Supporting Information

Quantitative Features of Osteo-Bioactive Ti Surfaces at the Atomic/Molecular Level

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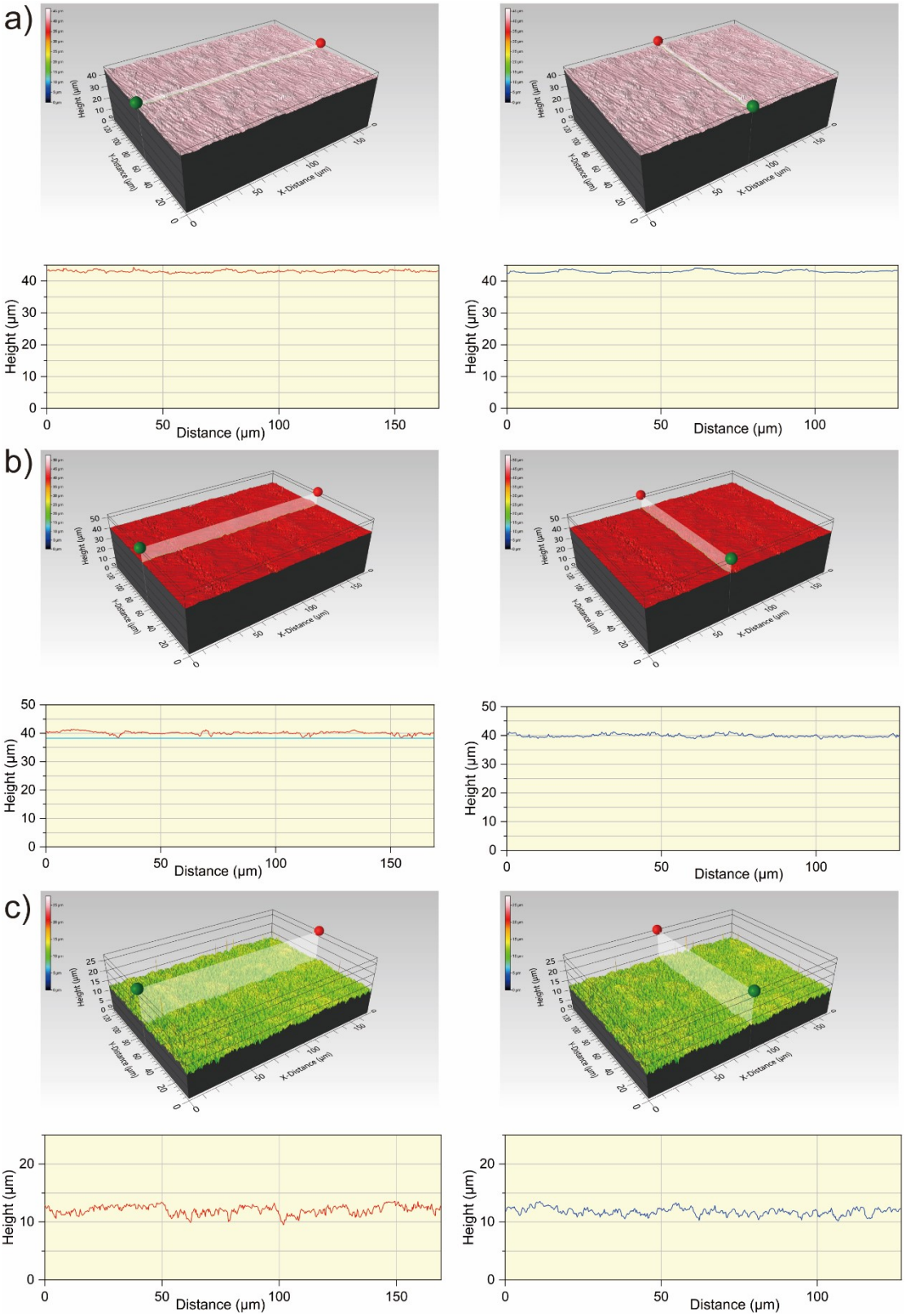
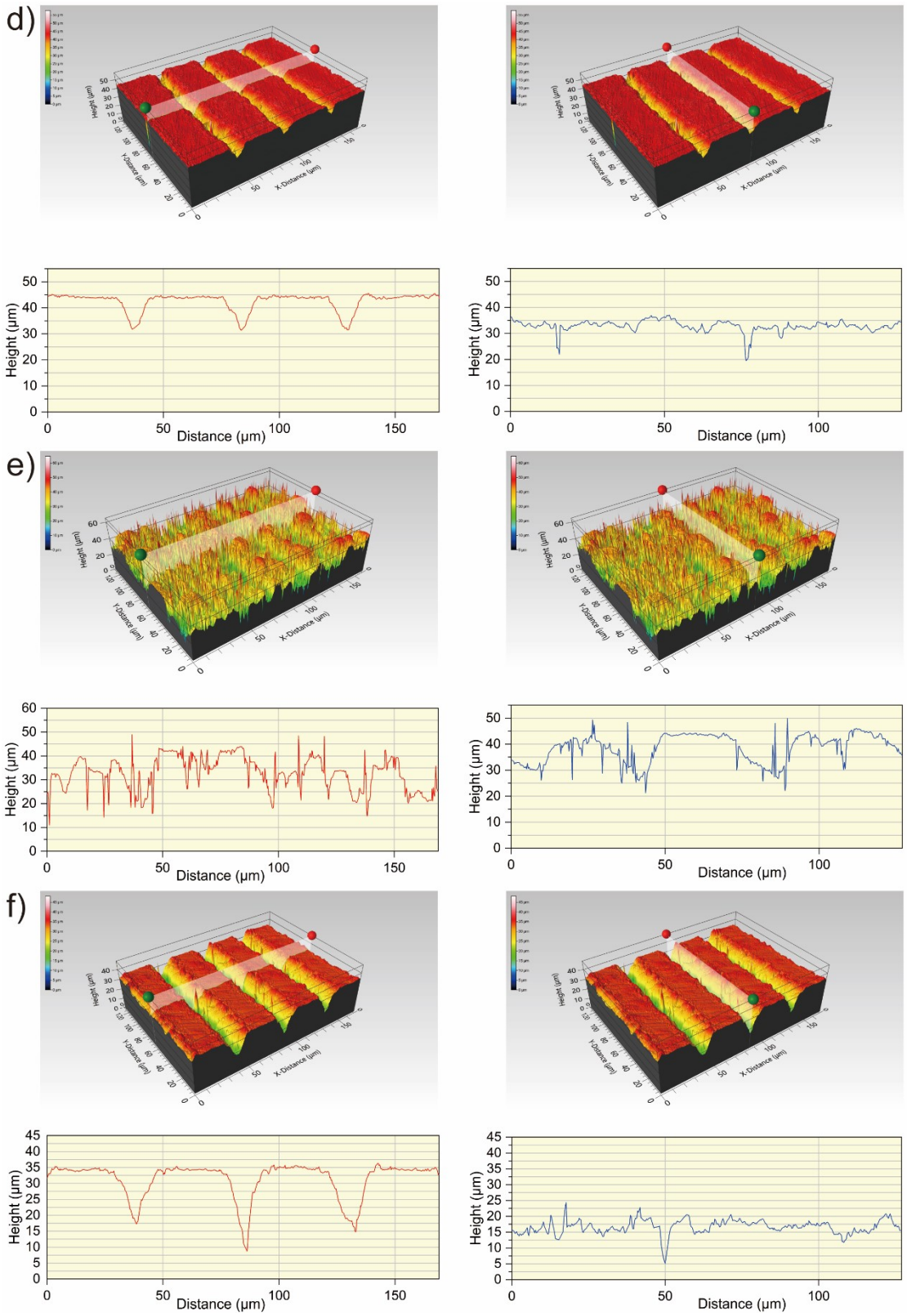
SI-1 Calculation Setup.

