y}{E^*} R \quad (2)$$

Here, σ_y denotes the yield strength, $E^* = E/(1 - \nu^2)$ is the effective elastic modulus, and R is the particle radius. With the characteristic thickness of the recoverable elastic region determined, the effective elastic energy storage volume can be estimated from this thickness together with the characteristic particle-substrate contact area. Although the actual contact area grows as the impact velocity increases, much of the newly added contact region is already plastically deformed and thus cannot store recoverable elastic energy [40]. Thus, the effective load-bearing area responsible for elastic energy storage and rebound can be scaled as $A_e \sim \alpha R^2$. Accordingly, the effective elastic energy storage volume inside the particle can be expressed as:

$$V_{eff} \sim A_e h_e \sim \alpha \frac{\sigma_y}{E^*} R^3 \quad (3)$$

For a particle undergoing severe plastic deformation, the elastic strain energy density is on the order of its upper limit, $u_e \sim \sigma_y^2/(2E^*)$ [27]. The stored recoverable elastic energy is therefore:

$$U_e \sim u_e V_{eff} \sim \alpha \frac{\sigma_y^3}{E^{*2}} R^3 \quad (4)$$

This scaling suggests that the internal recoverable elastic energy becomes independent of further increases in incident velocity. This assumption holds only in the high-velocity regime, in which severe plastic deformation causes the effective elastic recovery region to saturate and prevents it from growing further with increasing indentation [41]. By contrast, for the low-velocity impacts, the

recoverable elastic energy still increases with incident velocity, and the above saturation assumption is no longer applicable [40]. In this regime, deformation remains elastoplastic and the velocity dependence may therefore be different from the high-velocity impacts. Based on energy conservation during the elastic recovery stage, the rebound velocity of the particle can be expressed as:

$$\frac{1}{2}mv_r^2 = \beta U_e = \alpha\beta \frac{\sigma_y^3}{E^{*2}} R^3 \quad (5)$$

Here, β is a conversion efficiency ranging from 0 to 1, which quantifies the fraction of recoverable elastic strain energy converted into the rebound kinetic energy of the particle while accounting for internal damping, elastic-wave radiation, and other irreversible losses. By further refining the above equation, we obtain:

$$\frac{1}{2} \times \frac{4}{3} \pi R^3 \rho v_r^2 = \alpha\beta \frac{\sigma_y^3}{E^{*2}} R^3 \quad (6)$$

Simplifying this relation yields the rebound velocity v_r .

$$v_r = \sqrt{\frac{3\alpha\beta}{2\pi} \frac{\sigma_y}{E^*}} \sqrt{\frac{\sigma_y}{\rho}} \quad (7)$$

Substitution into the definition of the coefficient of restitution gives:

$$e_n = \frac{v_r}{v_i} = \sqrt{\frac{3\alpha\beta}{2\pi} \frac{\sigma_y}{E^*}} \left(\frac{v_i}{\sqrt{\sigma_y/\rho}} \right)^{-1} = k_1 \left(\frac{v_i}{\sqrt{\sigma_y/\rho}} \right)^{-1} \quad (8)$$

Here, k_1 is a fitting parameter that accounts for particle size and shape, interfacial conditions, and additional dissipation mechanisms. The parameter v_i denotes the initial impact velocity of the particle. To consistently characterize high-velocity impacts across different material properties, we introduce a dimensionless velocity, v/v_0 , defined as the impact velocity normalized by the characteristic velocity $v_0 = \sqrt{Y/\rho}$, where Y is the indentation hardness and ρ is the material density [42, 43]. Because indentation hardness Y can be more conveniently and accurately obtained from indentation simulations than the yield strength σ_y , it is commonly used in molecular simulations of high-velocity impact. Although the instantaneous flow stress evolves during impact, high-velocity microparticle impact studies show that the dynamic indentation hardness can be approximated as a constant, so the rebound response is represented by an impact-averaged dynamic strength. Thus, strain hardening is incorporated through the indentation hardness Y in the semi-analytical scaling. Material hardening can also affect the restitution response of elastoplastic impacts; Lyashenko and Popov [44] showed that incorporating strengthening of the plastically deformed material improves the description of experimentally observed restitution behavior. The correlation between indentation hardness Y and yield strength σ_y has been widely investigated, with the approximate relation $Y \approx$

$3\sigma_y$ commonly adopted [45]. Accordingly, Eq. (8) can also be expressed as:

$$e_n = k \left(\frac{v_i}{v_0} \right)^{-1} \quad (9)$$

The prediction given by Eq. (9) matches both the simulation and experimental data well, yielding a fitting coefficient of $k = 0.81$ and a coefficient of determination of $R^2 = 0.92$. As shown in Fig. 3(a), the semi-analytical model identifies an inverse power-law dependence of the coefficient of restitution on dimensionless velocity. The same scaling behavior is observed in the present MD results and in the experimental data reported in Ref. [38] for various metallic materials, including copper, aluminum, zinc, and nickel. This common trend suggests that the power-law scaling captures a generic feature of high-velocity particle rebound over the dimensionless velocity. Although the scaling law was derived for a particle impacting a rigid substrate, its form is expected to remain valid for impacts involving a deformable substrate, whereas the corresponding prefactor may change owing to the altered partitioning of deformation and energy dissipation between the two bodies. A systematic finite-element comparison found that replacing a deformable substrate with a rigid wall reduced the prefactor by about 11% and increased plastic dissipation by about 12% [46]. Indeed, comparable inverse power-law scaling relations for high-velocity impact have been documented in previous studies. For instance, the elastoplastic particle impact rigid plate model proposed by Thornton and Ning showed that the coefficient of restitution can be formulated in terms of the initial velocity and follows a $-1/4$ scaling when elastoplastic deformation dominates [7, 39]. With progressively increasing impact velocity, the restitution-velocity relation evolves successively through $-1/4$, $-1/2$, and -1 power-law scaling, reflecting the transition from elastoplastic to fully plastic and finally to a deeply plastic deformation [47]. It indicates that the deformation-regime transition induced by increasing impact velocity is linked to the evolution of the internal microstructure of the particle. As the deformation state evolves from the elastoplastic stage to the deeply plastic stage, plastic dissipation becomes the dominant dissipation mechanism in the high-velocity impact.

