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NEUTRON LAUE AND X-RAY DIFFRACTION STUDY OF A NEW CRYSTALLOGRAPHIC SUPERSPACE PHASE IN N-NONADECANE–UREA

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Aperiodic composite crystals present long-range order without translational symmetry. These materials may be described as the intersection in three dimensions of a crystal which is periodic in a higher-dimensional space. In such materials, symmetry breaking must be described as structural changes within these crystallographic superspaces. The increase in the number of superspace groups with the increase in the dimension of the superspace allows many more structural solutions. We will present recent results obtained by complementary Laue neutron diffraction and X-ray diffraction techniques on n-nonadecane-urea, a nice illustration of aperiodic materials. Within this original family of alkane-urea composites, we will illustrate how structural phase transitions are characterized by changes of intermodulation and described by increasing the rank of the associated crystallographic superspaces.

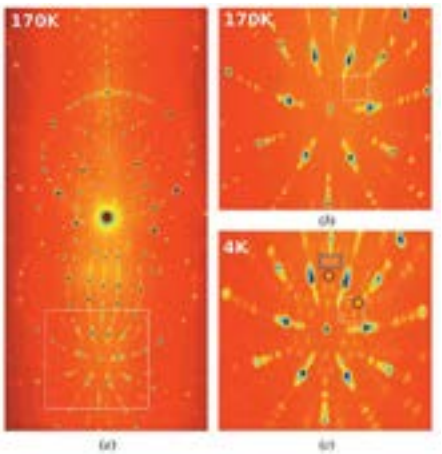

Figure 1:

(a) Laue diffraction image of n-nonadecane–urea at T=170K (phase I)
(b) Expansion of the selected region of the diffraction pattern at 170K
(b) same area at 4K

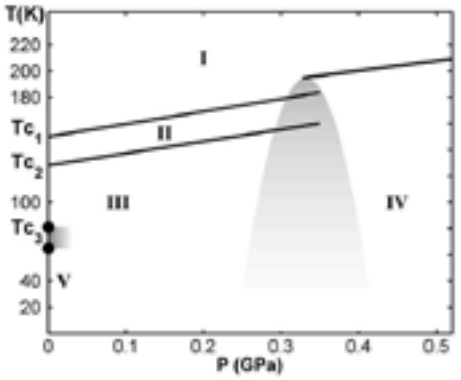

Figure 2:

Phase diagram (T,P) of the fully deuterated n-nonadecane–urea [1,2]. All the phases, I, II, III, IV and V, require a description within a crystallographic superspace. Shaded region indicates the metastable region between the ordered low-pressure and high-pressure phases. The two points associated with TC3 mark the metastability limit between phase III and phase V [1]

Recent Publications

1. Zerdane S., Mariette C., Mc Intyre G., Lemée-Cailleau M.H., Rabiller P., Guerin L., Ameline J.C., Toudic B. (2015) Neutron Laue and X-ray diffraction study of a new crystallographic superspace phase in n-nonadecane-urea, Acta Cryst B71, 293-299

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5. Huesges Z., Lucas S., Wunderlich S., Yokaichiya F., Prokes K., Schmalzl K., Lemée-Cailleau M.H., Pedersen B., Fritsch V., Löhneysen H.V., Stockert O.

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Biography

Marie-Hélène Lemée-Cailleau is expert in phase transition of molecular solids under various external controlled parameters, like temperature, pressure or light. Her speciality is single crystal neutron diffraction, using either monochromatic or polychromatic techniques, as well as X-ray diffraction (table-top or synchrotron), and all related structural analysis. She is physicist in the Science division of the Institut Laue Langevin, the European Neutron Source, located in Grenoble, France, and member of the French and European Crystallographic associations. (orcid.org/0000-0003-4733-4334).

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