MS13-1-19 Raman spectroscopy approach to determine crystallographic and molecular orientation of rubrene molecular films
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Abstract
Understanding and engineering molecular crystals are of great importance to reach a high performance of molecular-based electronics o biocompatible devices. Rubrene, a tetraphenyl derivative of tetracene, has been recognized to possess high mobility in single-crystal structures. We report ex-situ polarized Raman analysis of rubrene thin films grown by hot-wall epitaxy deposited onto mica substrates. Usually, polarized photons are used to distinguish molecular anisotropy in organic molecules, scaffolds for cell culture, and biological cell growth among other applications. Raman spectroscopy aid to determine both molecular anisotropy and chemical identity of the analyzed species.
We took the advantage of the Raman tensor properties i.e. group symmetry and polarized scattered photons to determine the molecular orientation of rubrene molecules in crystalline films. The Raman measurements were performed by shining the films at 90° with polarized laser light of 784 nm and collecting the Raman light in the backscattering configuration by rotating the in-plane sample at several angles. Since rubrene films exhibit three progressive stages of molecular growth i.e. from an amorphous matrix to spherulites and a final phase of coalescence, it is found that the Raman breathing mode 1003 cm–1 represents the rubrene fingerprint and is independent of the growth stage. Therefore, various internal modes of the phenyl groups were considered to compute the molecular orientation. In order to probe film anisotropy and molecular orientation, each angle was measured at two different polarizations. Thus, a set of Raman tensors was obtained and solved with an iterative “back-and-forth” method to determine the molecular orientation and to determine dipole-dipole interactions within the molecular crystal. Results revealed the advantage of Raman spectroscopy to probe crystallographic properties of molecular solids by using lower energies compared with other techniques.

References
Svenningsson, L., & Nordstierna, L. (2020). Polarized Raman Spectroscopy Strategy for Molecular Orientation of Polymeric Fibers with Raman Tensors Deviating from the Molecular Frame. ACS Applied Polymer Materials, 2(11), 4809–4813. https://doi.org/10.1021/acsapm.0c00762