To further clarify why the coefficient of restitution tends to converge among different materials at a given dimensionless velocity, we investigated in depth the evolution of dislocation microstructures within the particles. Fundamentally, plastic deformation in metals arises from the microscopic process by which a crystal under applied stress accommodates deformation through the continuous glide, multiplication, and interaction of dislocations, i.e., line defects within the lattice, ultimately leading to permanent macroscopic shape change. In this regard, dislocation density can be used to characterize the intensity of plastic deformation in the particle. It has been shown that, under the same absolute velocity, materials with lower yield strength exhibit earlier plastic activation and develop more extensive plastic deformation. However, as shown in Fig. 3(b), once the impact velocity

is normalized by the characteristic velocity v_0 , the dislocation density curves for different materials under high-velocity impact collapse onto nearly unified trend. In other words, at a given dimensionless velocity, plastic deformation dissipation tends to converge across materials. This result indicates that the extent of plastic dissipation during high-velocity impact is governed primarily by the dimensionless velocity, in which the impact loading is scaled by the material yield strength, rather than by the absolute impact velocity alone. This further implies that particles experience a comparable overall extent of plastic deformation at the same dimensionless velocity, regardless of differences in material yield strength. Accordingly, the near coincidence of dislocation density among different materials offers a microstructural mechanistic explanation for the observed convergence of their coefficients of restitution under the same dimensionless velocity. Also, it explains why the semi-analytical model can describe the scaling behavior of high-velocity rebound across different materials: at the same dimensionless velocity, the degree of plastic deformation becomes nearly equivalent.

To further assess the robustness and applicability of the rebound behavior established above, we examined the effects of particle size and interfacial adhesion. Under the present non-adhesive impacts, dimensional analysis shows that particle size enters the governing dimensionless formulation primarily through the adhesion number, suggesting that the rebound response should depend only weakly on particle size when adhesion is negligible. Consistent with this prediction, additional simulations show that increasing the particle radius from $40r_0$ to $100r_0$ changes the coefficient of restitution e_n by less than 12% at the low velocity impacts, with even smaller variations at higher velocities. Although this weak size dependence relies on negligible adhesion, we nevertheless explored the role of interfacial adhesion. Additional adhesive simulations show that increasing the interfacial strength progressively reduces e_n and can eventually lead to impact bonding. The adhesive contribution to energy dissipation varies non-monotonically with surface roughness, increasing initially and then decreasing as roughness becomes larger. This reflects a competition between enhanced adhesive contact at small roughness and reduced effective contact area due to contact localization at larger roughness. These results indicate that the rebound trend exhibits only weak particle-size dependence in the non-adhesive impacts, while appreciable adhesion can substantially modify the rebound response. The complete dimensional analysis, particle-size simulations, and interfacial adhesion analyses are provided in the Supplementary Material.

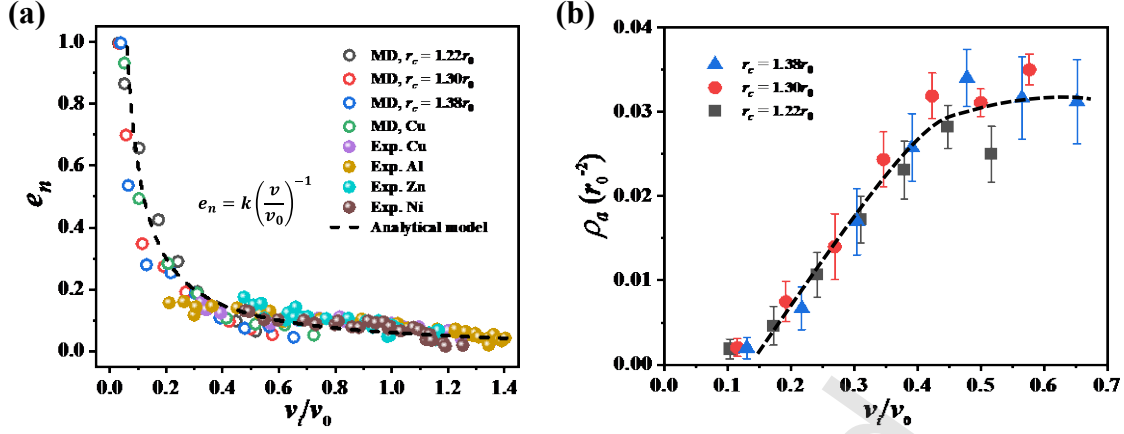


Fig. 3. (a) Coefficient of restitution as a function of dimensionless velocity for particles of different materials on smooth surfaces, compared with analytical models. The data include MD simulations for Morse materials and copper, as well as micro-ballistic impact test results for copper, aluminum, zinc, and nickel particles [38]. (b) Equivalent dislocation density as a function of dimensionless velocity for various plastic Morse materials.

3.2 Dual role of roughness in impact energy dissipation under normal impact

Based on the foregoing analysis of normal impact on smooth surfaces, this section further investigates how rough surfaces influence energy dissipation during particle collision. Real engineering surfaces are typically not smooth, but possess roughness to varying extents. Accordingly, understanding the role of surface roughness in energy dissipation is of clear practical significance. Our results indicate a pronounced velocity dependence in the influence of surface roughness on energy dissipation. At low velocities of $v_i/v_0 < 0.1$, the coefficient of restitution significantly decreases on rough surfaces compared to smooth surfaces, showing that rough surfaces markedly intensify energy dissipation and yield lower restitution than smooth surfaces. At high velocities, however, the trend reverses: the coefficient of restitution exhibits a slight increase with increasing roughness, implying a partial suppression of overall particle plastic dissipation. Thus, the role of surface roughness is not a simple monotonic enhancement of plastic dissipation. Instead, its mechanical effect varies with velocity through changes in contact mode, local interfacial deformation, and overall particle deformation.

