A First-Principles Polarized Raman Method for Determining Whether a Sample is Crystalline or Isotropic

ANDREW WEISMAN, Columbia University, KATERI DUBAY, University of Virginia, KATHERINE WILLETS, The University of Texas at Austin, RICHARD FRIESNER, Columbia University — We have discovered a simple way to apply basic vibrational Raman spectroscopy to unambiguously determine whether a region of a sample is crystalline or isotropic. Unlike previous methods for determining crystallinity, ours is completely general and rigorously founded in the theory of Raman scattering; it applies independently to any mode of any material and requires no previously established relationships between peak parameters and degree of crystallinity. By applying this technique while scanning an unknown, heterogeneous sample, the borders of the crystalline and isotropic regions can be delineated clearly, after which more developed methods can be applied to determine the orientations of the crystalline regions, thereby completely characterizing the molecular structure of the sample.