

Aggregate elasticity and compaction performance: powder Brillouin light scattering

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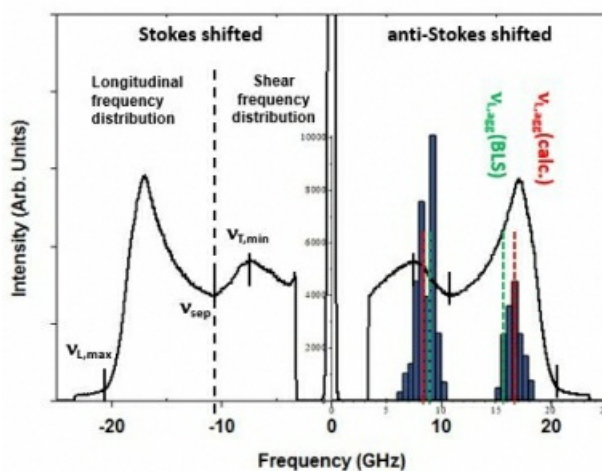
To assist the rational design of solid dosage forms, an improved structure-mechanics relationship is needed, i.e. identifying those structural elements (hydrogen bonding, crystal packing, dispersive interactions and slip planes) that most prominently contribute to bulk phase mechanics. Challenging this development, organic molecules typically crystallize into low-symmetry space groups and the expressed mechanical properties are often highly anisotropic. As a result, the availability of comprehensive mechanical data is sparingly available for molecular solids and thus limits its integration with developing models of powder compaction performance. For this seminar, the aggregate elasticity of three series – caffeine co-crystals, p-aminobenzoates and point-substituted nitro-benzoic acids – will be discussed in relation to their respective intermolecular interaction topologies and tableting performance.

Brillouin light scattering, an inelastic light scattering technique traditionally used for single-crystal elasticity, is being developed into a powder-based approach (powder BLS).[1,2] In powder BLS, rather than spectra composed of discrete acoustic modes a distribution of acoustic frequencies are observed. These distributions are material specific and sensitive to the strength and anisotropy of the intermolecular interaction potential. To further aid the interpretation of these spectra, predicted acoustic frequency distributions are calculated using materials with experimentally determined elastic constants.

Furthermore, through our assignment of powder BLS characteristic frequencies, the zero-porosity, aggregate elastic moduli are obtained. An initial validation of this approach is discussed with respect to acetylsalicylic acid, a material with well-characterized mechanics. The mechanical properties of our series will be further discussed in association with the compressibility, compactability and slip-mediated plasticity of each material series. Overall, the complementary approach of using both structural and the acoustic inputs uniquely provided from powder BLS is anticipated to expand our comprehension of the structure-mechanics relationship and its role in tableting performance.

[1] Singaraju, A. B. & Stevens, L. L. (2016) Cryst. Growth Des., 16, 4383 - 4391

[2] Singaraju, A. B. & Stevens, L. L. (2016) Mol. Pharmaceutics, 13, 3794 - 3806



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