We begin with the low-velocity regime, corresponding to a dimensionless velocity smaller than 0.1. As shown in Fig. 4(a), for a representative roughness of $R_a/R = 0.175$, the normal coefficient of restitution for impact on a rough surface is significantly lower than that for a smooth surface and lies far below the value predicted by the semi-analytical model. By contrast, when the dimensionless velocity exceeds 0.1, the restitution coefficient for the rough surface is in good agreement with the analytical prediction, suggesting that, in the high-velocity regime, the difference between smooth and

rough surfaces becomes minor and the roughness effect on energy dissipation is relatively limited. The strain distribution at the particle bottom in Fig. 4(b) further shows that, for a smooth surface, deformation at the particle-substrate interface remains relatively uniform and no obvious plastic zone develops near the interface. Under such conditions, the dissipation is governed mainly by viscoelastic dissipation and elastic-wave propagation [48]. On a rough surface, by contrast, the asperities come into contact first and induce much stronger local stress concentration. Consequently, pronounced local plastic deformation may develop even though the overall shape of the particle does not deform severely, and the resulting deformation pattern is highly nonuniform and spatially random. Surface asperities strongly localize the contact stress, so that the local stress can substantially exceed the material yield strength and initiate plastic flow [12]. Although these local plastic events do not strongly alter the overall particle shape, they markedly enhance energy dissipation and thus lead to a lower coefficient of restitution. This interpretation agrees with the finite element findings, according to which surface roughness increases plastic dissipation through changes in contact mode and intensified local plastic deformation [13].

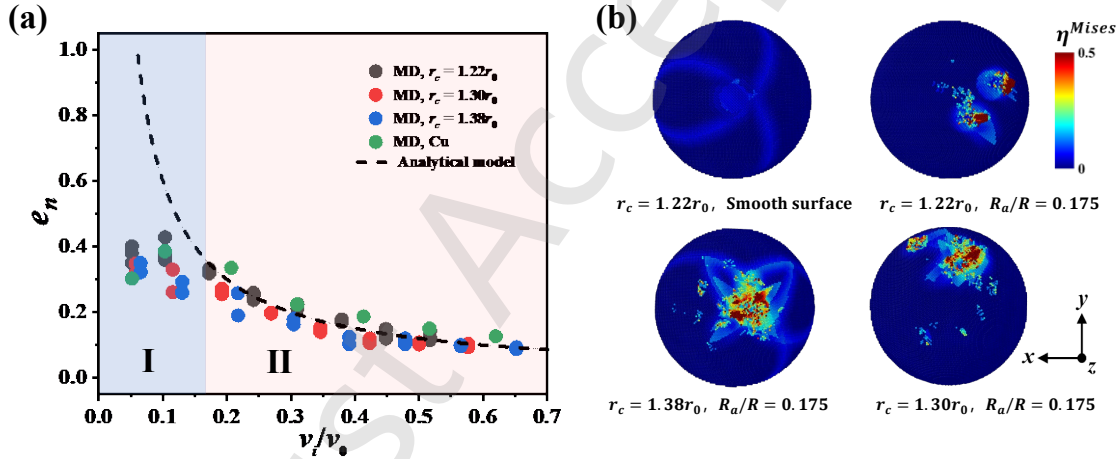


Fig. 4. (a) Coefficient of restitution as a function of dimensionless velocity for Morse materials with different plasticity at a roughness of $R_a/R = 0.175$, compared with the analytical model for a smooth surface; (b) Comparison of plastic deformation contours at the particle bottom between smooth and rough surfaces for a low-velocity impact at $v_i/v_0 = 0.1$.

To clarify the specific role of roughness itself, we compared the trend of the coefficient of restitution at a fixed impact velocity across different roughness levels ranging from $R_a/R = 0.075$ to $R_a/R = 0.275$. As shown in Fig. 5(a), in the low-velocity regime, the coefficient of restitution decreases monotonically as surface roughness increases, with an overall reduction of about 60% from the smooth surface to the rough surface with $R_a/R = 0.275$. The reason is that larger roughness produces more pronounced asperity topography, leading to stronger stress concentration in the local contact zone and thereby facilitating the onset of local plastic deformation [16]. As roughness

increases, plastic dissipation during impact becomes progressively stronger, with more of the initial kinetic energy being consumed by localized irreversible deformation, and the coefficient of restitution therefore decreases continuously. In other words, the primary role of a rough surface is to amplify plastic dissipation within microscale regions of the interface in the low-velocity regime; even without extensive deformation of the entire particle, the rebound capability can still be significantly weakened. This further explains the pronounced deviation of the restitution coefficient on rough surfaces from the analytical prediction based on smooth surfaces, since that model does not account for the local nonuniform plastic dissipation caused by asperities.

