Electronic Supplementary Material

Surface removal of a copper thin film in an ultrathin water environment by a molecular dynamics study

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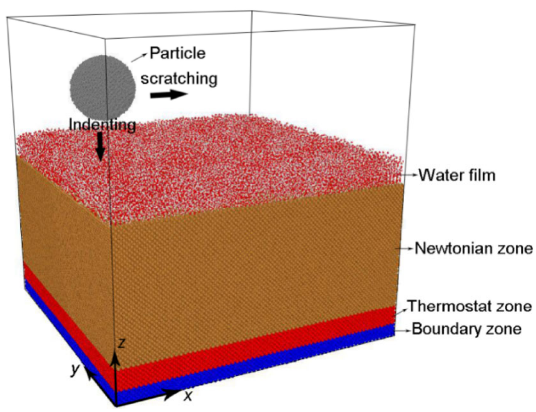

Fig. S1 Schematic model of the MD simulation system.

Table S1 Parameters used in the MD simulations.

Properties	Parameters
Abrasive particle	Diamond, sphere with radius of 2.5 nm, 11,976 atoms
Water film	Density of 1.0 g·cm^{-3}, thickness (H): 0.3 nm, 0.5 nm, and 1.0 nm
Workpiece	Cu (FCC), $68a \times 68a \times 35a$ (a = 0.3615 nm), 656,608 atoms
Potential for Cu thin film	EAM potential: $E_i = F_\alpha\left(\sum_{j\neq i}\rho_\beta\left(r_{ij}\right)\right)+\frac{1}{2}\sum_{j\neq i}\phi_{\alpha\beta}\left(r_{ij}\right)$
Potential for particle–Cu film	Morse potential: $E = D_0\left[e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)}\right]$ $r < r_c$ where D_0 = 0.1 eV, α=1.7 Å^{-1}, and r_0=0.22 nm
Potential for water molecules	O–O, ε = 0.1554 kcal/mol, δ = 0.31655 nm
Potential for water–particle	O–C, ε = 0.1 kcal/mol, δ = 0.3275 nm
Potential for water–workpiece	O–Cu, ε = 0.2708 kcal/mol, δ = 0.28877 nm
Scratching	Depth: –0.2 nm, 0.1 nm, 0.5 nm, 1.0 nm; distance: 9.0 nm; v = 10 m·s^{-1}

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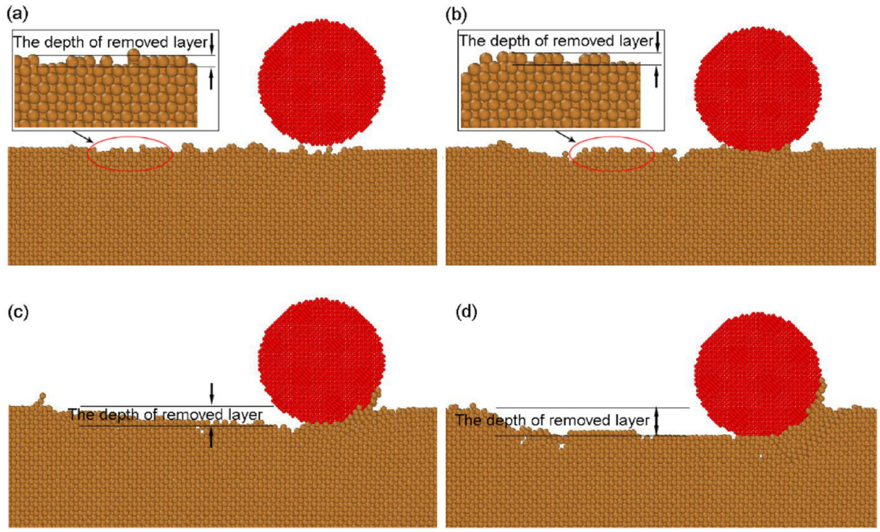

Fig. S2 Snapshots of the worn morphology of a slice (with 0.5 nm thickness) of the *xz* plane under various scratching depths (*h*): (a) –0.2 nm, (b) 0.1 nm, (c) 0.5 nm, and (d) 1.0 nm, at a scratching distance of 9 nm, for nanoscratching with a water film of 1.0 nm thickness.

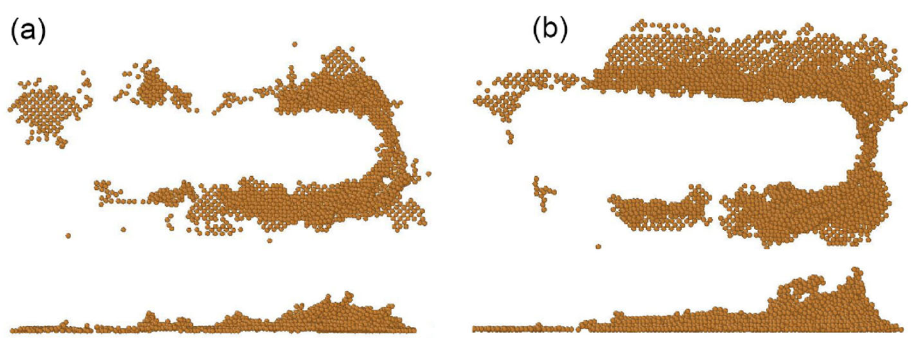

Fig. S3 Snapshots of the ridge morphology for nanoscratching with a water film thickness of 1.0 nm at a scratching depth of (a) 0.5 nm and (b) 1.0 nm.

