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Translational Disorder and Crystal Growth Mechanisms in Channel Inclusion Compounds. M.D. Hollingsworth[1], J. Bacsa[1], C.F. Campana[2] and M.L. Peterson[1], from the [1]Chemistry Dept., Kansas State Univ., Manhattan, KS 66506 and [2]Bruker AXS Inc., 5465 East Cheryl Parkway Madison, Wisconsin 53711.

We have synthesized a large number of commensurate inclusion compounds of urea that undergo ferroelastic domain switching (reorientation under applied anisotropic stress). Because they can exhibit several types of disorder and twinning, many of these channel structures require non-routine methods for structure solution. Of interest is 1,11-undecanedioic acid/urea (1:9), in which two repeats of the guest (length = 16.5Å) match three repeats of the 11.0Å urea helix ($2c_g' = 3c_h'$). This material exhibits macroscopic, non-merohedral rotational twinning and a type of static translational disorder of guests in which domains are displaced along the channel axis by 11.0Å. The small lateral extent of these domains leads to a dramatic loss of intensity in 2/3 of the layer lines ($l \neq 3n$). Structure solution and refinement was achieved by using only the data with $l = 3n$ (for an 11.0Å cell). Comparison of this structure and refinement with a heavily constrained structure using all of the layer line data (for a 33Å cell) illustrates several knotty issues. The translational disorder exhibited in this system provides a static component to surface roughening during crystal growth.