However, under high-velocity impact, the effect of surface roughness on energy dissipation is completely opposite to that observed at low velocities. As shown in Fig. 5(a), when the dimensionless velocity is 0.52, the coefficient of restitution exhibits a slight increase with increasing roughness. Specifically, as the roughness increases from 0.075 to 0.275, the restitution coefficient rises by approximately 60%, in direct contrast to the low-velocity regime. To clarify the origin of this anomalous trend, we further analyzed the evolution of dislocation microstructures within the particle after high-velocity impact. As shown in Fig. 5(b), the dislocation density decreases monotonically as roughness increases, while the dislocation structure ceases to spread deeply within the particle and becomes increasingly confined to the vicinity of the contact interface. As seen from the dislocation microstructures in Fig. 5(c), under smooth or low-roughness conditions, the particle experiences intense bulk plastic deformation during high-velocity impact. It is significantly flattened, and contains dislocations distributed throughout the particle interior, indicating substantial volumetric plastic dissipation. In contrast, at large roughness, mutual embedding occurs between the particle and the rough substrate, resulting in mechanical interlocking. This mechanical interlocking constrains large-scale lateral spreading and particle-scale bulk plastic flow, redirecting plastic deformation from a bulk deformation mode to a localized deformation mode, and thus weakening the overall plastic dissipation of the particle. Accordingly, in the high-velocity regime, rough surfaces slightly increase the coefficient of restitution by suppressing overall particle-scale plastic dissipation through mechanical interlocking. The reversal in the roughness dependence of the coefficient of restitution may occur over a transition velocity range, which may depend on material properties as well as characteristic roughness parameters, including roughness amplitude and spectral features. In addition, in the high-velocity regime, severe plastic deformation causes the coefficient of restitution after impact to remain at a very low level, typically below 0.2, with only limited variation with surface roughness [38]. To assess the effect of other spectral features and determine whether the identified mechanism depends on the specific spectral characterization of the rough surface, additional sensitivity analyses were performed. Since roughness R_a alone does not uniquely characterize a self-

affine surface, the Hurst exponent and the PSD roll-off wavelength were varied independently while R_a was held fixed. These variations produced only modest quantitative changes in the coefficient of restitution, within approximately 12% over the ranges examined, without altering the identified velocity-dependent dual role of surface roughness. The complete sensitivity analyses and corresponding results are provided in the Supplementary Material.

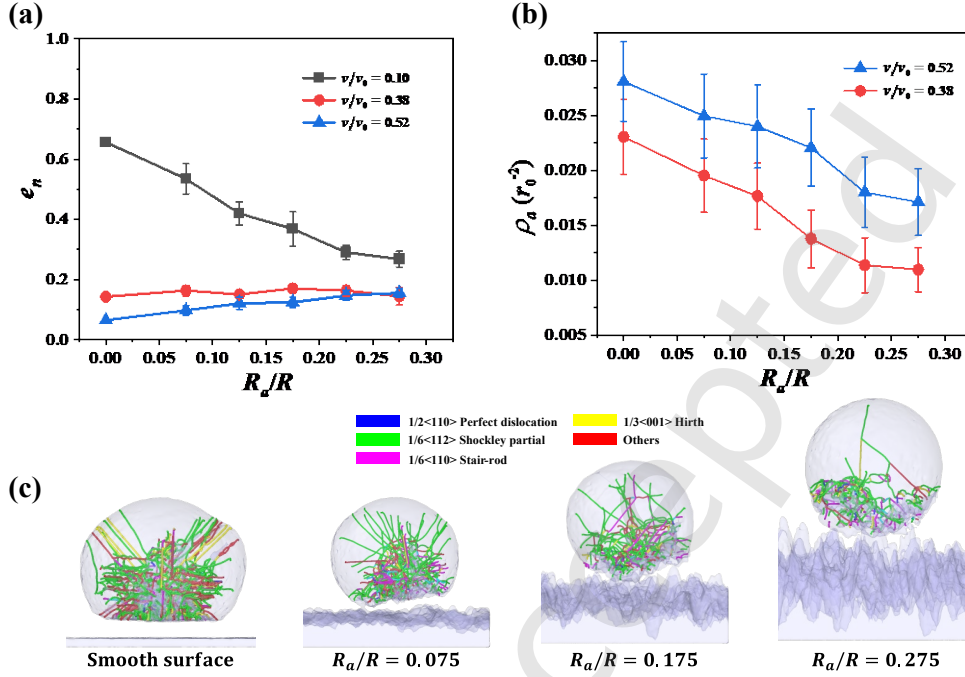


Fig. 5. (a) Variation of the restitution coefficient with surface roughness at high and low velocities; (b) Equivalent dislocation density with surface roughness under high-velocity impact; (c) Corresponding dislocation microstructure within the particle under high-velocity impact.

Importantly, the slight increase in the coefficient of restitution at high velocities does not imply that rough surfaces restore the elastic rebound energy. Instead, it reflects a transition in the way surface roughness governs energy dissipation. At low velocities, roughness mainly enhances dissipation by inducing local plastic deformation. At high velocities, however, mutual embedding between the particle and the rough surface leads to mechanical interlocking [49], which redirects dissipation from extensive global plastic deformation to a more localized interfacial region. This trend does not persist at extremely large roughness. When asperities become sufficiently large and approach the particle scale, intense local indentation and stress concentration may trigger particle damage, cracking, and even failure, introducing additional dissipation and shifting the rebound response toward a damage-dominated regime. In summary, the results reveal that surface roughness plays a velocity-dependent dual role in governing impact-induced energy dissipation: roughness enhances localized plastic dissipation at low velocities, whereas it constrains particle-scale plastic flow at high

velocities. This provides a deeper understanding for particle rebound, deposition, and deformation-mode transitions on rough surfaces.

3.3 Deformation mode transition from compression to ploughing under oblique impact

Building on the preceding analysis of particle head-on impact on rough surfaces, this section further investigates the deformation and rebound behavior of particles under high-velocity oblique impact. In oblique impact, the incident angle θ is defined as the angle between the initial velocity vector and the normal to the substrate surface. Unlike normal impact, oblique impact simultaneously involves normal indentation and tangential sliding, with corresponding normal and tangential velocity components $v_n = v_i \cos\theta$ and $v_t = v_i \sin\theta$, respectively. Therefore, the coefficient of restitution is governed collectively by impact velocity, incident angle, and surface roughness. The tangential coefficient of restitution is the signed ratio of post- to pre-impact tangential center-of-mass velocities [23]. The center-of-mass definition is used because severe deformation creates a finite, continuously changing contact patch, so a unique material contact point cannot be identified without an additional geometrical convention. Here, the evolution of the coefficient of restitution during oblique impact is linked to the particle deformation mode, with particular focus on how incident angle modifies the balance between normal and tangential dissipation [50].