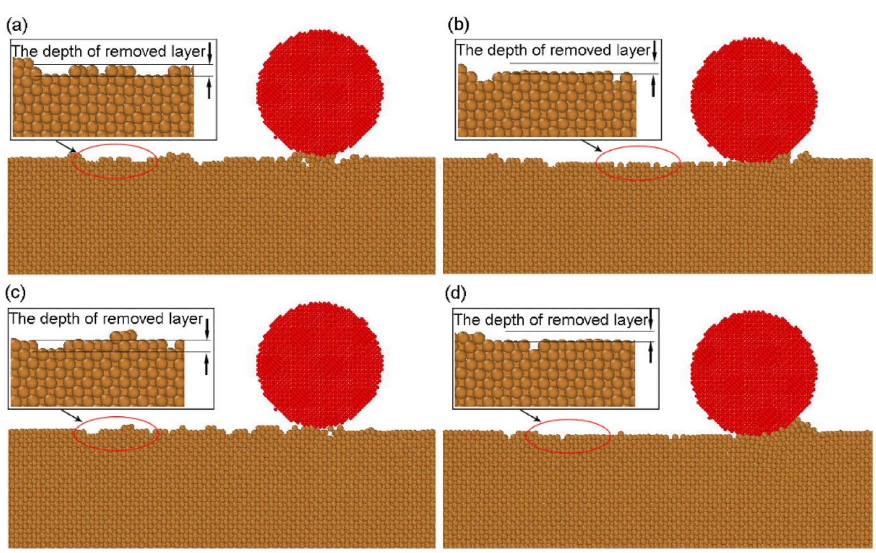

Fig. S4 Snapshots of the worn morphology of the cross-sectional views of the *xz* plane with the omission of the water film under various water film thicknesses (*H*) and scratching depths (*h*), $H = 0.3$ nm: (a) $h = -0.2$ nm, (b) $h = 0.1$ nm; $H = 0.5$ nm: (c) $h = -0.2$ nm, (d) $h = 0.1$ nm.

For dry nanoscratching, Figs. S5(a) and S5(b) show that the monoatomic layer removal occurs at a scratching depth of 0.1 nm, whereas the Cu surface is still maintained with its perfect lattice structure at a scratching depth of –0.2 nm.

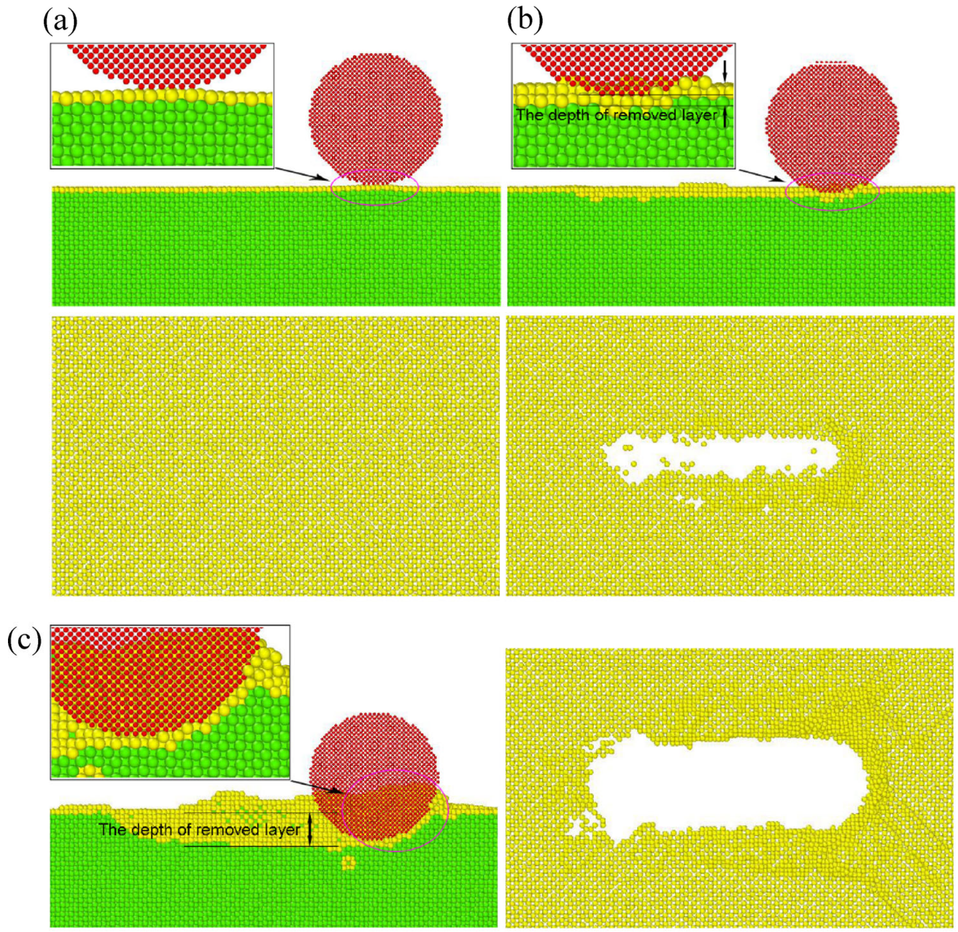

Fig. S5 Snapshots of the worn morphology of the cross-sectional views of the *xz* plane and plane views of the *xy* plane under various scratching depths (*h*): (a) –0.2 nm, (b) 0.1 nm, and (c) 1.0 nm, at a scratching distance of 9 nm, for the dry nanoscratching process. Yellow and green spheres represent the initial surface of the Cu atoms, and other Cu atoms, red represent the abrasive particle.

As the scratching depth increases to 1.0 nm in Fig. S5(c), the abrasive particle contacts the Cu atoms and results in a large removed zone. Practically all the surface Cu atoms in contact with the particle are removed during the scratching process. As the particle moves forward, numerous deformed atoms accumulate to form clusters or chips ahead of the particle. Concurrently, the remarkable ridges along both the left and right sides of the particle were produced. After the particle passes by, a groove is formed.