Molecular dynamics calculations were performed using NAMD 2.10 code [1]. For all systems, periodic boundary conditions were imposed, and a TIP3P water model was utilized. A cutoff distance of 12 Å was established for both real-space electrostatic and van der Waals interactions. Long-range electrostatic interactions were characterized using the Particle–Mesh–Ewald method. During the calculations, a time step of 1 fs was chosen, and the rigid bond model was applied to hydrogen atoms via the SHAKE algorithm. The behavior of TIP3P water molecules and ions was described by the CHARMM36 force field. TiO_2 was simulated using parameters that we specifically tailored. The theoretical foundation for this fitting was based on the first-principles calculation results obtained by Matsui et al [2]. The force-field parameters for the functional group were developed using the Force Field Toolkit (ffTK) plugin within the VMD package. The atomic charges of hydroxyl and phosphate were defined in accordance with a comparable structure within the CHARMM36 force field.


a)
b)
c)
Height (µm)
X-Distance (µm)
Y-Distance (µm)
Distance (µm)
0
50
100
150
10
20
30
40


d)
e)
f)
Height (µm)
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X-Distance (µm)
Y-Distance (µm)

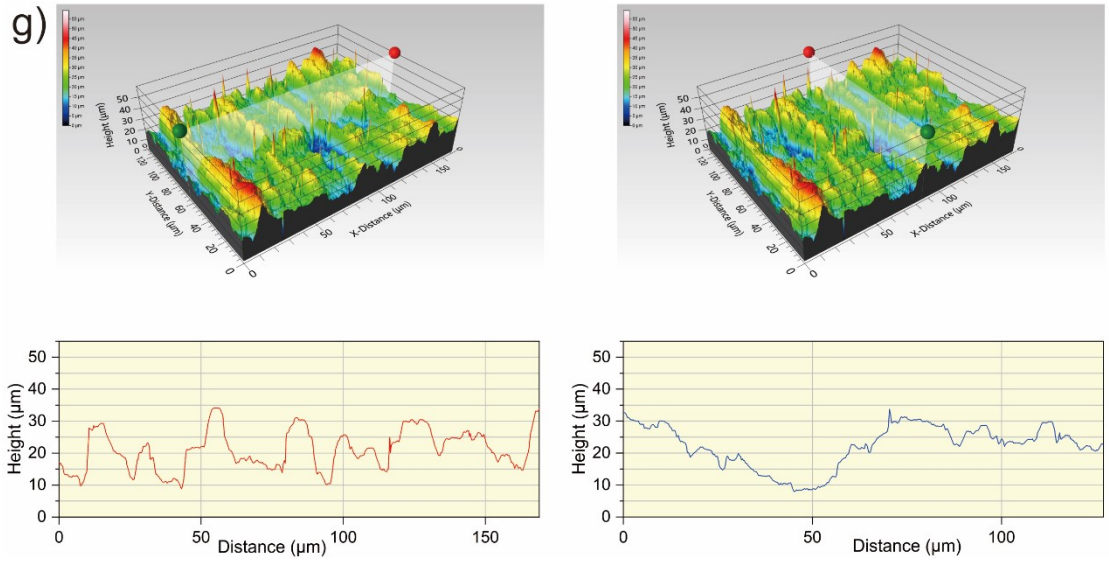

Figure S1 Three-dimensional (3D) surface profiles and sample ridge shape profiles in detail. a) Ti, b) 0.1W-0.065, c) 0.1W-0.01, d) 0.3W-0.065, e) 0.3W-0.01, f) 0.5W-0.065, g) 0.5W-0.01.