We first examine the normal coefficient of restitution, whose evolution under oblique impact remains broadly consistent with that in head-on impact. As shown in Fig. 6(a), the normal coefficient of restitution decreases monotonically with increasing impact velocity, indicating progressively stronger plastic dissipation arising from normal compressive deformation. With increasing incident angle, the normal velocity component decreases while the tangential component increases. Consequently, the degree of normal indentation is reduced, the particle undergoes weaker plastic deformation, and the normal coefficient of restitution correspondingly increases. Conversely, at small incident angles, the larger normal velocity component makes the particle more susceptible to intense normal compressive deformation, and the normal coefficient of restitution decreases markedly. Comparison with available oblique-impact measurements and the experimental validation shows that the predicted e_n and e_t are generally consistent with the measured ranges and their velocity and angle dependent trends [23, 51-53], providing additional experimental support for the present simulations. This trend agrees well with the experimental observations in sphere oblique impact [21, 54]. Wu et al. [55] similarly showed that the normal rebound response changes with impact angle, highlighting the important role of incident angle in determining particle rebound under oblique impact.

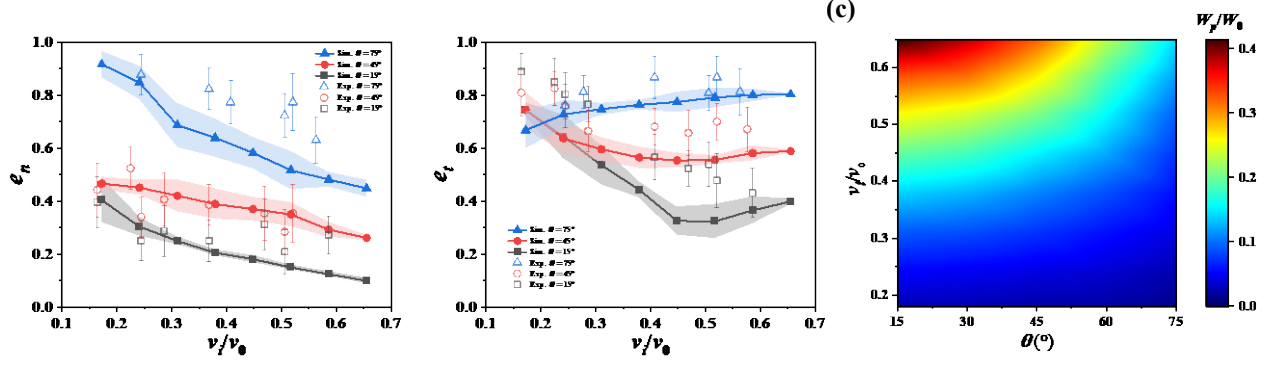


Fig. 6. Evolution of the restitution coefficient and plastic dissipation with impact velocity at different impact angles for $R_a/R = 0.075$: (a) normal restitution coefficient; (b) tangential restitution coefficient; (c) total plastic dissipation energy. In (a) and (b), solid symbols represent the present simulation results, shaded bands indicate the standard deviations of replicate simulations, and open symbols with error bars denote experimental data from Refs. [23, 51-53].

Compared with the normal coefficient of restitution, the tangential coefficient of restitution more clearly reflects the distinctive features of oblique impact. As shown in Fig. 6(b), the tangential coefficient of restitution exhibits different velocity-dependent trends at different incident angles. At a small angle of $\theta = 15^\circ$, it decreases as impact velocity increases and gradually approaches a plateau at high velocities, whereas at a large incident angle of $\theta = 75^\circ$, it instead increases with impact velocity. These results suggest that tangential rebound is governed not simply by the initial tangential velocity, but by the change in the dominant energy dissipation mechanism associated with incident angle. To investigate this transition in the dominant dissipation mechanism, we further examined the dependence of the total plastic dissipation energy W_p on both velocity and incident angle. The total plastic dissipation energy W_p can be decomposed into the normal plastic dissipation W_n and the tangential plastic dissipation W_t , which can be expressed as

$$W_p = W_n + W_t = \int F_n d\delta_n + \int F_t d\delta_t \quad (10)$$

Here, F_n and F_t are the normal compressive and tangential frictional contact forces, respectively, and δ_n and δ_t are the corresponding normal indentation and tangential sliding distances over which these forces act.

As shown in Fig. 6(c), for a small incident angle of $\theta = 15^\circ$, the total plastic dissipation rises sharply with increasing impact velocity. As the dimensionless velocity increases from 0.17 to 0.65, the increase in total plastic dissipation is about three times that at a large incident angle of $\theta = 75^\circ$, showing that strong plastic dissipation is induced by normal compressive deformation at small incident angles. At a large incident angle of $\theta = 75^\circ$, however, the velocity dependence of total

plastic dissipation is much weaker than that at small incident angles. In this case, tangential plastic dissipation increases only slowly with velocity and remains substantially lower than the total plastic dissipation at $\theta = 15^\circ$. As a result, the tangential coefficient of restitution shows a gradual increase with velocity at large incident angles, but a rapid decrease at small incident angles. The marked contrast in plastic dissipation between different incident angles originate from a transition in the particle deformation mode. When the incident angle is small, the particle motion approaches a head-on impact, and the overall dissipation arises mainly from plastic deformation caused by strong normal compression. At large incident angles, the particle tends instead to graze along the rough surface. Under these conditions, normal penetration is limited whereas tangential sliding is strongly enhanced, making the local contact region of the particle more susceptible to scratching and plowing wear, which then become the main modes of energy dissipation [20, 56].

