Supplemental Material

Numerical investigation of the role of osteopontin on the mechanical strength of biological composites

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S1. Hydroxyapatite surface

In this paper, the hydroxyapatite surface is a {100} crystal surface modelled near to the OH groups, as shown in Figure S1. Previous research suggested that this surface is the primary hydroxyapatite surface observed in biological materials (Sato et al. 2002; Corno et al. 2011).

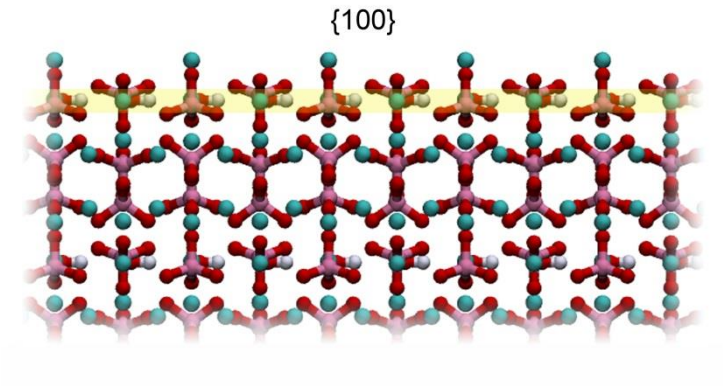

Figure S1. Hydroxyapatite {100} crystal surface modelled near to the OH groups (highlighted in yellow). H, O, P and Ca are represented by the colours white, red, purple and cyan, respectively.

S2. Hydroxyapatite parameters

The MD simulations used the GROMOS force field (van Gunsteren and Berendsen 1987; van Gunsteren et al. 1996) added with the hydroxyapatite parameters (Hauptmann et al. 2003; Pan et al. 2007). The Hauptmann force field (Hauptmann et al. 2003) describes the van der Waals interactions using the Born-Mayer-Huggins (BMH) equation, i.e.,

$$V_{BMH} = w(\rho_i + \rho_j) \times \exp\left(\frac{R_i + R_j - r_{ij}}{\rho_i + \rho_j}\right) - \frac{C_i C_j}{r_{ij}^6} \quad \text{(S1)}$$

where r_{ij} is the distance between particles i and j, the value of w is 1.1552×10^{-19} J·Å^{-1} (Yuen et al. 1974), ρ, R and C are the BMH parameters. However, the Lennard-Jones (LJ) equation is used in the GROMOS force field (van Gunsteren and Berendsen 1987; van Gunsteren et al. 1996). Hence, in this paper, the MD simulations employed the LJ parameters converted from the BMH parameters. Previous study has successfully converted the BMH parameters to LJ parameters (Pan et al. 2007). Both the BMH and LJ parameters are shown in Table S1. Here, the LJ parameters for the interactions between the osteopontin and hydroxyapatite were computed using the Lorentz-Berthelot (LB) combination rule (Hirschfelder et al. 1954), i.e.,

$$V_{LJ} = 4\varepsilon_{ij}\left(\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right) \quad \text{(S2)}$$

$$\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2} \quad \text{(S3)}$$

$$\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j} \quad \text{(S4)}$$

where r_{ij} is the distance between particles i and j, ε and σ are the LJ parameters. The electrostatic interactions were computed using the Coulomb's law equation, i.e.,

$$V_C = \frac{1}{4\pi\varepsilon_0}\frac{q_i q_j}{\varepsilon_r r_{ij}} \quad \text{(S5)}$$

where r_{ij} is the distance between particles i and j, ε_0 is the vacuum permittivity, ε_r is the relative permittivity, q is the partial atomic charges. The partial atomic charges, q employed in the MD simulations are shown in Table S1.

Table S1. Born-Mayer-Huggins parameters (ρ, R, C), Lennard-Jones parameters converted from the Born-Mayer-Huggins parameters (ε, σ), and partial atomic charges (q) (Hauptmann et al. 2003; Pan et al. 2007). O(P) and O(H) represent the oxygen in the phosphate and hydroxide groups, respectively.

Atom	ρ (Å)	R (Å)	C (10^{-9} J$^{1/2}$·Å^3)	ε (kJ·mol^{-1})	σ (nm)	q (C)
Ca	0.080	1.30	1.2151	0.5159	0.29067	+2.0
P	0.150	1.70	6.8351	4.1014	0.34919	+2.6
O(P)	0.135	1.30	2.2784	1.0757	0.30044	–1.4
O(H)	0.111	1.30	1.5189	0.4744	0.31073	–1.6
H	0.010	0.10	0.0015	0.0000	0.00000	+0.6

References

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