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*Correlating crystal structure, nanomechanical, and compaction behavior of febuxostat polymorphs*

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A xanthine oxidase inhibitor, Febuxostat exhibits unprecedented solid forms with a total of 40 polymorphs and pseudo-polymorphs have been revealed in patent applications. Polymorphs differ in molecular arrangement and conformation, intermolecular interactions, and various physicochemical properties including mechanical properties. Febuxostat Form Q (FXT Q) and Form H1 (FXT H1) were investigated for single crystal structure, nanomechanical parameters and bulk deformation behavior. FXT Q showed greater compressibility, densification and plastic deformation as compared to FXT H1 at a given compaction pressure. Lower mechanical hardness of FXT Q (0.214 GPa) as compared to FXT H1 (0.310 GPa) was found to be consistent with greater compressibility and lower mean yield pressure (38 MPa) of FXT Q. Superior compaction behavior of FXT Q was attributed to presence of active slip systems in crystal lattice which offered greater plastic deformation under mechanical stress. By virtue of greater compressibility and densification, FXT Q showed higher tableting performance over FXT H1. Significant correlation was found with such anticipation that the preferred orientation of molecular planes into crystal lattice translated nanomechanical parameters to bulk compaction process. However, the prediction of compactibility or tableting performance of materials based on true density or molecular packing still remains warranted wherein slip-planes may cause deviation in structure-property relationship. This study corroborated how molecular level crystal structure confers a bridge between particle level nanomechanical parameters and bulk level deformation behavior.

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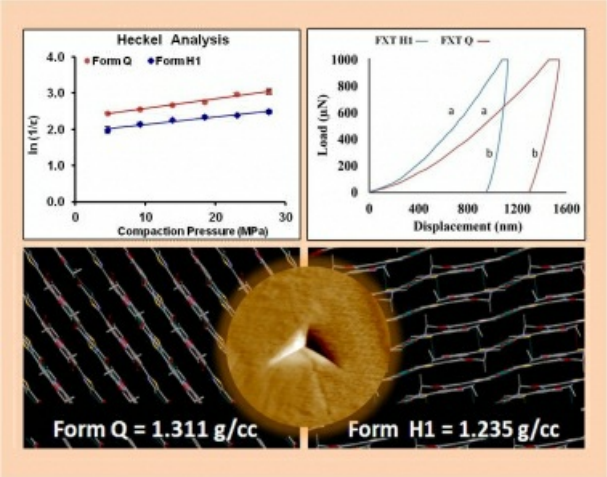


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