To quantitatively characterize the deformation-mode transition during oblique impact, we examined the relative contributions of tangential and normal contact force work, expressed as the ratio of tangential plowing-wear dissipation W_t to normal compressive-deformation dissipation W_n . As shown in Fig. 7, the ratio W_t/W_n is governed primarily by incident angle and shows only a relatively weak dependence on impact velocity. When the incident angle is small (15°), the work done by the tangential contact force is far below that by the normal contact force, with a ratio of about 0.1. This indicates that the dissipation is dominated by normal compressive plasticity, and that the particle therefore deforms primarily in a compression-dominated mode (Fig. 8) [57]. Under small angle impact, the normal velocity component is large whereas the tangential component is small. The particle therefore undergoes intense normal plastic compression and becomes strongly embedded in the rough surface, while continuous tangential sliding is inhibited because the tangential motion is insufficient to overcome the asperity-induced resistance [58]. The resulting deformation is characterized by pronounced compressive plasticity in both the contact region and the particle interior, with an approximately symmetric distribution.

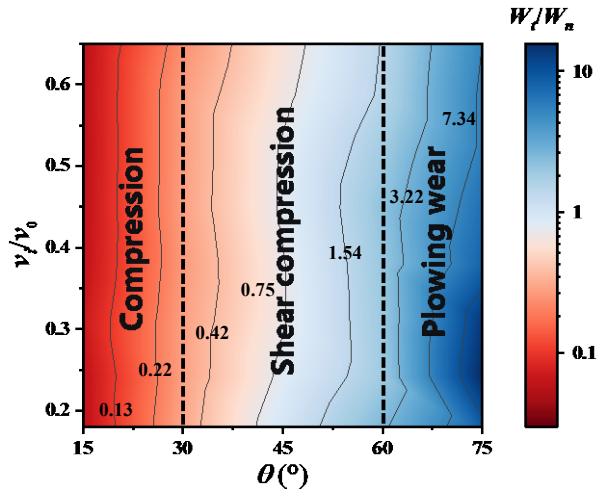


Fig. 7. The work ratio between tangential and normal contact forces, W_t/W_n , with impact angle and impact velocity at roughness $R_a/R = 0.075$. Based on the magnitude of W_t/W_n , the overall plastic deformation mode of the particle can be classified into three types: compression for $W_t/W_n \approx 0.1$, compression-shear for $W_t/W_n \approx 1$, and ploughing for $W_t/W_n \approx 10$.

At a large incident angle of 75° , the situation is reversed: tangential work substantially exceeds normal work, with the ratio reaching about 10. Under these conditions, the dissipation is governed mainly by tangential plowing wear, and the deformation mode becomes plowing wear (Fig. 8) [59]. Under large angle impact, the particle exhibits only limited normal embedding, but the large tangential velocity component allows it to slide along the rough surface while overcoming some asperity resistance. The overall particle shape therefore remains largely intact, and the plastic deformation is concentrated mainly in the bottom contact layer, where typical plowing-wear features are observed [25]. At a moderate incident angle of 45° , the work contributions in the tangential and normal directions are nearly equal, giving a ratio of about 1. This indicates that the particle experiences both pronounced indentation and significant sliding, corresponding to a compression-shear coupled deformation mode (Fig. 8). Under this condition, the particle experiences partial embedding together with partial sliding, leading to pronounced compressive and shear plastic deformation both at the bottom region and within the particle interior, with a clearly asymmetric deformation pattern. These results show that the mode transition in oblique impact is not simply a qualitative morphological impression, but can be unambiguously identified from the relative contributions of tangential and normal dissipation.

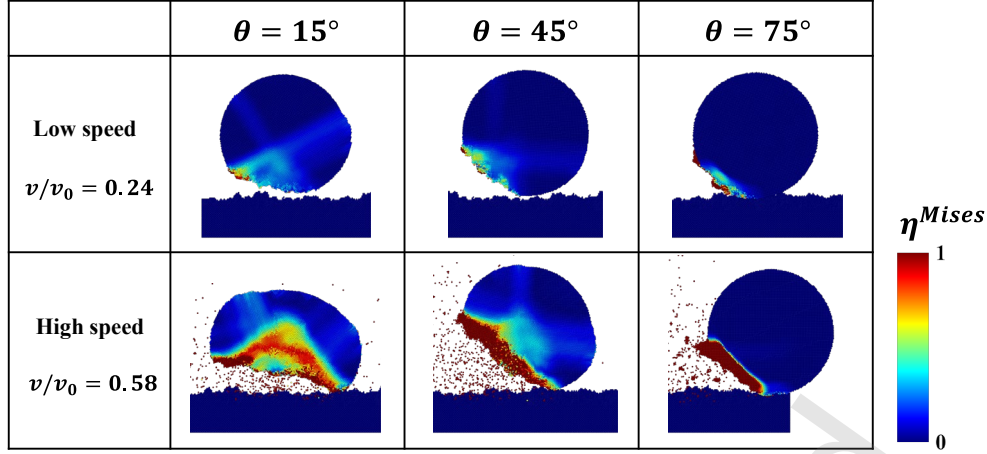


Fig. 8. Deformation modes of particle impact on rough surfaces under different incident angles.

On the other hand, the deformation mode shows relatively little sensitivity to surface roughness. Comparing the dissipation ratios at a large incident angle of 60° for different roughness levels, Fig. 9(a) shows that tangential plowing-wear dissipation consistently exceeds normal compressive-deformation dissipation by a substantial margin, indicating that plowing wear remains dominant throughout. Even with varying roughness, the tangential-to-normal dissipation ratio stays markedly greater than 1, implying that roughness mainly modulates the severity of plowing wear rather than changing the deformation mode itself. As shown in Fig. 9(b), larger roughness gives rise to more pronounced asperities, which increase tangential resistance; as the hindrance to tangential sliding becomes stronger, local wear at the particle bottom becomes correspondingly more severe [60]. In summary, the deformation mode in high-velocity oblique particle impact is controlled mainly by incident angle, with only weak sensitivity to impact velocity and surface roughness. At small incident angles the response is compression-dominated, at large incident angles it is plowing-dominated, and at intermediate angles the deformation is governed by a coupled compression-shear mode. This pattern is of substantial importance for understanding particle rebound, wear behavior, and energy dissipation mechanisms under different impact conditions.

