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Towards Understanding Defect Formation Evolution During Cryogenic Milling of Crystalline Organics

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ABSTRACT

Dynamics of defects at the molecular level and the effect on the mechanical properties at the bulk level of materials are of interest in the pharmaceutical and food industries for achieving the desired functionality and stability. Unfortunately, the material sciences in these industries remains suboptimal compared to other industries engaged in materials processing. The effectiveness of the defected material on solubility, mechanical properties and stability can be neutralized if the crystallinity or crystalline phase changes unexpectedly during processing or storage (environmental conditions of temperature and humidity), negating any solubility or processability advantage resulting in a change in the drug's ability to be absorbed properly in the body or having long shelf-life. The behavior of materials at the nano/micron scale is poorly understood in part due to the complexity of the particulate organics (soft composites) involved and the lack of characterization that enables assessment and quantification of crystal defects such as dislocations, stacking faults, grain boundaries and phase boundaries.

In this presentation, the effects of defect formation on mechanical deformation of crystalline organics that breaks down the crystal structure by the accumulation of defects will be discussed experimentally and computationally. Data will be shown to illustrate structural characterization and how transformations induced by processing multi-component particulate systems play an important role in their physical and mechanical properties followed by a discussion of how the properties of the composite organics are altered by both the process and environmental conditions(temperature and moisture). Simulations of diffraction on different structures and structures with different defect content using Rietveld-based least-squares models can enable quantitative documentation of changes in organic soft materials. Small Angle X-ray Scattering (SAXS) and conventional diffractometry combined with *in situ* capabilities will enable a full spectrum assessment of phase and structural evolution. Finally, it will be concluded that this is still a complex problem with many aspects that need further exploration.

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