MS26-O3 Phase transitions and critical phenomena in aperiodic composite crystals

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These last decades, the concept of order has broadened to analyze materials which have long-range order with symmetries that are incompatible with periodicity. These aperiodic compounds are described in the frame of a higher-dimensional analogue of the physical space called crystallographic superspace, and these crystals are periodic structures in these superspaces [1]. Aperiodic crystals are usually classified into three categories: incommensurately modulated phases, quasicrystals and aperiodic composites. Aperiodicity in composite materials may appear rather naturally due to the possible misfit of the host and the guest parameters along their crystallographic directions. A prototype series is given by the alkane chains confined in honeycomb–like urea sublattices.

We will first present symmetry breakings in this prototype family and show the richness of phases appearing in higher dimension spaces [2]. We will report on pretransitional phenomena in such a high-dimensional space, generalizing the critical results previously reported at a lower dimensionality [3]. Very high-resolution diffraction data reveal anomalously large correlation lengths along the aperiodic direction, with all correlation lengths diverging at *T*cl. This could be explained by low-frequency phason excitations that soften at *T*cl at the critical wave vector, in accordance with an increase in the critical diffuse scattering intensity.

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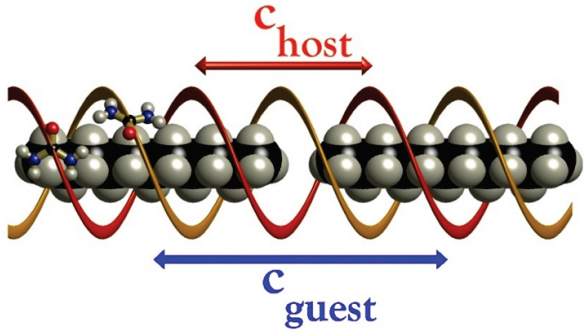

Figure 1. Aperiodic confinement of alkane in honeycomb–like urea sublattice

Keywords: composite crystal, phase transition, superspace crystallography

MS26-O4 Allotwinning: the overlooked form of twinning

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Twinning is the association of equivalent macroscopic domains with a well-defined crystallographic orientation relationship [1]. A related, but often overlooked, phenomenon is allotwinning, the oriented association of *different* polytypes of the same compound [2]. Whereas the structural characterization of twinned crystals has become routine in the last years, only few structures of allotwins were published. Nevertheless, allotwinning is more common than expected and therefore needs to be addressed.

Two inorganic compounds ($K_2HAsO_4 \cdot 2.5H_2O$, $KAgCO_3$) and one metalorganic iron pincer-complex, crystallizing as allotwins are presented and the problems and pitfalls encountered during data reduction and structural characterization are discussed.

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Keywords: twinning, polytypism, data reduction, structure refinement