Surface Roughness

Many surfaces have a roughness on all length scales, including the atomistic scale that can be described by the self-affine fractal scaling. This method has a so-called Hurst exponent which plays a crucial role in determining the roughness. The Random Midpoint Displacement (RMD) method with the Hurst exponent is used to generate rough surfaces, and the surface boundaries are periodic.

The principle is as follows: it starts at an initial square with random values at the four corners. Let us have one corner's value at:

$$[x_0, y_0, f(x_0, y_0)],[x_1, y_0, f(x_1, y_0)],[x_0, y_1, f(x_0, y_1)],[x_1, y_1, f(x_1, y_1)]$$

In the first step, a vertex is added in the middle, and the vertex is denoted by

$$[x_{1/2}, y_{1/2}, f(x_{1/2}, y_{1/2})]$$

where

$$x_{1/2} = \frac{1}{2}(x_0 + x_1) \quad (1)$$

$$y_{1/2} = \frac{1}{2}(y_0 + y_1) \quad (2)$$

$$f(x_{1/2}, y_{1/2}) = 1/4(f(x_0, y_0) + f(x_1, y_0) + f(x_0, y_1) + f(x_1, y_1)) + \sigma_1 \quad (3)$$

$$\sigma_i = \frac{1}{2^{H \times i}}\sigma \quad (4)$$

The added vertex is shifted in the z-coordinate direction by a random value denoted by σ_i .The Hurst exponent H is 0.8. In the *i*-th iteration step the variation σ_i must be modified according to Eq. 4. The random number σ is generated with a Gaussian distribution. This procedure is recursively repeated for each sub-square and then for every one of their descendants and so on, as shown in Figure S1.

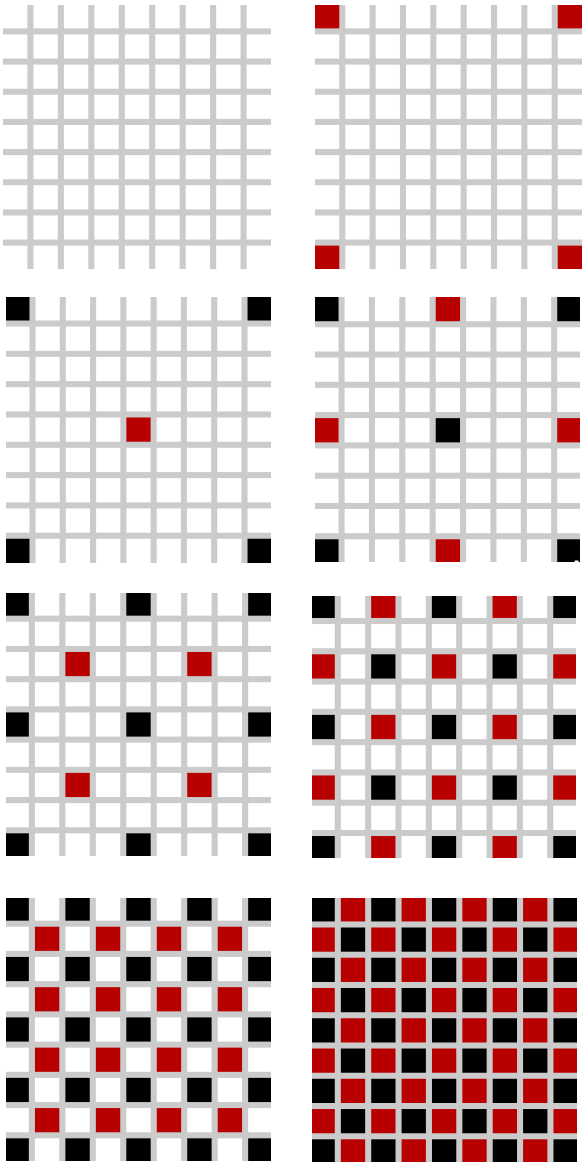

Figure S1. A schematic view of original RMD process within first 8 iterations. The dark areas mean the surface point from previous iteration while the red areas present the surface profile in the current iteration.

However, the original RMD starts at the centre of the surface, and the iteration divides the surface into predefined smallest squares. It is evident from Eq.3 and 4 that the first iteration has the greatest influence on the final shape of a surface, so it is highly likely to generate a surface with a few, albeit large asperities. This will not be good if one wants to simulate a multi-asperity contact. To solve this problem, the surface is first divided into 16 squares of equal size (4×4 in this paper). The RMD is applied within each square so that the whole surface has more asperities, but because a periodic boundary is required in MD simulation, periodicity should be

considered in the original RMD algorithm. Specifically, within one of the 16 squares shown in Figure S2, the surface height at the boundary (both boundary between sub-squares and system mirrors) should be averaged with the neighbouring squares. Finally, to create surfaces with the required RMS 0.8 nm , the heights of the surface can be scaled accordingly.

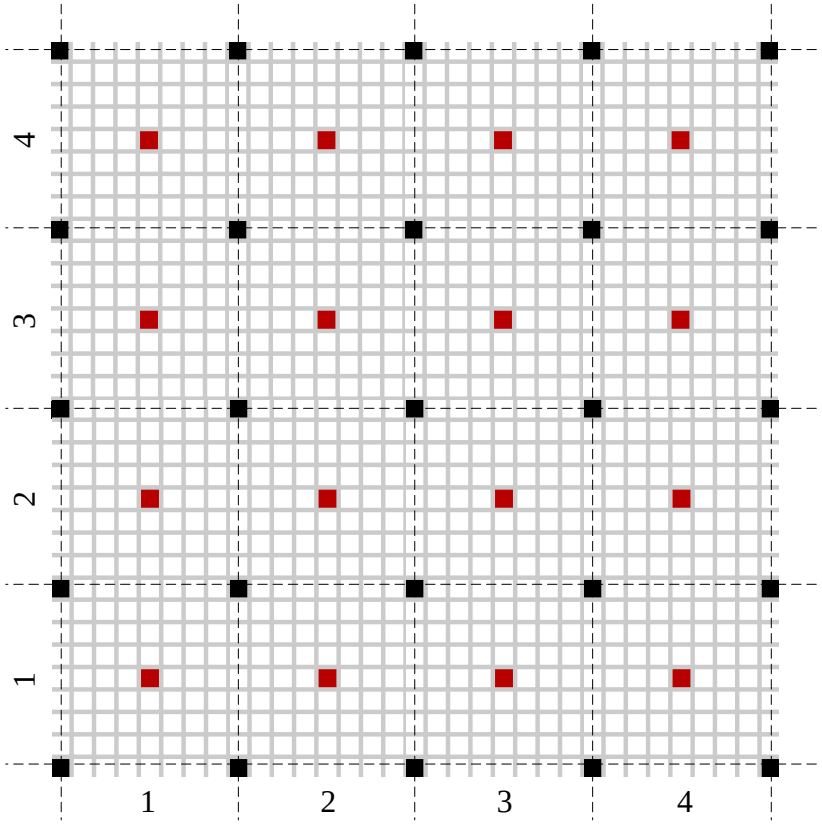

Figure S2 The simulation domain is divided into 16 (4×4) sub-squares. In each sub-square, the RMD is carried out.