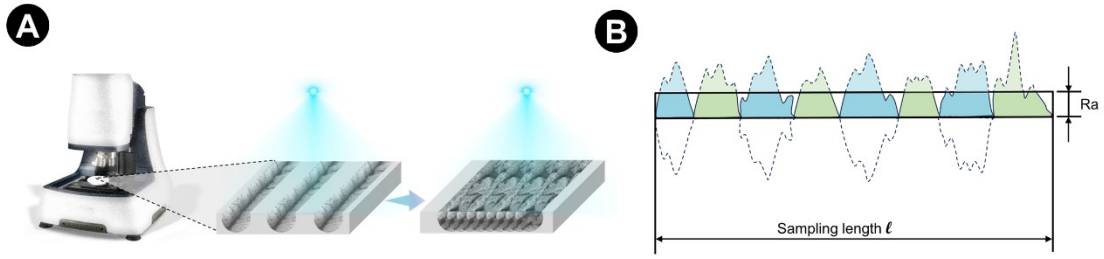

Figure S2 Schematic of optical profilometer imaging and definition of surface roughness Ra. From the measurement area of the optical profilometer, it can be seen that as the laser etching line increases, the roughness within the test area will increase gradually. Regarding Ra, the arithmetic mean roughness, it represents the average absolute value of roughness over a reference length. Originally, the blue region in the graph indicates areas below the mean line, but for the purpose of calculation, we take the absolute value of these deviations to determine Ra. This absolute value is relative to the average height of the surface. More accurately, Ra is the average deviation of the heights of each point on the surface from the mean height.

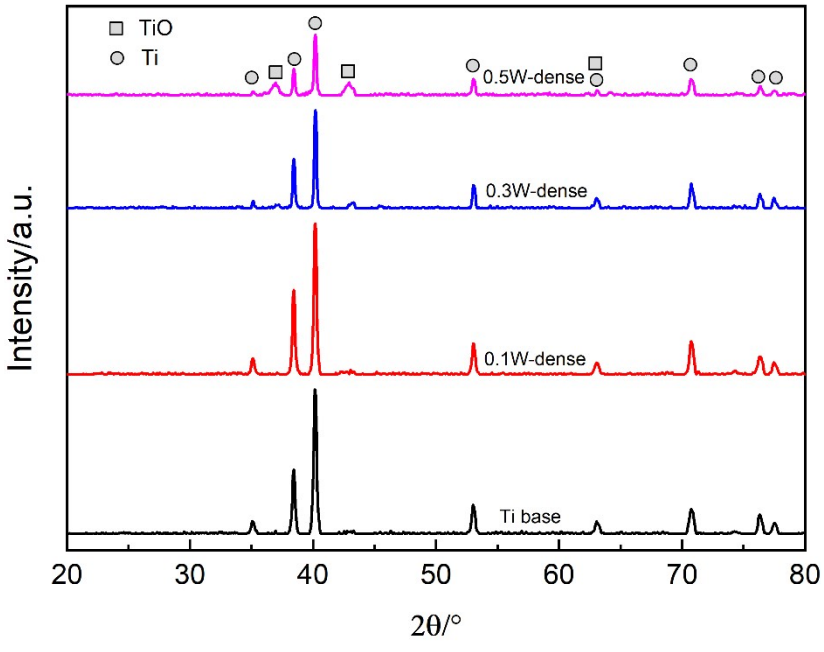

Figure S3 XRD diagram of the Ti samples after modifications.

SI-2 Transfer of standard deviation

Add or subtract: $(X\pm u_x)+(Y\pm u_y)=(X+Y)\pm\sqrt{u_x^2+u_y^2}$

$$(X\pm u_x)-(Y\pm u_y)=(X-Y)\pm\sqrt{u_x^2+u_y^2}$$

multiply or divide: $(X\pm u_x)(Y\pm u_y)=XY\pm XY\sqrt{\left(\frac{u_x}{X}\right)^2+\left(\frac{u_y}{Y}\right)^2}$

$$\frac{X\pm u_x}{Y\pm u_y}=\frac{X}{Y}\pm\frac{X}{Y}\sqrt{\left(\frac{u_x}{X}\right)^2+\left(\frac{u_y}{Y}\right)^2}$$

where u_x and u_y represent the standard deviation of X and Y, respectively.

