Contributions of Raman Spectroscopy to Powder X-ray Diffraction for Solid-State Characterization

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Powder X-ray diffraction (PXRD) serves as the primary benchmark for phase identification in solid-state materials. However, structural models based solely on long-range periodic order may overlook local complexities that influence material properties. This presentation provides a critical review of Raman spectroscopy as a complementary probe to X-ray diffraction, highlighting its sensitivity to local coordination, short-range order, and the dynamics of light-atom sublattices.

Through case studies involving pharmaceuticals and functional materials, we examine instances where vibrational spectroscopy resolves structural ambiguities present in diffraction data. The discussion correlates the bond polarizability probed by Raman with the electron density distributions mapped by X-rays. Particular emphasis is placed on investigations under extreme conditions, such as high pressure and variable temperature, where vibrational modes may indicate subtle phase transitions, soft-mode behavior, or bond stiffening that precede macroscopic lattice changes. Furthermore, the impact of instrumental parameters on data fidelity is addressed to contextualize the reliability of spectral results. This work supports the current initiative to integrate vibrational data into crystallographic databases, demonstrating that a multi-technique approach enhances the accuracy of solid-state characterization.