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Prioritized adsorption of acid amino acids secreted from bacterial EPS contributes to the crystal lattice preferred orientation

YANYANG ZHAO

Shandong University of Science and Technology

Presenting Author: zhaoyysdust@163.com

The lattice structure of biominerals are commonly different from chemically-synthesized minerals [1, 2], but the reasons for these are not fully understood. A facultative anaerobic bacterium, *Enterobacter ludwigii* SYB1, is used in experiments to document its biomineralization. X-ray diffraction (XRD) spectra showed that calcite, monohydrocalcite (MHC), and dypingite formed in samples with bacterial cells. It was also found that the (222) plane of MHC was the preferred orientation compared to standard data. Scanning Transmission Electron Microscopy (STEM) analysis of cell slices provides direct evidence of concentrated calcium and magnesium ions on the surface of extracellular polymeric substances (EPS). In addition, high-resolution transmission electron microscopy (HRTEM) showed that crystallized nanoparticles were formed within the EPS. 17 kinds of amino acid were identified within both biotic MHC and the EPS of SYB1, while the percentages of glutamic and aspartic acid in MHC increased significantly ($p<0.05$). Further, the adsorption energy was calculated for various amino acids on 7 diffracted crystal faces, with preferential adsorption demonstrated on (111) and (222) faces. At the same time, the lowest adsorption energy was always that of glutamic and aspartic acid for the same crystal plane (Figure 1). These results suggest that aspartic acid and glutamic acid always mix preferentially in the crystal lattice of MHC, and that differential adsorption of amino acids on crystal planes can lead to their preferred orientation.

[1] Weiner S, Dove P M. (2003), Reviews in mineralogy and geochemistry, 2003, 54(1): 1-29.

[2] Zhuang D, Yan H, Tucker M E, et al. (2018), Chemical Geology, 2018, 500: 64-87.