SI-3 Calculation of nucleation site density

First, calculate the density of O and Ti atoms (/nm^2) on the smooth surface according to Table 2. It is known that the total density of Ti and oxygen atoms (Ti+O) on the surface is ρ(Ti+O)=20.01±5.44/nm^2, and From, the percentages of O and Ti atoms are 31.16% and 9.51% shown in Table 2, respectively. the density of O atoms and Ti atoms on the surface can be calculated:

Density of O atoms：ρ(O) =(20.01±5.44)×31.16%=6.24±1.70 /nm^2

Density of Ti atoms：ρ(Ti)= (20.01±5.44)×9.51%=1.90±0.52 /nm^2

Table 3 shows that O atoms on the smooth surface come from two parts, namely TiO_2 and- OH, and TiO_2 accounted for 50.59%, -OH accounted for 49.41%, thus the densities of TiO_2 and -OH can be calculated respectively:

Density of TiO_2：ρ(TiO_2) = [(6.24±1.70)×50.59%]/2 =1.58±0.43/nm^2

Density of -OH：ρ(-OH) = (6.24±1.70)×49.41% = 3.08±0.84/nm^2

The calculations for the other regions are shown below:

0.1W-line

Density of O atoms：ρ(O) =(20.01±5.44)×32.41%=6.49±1.76 /nm^2

Density of Ti atoms：ρ(Ti)= (20.01±5.44)×11.82%=2.37±0.64 /nm^2

Density of TiO_2：ρ(TiO_2) = [(6.49±1.76)×57.05%]/2 =1.85±0.50/nm^2

Density of -OH：ρ(-OH) = (6.49±1.76)×42.95% = 2.79±0.76/nm^2

0.1W-dense (0.1W-0.01)

Density of O atoms：ρ(O) =(20.01±5.44)×35.74%=7.15±1.70 /nm^2

Density of Ti atoms：ρ(Ti)= (20.01±5.44)×14.63%=2.93±0.80 /nm^2

Density of TiO_2：ρ(TiO_2) = [(7.15±1.70)×65.06%]/2 =2.33±0.55/nm^2

Density of -OH：ρ(-OH) = (7.15±1.70)×34.94% = 2.50±0.59/nm^2

0.3W-line

Density of O atoms：ρ(O) =(20.01±5.44)×46.20%=9.24±2.51 /nm^2

Density of Ti atoms：ρ(Ti)= (20.01±5.44)×18.46%=3.69±1.00 /nm^2

Density of TiO_2：ρ(TiO_2) = [(9.24±2.51)×75.53%]/2 =3.49±0.95/nm^2

Density of -OH：ρ(-OH) = (9.24±2.51)×24.47% = 2.26±0.61/nm^2

0.3W-dense (0.3W-0.01)

Density of O atoms：ρ(O) =(20.01±5.44)×47.77%=9.56±2.60 /nm^2

Density of Ti atoms：ρ(Ti)= (20.01±5.44)×21.37%=4.28±1.16 /nm^2

Density of TiO_2：ρ(TiO_2) = [(9.56±2.60)×75.42%]/2 =3.61±0.98/nm^2

Density of -OH：ρ(-OH) = (9.56±2.60)×24.58% = 2.35±0.64/nm^2

0.5W-line

Density of O atoms：ρ(O) =(20.01±5.44)×43.75%=8.75±2.38 /nm^2

Density of Ti atoms：ρ(Ti)= (20.01±5.44)×22.70%=4.54±1.23 /nm^2

Density of TiO_2：ρ(TiO_2) = [(8.75±2.38)×69.41%]/2 =3.04±0.83/nm^2

Density of -OH：ρ(-OH) = (8.75±2.38)×30.59% = 2.68±0.73/nm^2

0.5W-dense (0.5W-0.01)

Density of O atoms：ρ(O) =(20.01±5.44)×45.23%=9.05±2.46 /nm^2

Density of Ti atoms：ρ(Ti)= (20.01±5.44)×24.68%=4.94±1.34 /nm^2

Density of TiO_2：ρ(TiO_2) = [(9.05±2.46)×64.69%]/2 =2.93±0.80/nm^2

Density of -OH：ρ(-OH) = (9.05±2.46)×35.31% = 3.20±0.87/nm^2

References

[1] J.C. Phillips, R. Braun, W. Wang, J. Gumbart, E. Tajkhorshid, E. Villa, C. Chipot, R.D. Skeel, L. Kalé, K. Schulten, J Comput Chem 26 (2005) 1781–1802.

[2] M. Matsui, M. Akaogi, Mol Simul 6 (1991) 239–244.