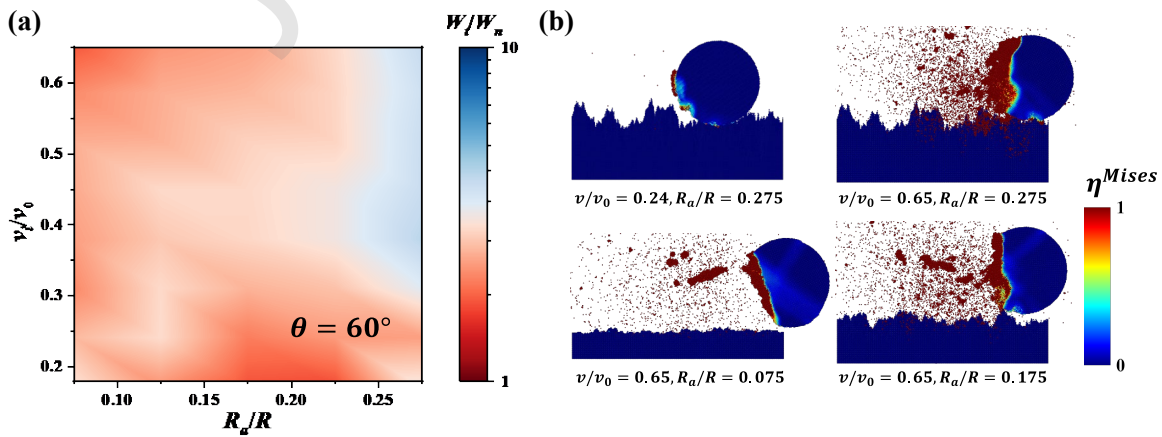


Fig. 9. (a) The tangential-to-normal work ratio W_t/W_n with surface roughness and impact velocity at a large impact angle of $\theta = 60^\circ$; (b) Corresponding strain contour maps of ploughing wear for the particle at an impact angle under different surface roughness.

4. Discussion on rebound of copper particle

The previous studies were primarily based on model materials, which possess generic physical and mechanical properties and are therefore well suited for elucidating the underlying physical mechanisms governing the observed behaviors. To assess the universality of the foregoing results, we further validated them using real metallic copper. Copper is a representative ductile metal with wide applications in additive manufacturing [61]. Therefore, MD simulations were carried out for copper particles impacting a rigid rough diamond surface. The collision model was constructed using the same configuration as described in the previous Section 2.1. The copper particles were modeled as face-centered cubic (FCC) single crystals with crystallographic orientations of x -[100], y -[010], and z -[001]. The interactions among copper atoms were described using an embedded atom method (EAM) potential [62], whereas the copper-carbon interactions were modeled using a Morse potential [63]. The copper particle radius was 100 Å, while the rigid diamond substrate measured 300 Å along both the x and y directions. The particles were assigned initial impact velocities ranging from 100 m/s to 600 m/s.

We first examined the variation of the coefficient of restitution for copper particles under normal impact onto rough surfaces. The results show that the behavior of copper is generally consistent with that of the model materials. As shown in Fig. 10(a), at low velocities of $v_i/v_0 = 0.1$, the coefficient of restitution of copper particles decreases monotonically as the roughness of the target surface increases. This trend is related to local plastic deformation induced by asperity contact: greater roughness leads to stronger stress concentration in the local contact region, so that plastic deformation occurs more readily, resulting in enhanced energy dissipation. At high velocities, the copper particles show the same anomalous behavior, namely, a slight increase in the coefficient of restitution with increasing surface roughness. Under high-velocity impact, severe plastic deformation occurs within the particles, leading to mutual embedding and mechanical interlocking [64]. Consequently, a rougher surface restricts plastic deformation of the particle and lowers the overall plastic dissipation. Thus, the copper simulations also validate the behaviors found for the model materials.

