Supporting Information

Promotion of collagen mineralization and dentin repair by succinate

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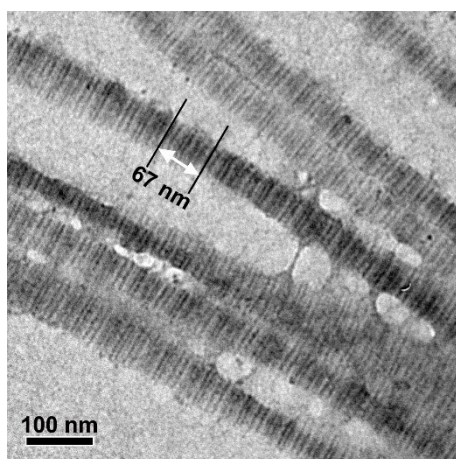
Fig. S1 TEM image of self-assembled collagen fibers are stained with uranyl acetate, which shows a typical 67 nm D-band.
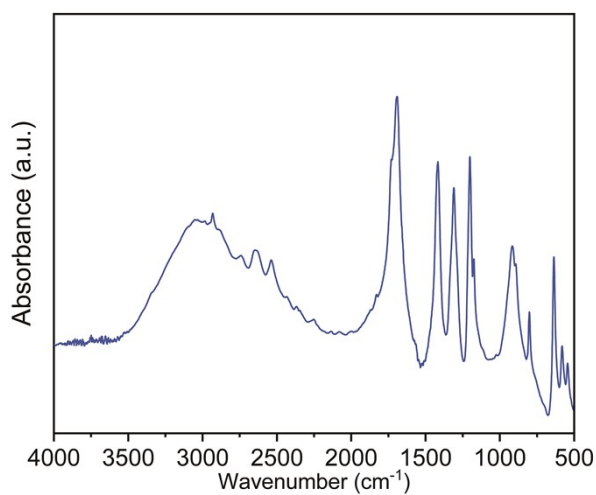

Fig. S2 FTIR spectrum of SA. The characteristic peaks of SA were detected at 2932, 2643 (O-H stretching), 1690 (C=O stretching), 1417 (symmetric stretching of COO-), 1309, 1202 (C-O stretching), 1175, 917 (O-H out of plane bending vibration) and 801 cm^{-1}, which were in accordance with previous results.[1]
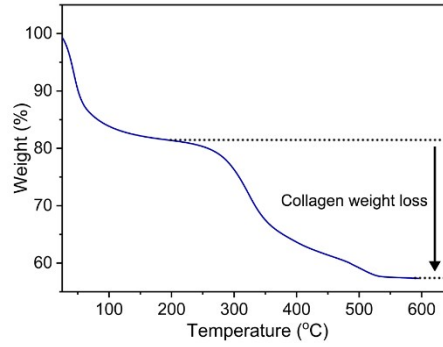
Fig. S3 Represented thermogravimetric analysis (TGA) curve of mineralized collagen hydrogel. The data is displayed as weight versus temperature. In the first stage, at T<200 °C, the weight loss was assigned to water, also called dehydration. In the second stage, 200-600 °C, the weight loss was assigned to organic materials, mainly collagen, also called organic decomposition. Based upon the TGA curve, the mineral-to-collagen mass ratio is calculated by Equation 1.

$$\frac{Mineral}{Collagen} = \frac{m_{600°C}}{m_{200°C} - m_{600°C}} \times 100\%$$

(1)

The relative strength of Peak calculation

In Fourier transform infrared spectroscopy (FTIR) of collagen fibers, the peak at 1454 cm^{-1} was assigned to the -CH$_2$ and -CH$_3$ bending vibration, which its intensity almost no change after SA treated the collagen fibers (Refer to Fig. 2a), and thus this peak could be chosen as a standard internal peak. The ratio of the integral area of the peak at 1400 and 1454 cm^{-1} could be defined as the relative strength (RS) for the peak at 1400 cm^{-1}, assigning to the symmetrical stretching of the carboxyl groups (-COO^{-1}), used for semiquantitative analysis of the intensity change of this peak between the pristine and SA-modified collagen. Therefore, the interaction between SA and collagen could be qualitatively analyzed by analyzing the difference in RS of the peak at 1400 cm^{-1}

between different samples.

The RS could be expressed as Eq. 2

$$RS = \frac{S_{1400}}{S_{1454}}$$ (2)

where the S_{1400} and S_{1454} values correspond to integral areas of the fitting peak for the peak at 1400 cm^{-1} and 1454 cm^{-1}, respectively (Fig. S4). Before calculating the RS, the pre-processing of FTIR spectra, including a quality test, baseline correction, and vector normalization, was required.
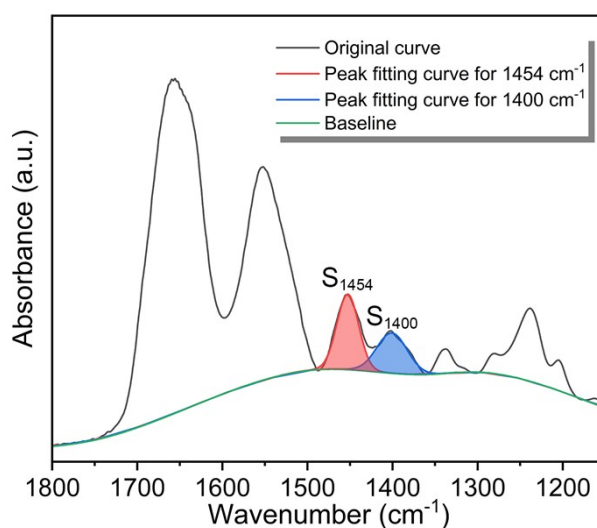
Fig. S4 The FTIR of pure collagen was displayed here as a schematic diagram to illustrate how to calculate the RS.

Langmuir adsorption isotherm of SA onto collagen

Analyzing the data of the adsorption of SA onto collagen and fitting the curve, we find it follows the Langmuir model. Assuming that there is no lateral interaction between adjacent adsorbed molecules when a single molecule occupies a single surface site, the Langmuir adsorption isotherm can be expressed as Equation 3.[2]

$$q = q_m \times \frac{bC_e}{1 + bC_e}$$
(3)

Where q_m is the maximum quantity of adsorbate adsorbed in a single monolayer (mg g^{-1}), b is the adsorption equilibrium constant, and C_e is the equilibrium concentration of adsorbate.

The adsorption experiments are performed at 37 °C. The q_m can be determined experimentally, and, based on the fitting curve, the value is around 12.078 mg/g. Meanwhile, the b is also calculated, and the value is around 0.185. Furthermore, the free energy change of the adsorption is given as:

$$\Delta G =- RT lnb$$
(4)

Where R is the universal gas constant (8.314 J mol^{-1} K^{-1}), and T is the absolute temperature (K). Here the value is 310.15 K. Therefore, according to thermodynamic law, we could calculate the ΔG of adsorption (4.35 kJ mol^{-1}), corresponding to the interaction energy between SA and collagen.[3]

References

1.   S. Krishnan, C. J. Raj, S. M. N. Priya, R. Robert, S. Dinakaran and S. J. Das, *Cryst. Res. Technol.*, 2008, **43**, 845-850.

2.   I. Langmuir, *J. Am. Chem. Soc.*, 1918, **40**, 1361-1403.

3.   Y. Liu, *J. Chem. Eng. Data*, 2009, **54**, 1981-1985.