Supporting Information

Correlations of Crystal Shape and Lateral Orientation in Bioinspired $CaCO_3$ Mineralization

Ming-Feng Liu,[a] Zihao Lu,[a] Zhisen Zhang,[*a] Chuanlian Xiao,[a] Ming Li,[a] Ya-Xi Huang,[*a] Xiang Yang Liu,[a,b] Yuan Jiang[*a]

[a.] College of Materials, Department of Physics, Research Institute for Biomimetics and Soft Matter, Fujian Provincial Key Laboratory of Soft Functional Materials, Xiamen University, Xiamen, 361005, P. R. China.

[b.] Department of Physics, Faculty of Science, National University of Singapore, Singapore 117542

E-mails:
yuan.jiang@xmu.edu.cn,
zhangzs@xmu.edu.cn
yaxihuang@xmu.edu.cn

1. Molecular simulation details

All the MD simulations in this work were performed in the NVT ensemble by Gromacs 4.5.2 package.[1, 2] The periodic boundary condition was applied to all of the three directions. A time step of 2 fs was used with atom coordinates saved every 10 ps, with a total simulation time of 30 ns. The last 10 ns trajectories were used to extract results in this work. A temperature of 298 K was maintained using the V-rescale method. The OPLS all-atom force field was used to describe PCL molecules.[3] And the adopted model of calcite is developed by Shen et al.[4], which is fitted from Raiteri's model[5]. The atoms in calcite remain fixed in all the simulations. The particle mesh Ewald (PME) summation[6] was used to calculate the long-range electrostatic interaction, with a cutoff of 1.3 nm for the separation of the direct and reciprocal space summation. The cutoff distance for the van der Waals interaction was 1.3 nm, and the parameters of the Lennard-Jones potential for the cross interactions between non-bonded atoms were obtained from the venerable Lorentz-Berthelot combination rule.[7] In all MD simulations, the system consisted ~11670 atoms with x, y, and z dimensions of 6.05 nm, 5.97 nm, and 9.00 nm, respectively, which were constructed by 1764 Ca^{2+}, 1764 CO_3^{2-} and 38 PCL molecules. The (110) face of calcite is in *x*-*y* plane. Five independent parallel simulations were carried out to obtain the reliable result.

References:

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2. Figures

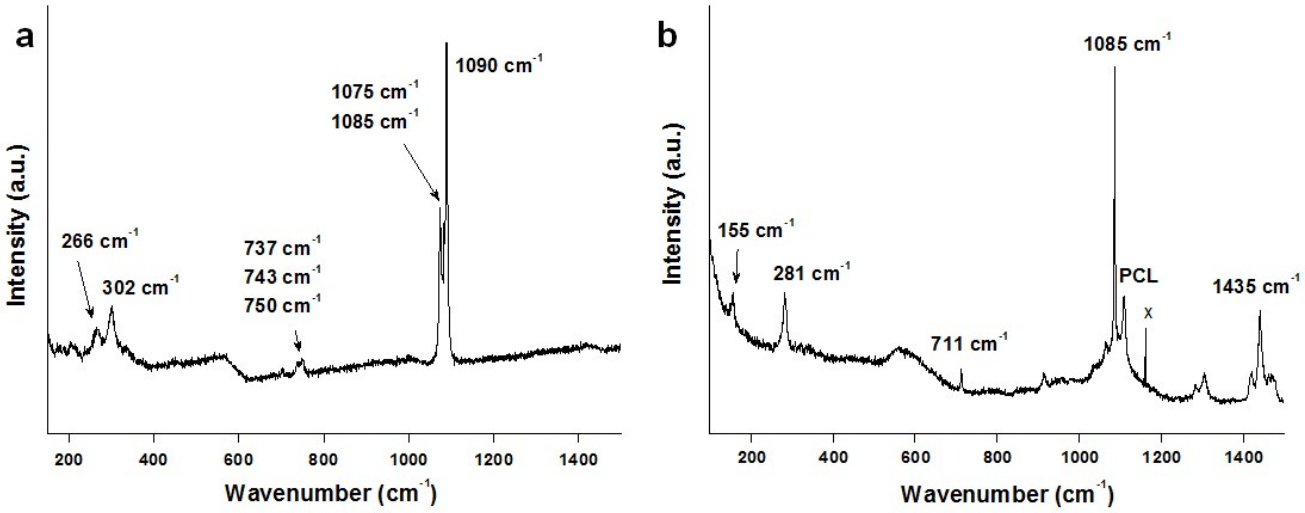

Figure S1. (a-b) Raman spectra of vateritic microdomains (a) and finally achieved calcitic microrods (b).