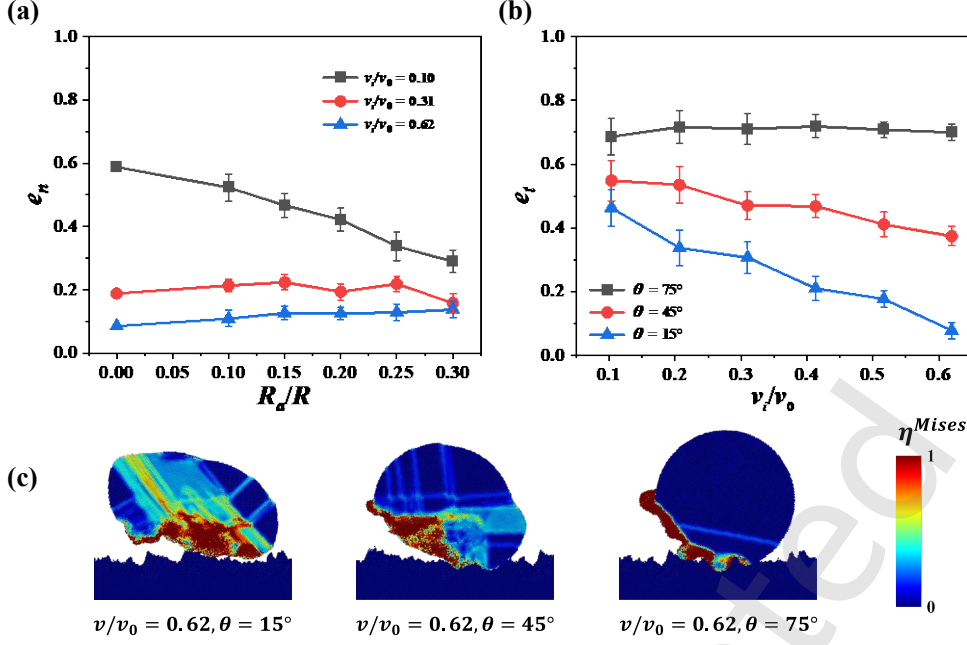


Fig. 10. (a) Variation of the normal restitution coefficient with surface roughness at low and high velocities. (b) Evolution of the tangential restitution coefficient with impact velocity under different impact angles at a roughness of $R_a/R = 0.1$; (c) Corresponding strain contour maps of the particle under different deformation modes.

Similarly, under oblique impact, copper particles show rebound trends consistent with those of the model materials. As shown in Fig. 10(b), the tangential coefficient of restitution decreases with impact velocity at a small incident angle of 15° , but increases slowly with impact velocity at a large incident angle of 75° . This evolution of the restitution coefficient is likewise linked to a transition in deformation mode. As shown in Fig. 10(c), under small-angle impact, the copper particle is strongly flattened, with intense compressive plastic deformation occurring in both the bottom region and the interior. By contrast, at large incident angles, the copper particle largely preserves its overall shape, with plastic deformation confined mainly to a local region near the bottom. In summary, the copper simulations confirm the rebound laws previously established from model materials, including the power-law dependence of restitution on dimensionless velocity in normal impact, the dual role of roughness in dissipation, and the incident angle dependent transition of deformation mode in oblique impact.

5. Summary and conclusions

In this study, we constructed the self-affine rough surfaces at the atomic scale to systematically investigate the rebound dynamics of high-velocity particle impacts on rigid rough surfaces by combining MD simulations with theoretical analysis. The study focuses on the effects of surface

roughness and impact angle on the collision process, revealing their influence on energy dissipation mechanisms and deformation mode transitions. The main conclusions are as follows:

(1) The MD simulations uncover a universal scaling for head-on particle rebound on smooth surfaces: the normal coefficient of restitution decreases with dimensionless velocity following an inverse power-law relation. The similar scaling trend is also observed in micro-ballistic impact experiments for various metallic materials. To rationalize this behavior, a semi-analytical model is developed based on the balance between recoverable elastic strain energy and rebound kinetic energy, which captures the observed power-law scaling. Dislocation microstructure analysis further supports that different materials exhibit nearly identical equivalent dislocation densities at the same dimensionless velocity, indicating comparable degrees of plastic deformation. It provides a microscopic explanation for the normalized rebound behavior and the apparent convergence of the coefficient of restitution across different material systems.

(2) The influence of surface roughness on the rebound behavior under head-on impact is velocity dependent. At low velocities, localized plastic deformation at the contact interface is obvious, leading to increased energy dissipation and a monotonic decrease in the coefficient of restitution with increasing roughness. At high velocities, an excessively rough surface restricts the full development of overall plastic deformation within the particle, resulting in an anomalous increasing trend of the coefficient of restitution with roughness. Dislocation microstructure analysis further supports that the dislocation density within the particle decreases during high-velocity impact on highly rough surfaces, corresponding to reduced plastic dissipation, which elucidates the microscopic mechanism underlying the anomalous restitution behavior.

(3) For oblique impact, the deformation mode primarily depends on the impact angle, with a weaker dependence on impact velocity and surface roughness. The deformation modes under oblique impact can be categorized into three types: normal-compression for $\theta < 30^\circ$, shear-compression for $30^\circ < \theta < 60^\circ$, and ploughing wear for $\theta > 60^\circ$. Under oblique impact, the normal coefficient of restitution decreases with increasing velocity but increases with increasing impact angle, consistent with the behavior observed under normal impact. In contrast, the tangential coefficient of restitution decreases with increasing velocity at small impact angles but increases with increasing velocity at large impact angles. This behavior is primarily attributed to the significant dominance of tangential work over normal work, with a ratio of $W_t/W_n \approx 10$, and lower overall plastic dissipation at large impact angles; whereas normal work dominates, with $W_t/W_n \approx 0.1$, and higher overall plastic dissipation at small impact angles. Accordingly, the tangential-to-normal work ratio provides a compact measure of contact-friction coupling and distinguishes among the deformation modes.

In summary, this study establishes a semi-analytical model for the normal coefficient of restitution under high-velocity normal impact, elucidates the mechanisms governing energy dissipation and rebound behavior in terms of surface roughness and impact angle during oblique impact, and identifies the transitions of deformation modes under different impact conditions. The findings deepen the understanding of the dynamic behavior of high-velocity particle impact and provide a theoretical basis for engineering applications such as cold spray process optimization and shot peening surface treatment.

Supplementary Material

See the Supplementary Material for the dimensional analysis and additional simulations addressing particle-size dependence, interfacial adhesion, and the effects of the Hurst exponent and roll-off wavelength on rebound behavior.

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CRediT authorship contribution statement

Haiyang Yao: Methodology, Investigation, Formal analysis, Validation, Writing –original draft, Data curation. **Fengxian Liu:** Investigation, Formal analysis, Validation, Writing – review & editing. **Keyan Huang:** Investigation, Formal analysis, Validation, Writing – review & editing. **Jianqiao Hu:** Conceptualization, Methodology, Formal analysis, Project administration, Funding acquisition. Writing – review & editing, supervision. **Hengxu Song:** Project administration, Funding acquisition. Writing – review & editing, supervision.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Compliance with Ethical Standards

Conflict of 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.

Ethical approval: This article does not contain any studies with human participants or animals performed by any of the authors.

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