

Understanding structural variations in elastic organic crystals by in situ high-pressure fourier transform infrared spectroscopy and nanoindentation study

Abstract

Organic crystals possessing elasticity are gaining wide attention due to their potential applications in technology. From a design perspective, it is of utmost importance to understand the mechanical behavior of these crystals and their ability to handle stress. In this paper, we present an in situ high-pressure Fourier transform infrared spectroscopy study on 2,5-dichloro-*N*-benzylidene-4-chloroaniline (DPA) and 2,6 dichloro-*N*-benzylidene-4-fluoro-3-nitro aniline (DFA) crystals at pressures ranging from ambient pressure to 21.5 and 14.5 GPa respectively along with nanoindentation studies, at room temperature. The infrared stretching wavenumber of the aromatic and aliphatic C–H, H–C=N, and C–Cl bands on compression showed blueshifts and increased widths, which reflect structure perturbation caused by changes in intermolecular interactions in the crystals. It was noted that both crystals DPA and DFA behave in a different fashion under high-pressure prompting the derivation of different models based on structural changes in the lattice. Further, nanoindentation studies corroborated pressure-induced molecular movement in both crystals.

Key words: Nanoindentation, Crystals, Aromatic compounds, Molecular interactions, Molecules