Versatile surface characterizations of Sum Frequency Generation(SFG) spectroscopy for polymers

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Abstract:

Vibrational Sum Frequency Generation (SFG) is a second order non-linear optical process, which can specifically probe molecular based on the non-centrosymmetric features. This capability has been extensively utilized to detect molecular species on 2D interface or to selective characterize 3D bulk crystal materials dispersed in amorphous matrix. 2D interface analysis using SFG can be explored to understand interfacial conformation and chain angles of the hydrophilic/hydrophobic polymer chains on a glass surface in response to external environmental conditions such temperature and humidity.

3D bulk crystalline analysis can be utilized for understanding of biopolymers, especially crystalline structures dispersed in amorphous matrix because matrix, such as cellulose and β-sheet structures because SFG signal non-crystalline materials are cancelled. Consequently, the SFG spectra can provide chemical information, collective chain directionality of crystalline structures as an insight for bio-mimicry based application engineering. However, considering the complexity of the SFG process and various parameters, the SFG spectral features should be evaluated by comparing with SFG simulation in a logical way. In this study, SFG numerical calculation has been demonstrated using DFT result.