Abstract Submitted
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Crystal modification and preferred orientation studies of 1,ω-alkanediols (ω =10-13) obtained from rapid glancing incidence X-ray diffraction experiments[1] GILGAMESH LUIS-RAYA, Universidad Politécnica de Pachuca, MARIUS RAMÍREZ-CARDONA, AACTyM Universidad Autónoma del Estado de Hidalgo, EUCARIO G. PÉREZ-PÉREZ, NAZARIO BAUTISTA-ELIVAR, LUIS ALBERTO ZAMORA-CAMPOS, FRANCISCO MARROQUÍN-GUTIÉRREZ, Universidad Politécnica de Pachuca — The crystal structure determination of four polycrystalline samples of 1,ω-alkanediols (CnH2n+2O2 with n = 10, 11, 12 ,13) was achieved from Glancing Incidence X-ray Diffraction (GIXD) data by combining lattice energy optimization, molecular replacement and rigid-body structural Rietveld refinements. The occurrence of either monoclinic (P21/c, Z=2) or orthorombic (P212121, Z=4) polymorphs is explained as function of a constant hydrogen bond energy (28.5 kJ/mol per molecule) in the series, the differences on hydrogen patterns and the different herringbone grade on the bilayer arrangement. From a multi-axial March-Dollase treatment, energetic and structural features yield remarkably differences on the textural behavior as well as on morphology of crystallites. In this work we show that crystalline structures of medium complexity and their microstructures can be solved from short counting times of GIXD experiments from standard radiation, and a molecular replacement procedure using crystal structures of compounds with higher chain lengths as reference data.

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Gilgamesh Luis-Raya
Universidad Politécnica de Pachuca

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