$Bi_2Mn_{4/3}Ni_{2/3}O_6$: This is a very unusual material as it adopts the perovskite structure with Bi^{3+} on the A site – there has only been one previous example of perovskite stable to ambient pressure synthesis, $BiFeO_3$. The material is spin-glass-like with a freezing temperature, T_f, of 35K due to competing exchange interactions on the B site of the perovskite structure and undergoes an incommensurate to "commensurate" transition above 410 K, which shows hysteresis. We have previously described the room temperature phase in 3+2 dimensional space group Ibmm(0-p0,q00)mm.ss ($\sqrt{2}a_p$ x $2a_p$ x $\sqrt{2}a_p$; p,q ~ ½).[1] Herein we will describe the temperature variation of the modulation vectors and the persistence of incommensurate cation order into the "commensurate" high temperature phase from combined synchrotron X-ray and time of flight neutron diffraction data.

$Bi_2Mn_{2/3}Ti_{2/3}Ni_{2/3}O_6$: This phases also crystallizes in the same superspace group as the manganese nickel analogue, in 3+2 dimensional space group Ibmm(0-p0,q00)mm.ss ($\sqrt{2}a_p$ x $2a_p$ x $\sqrt{2}a_p$; p,q ~ ½). It's room temperature structure based combined synchrotron X-ray and time of flight neutron diffraction will be discussed.

Bi_2CoTiO_6: This metastable high pressure double perovskite unusually shows no cation order but does show an incommensurate modulation, like several other similar phases. The combined refinements show that this material crystallizes in the polar superspace group I2cm(0p0)000 (p ~ -2/3).

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Huge period *vs* aperiodicity in organic host guest systems.

Philippe Rabiller,[a] Laurent Guérin,[a] Céline Mariette,[a] Bertrand Toudic,[a] Claude Ecolivet,[a] Mark Hollingsworth,[b] [a]*Institut de Physique, Rennes, UMR 6251 CNRS Université de Rennes 1 35000 Rennes (France).* [b]*Department of Chemistry, Kansas State University, Manhattan (USA).* E-mail: philippe.rabiller@univ-rennes1.fr

Supramolecular chemistry and crystal engineering enable very attractive aperiodic host-guest architectures, where guest molecules are confined with their own periodicity into nanochannels [1]. The diffraction patterns of these aperiodic materials exhibit sharp Bragg peaks characteristic of long-range order, although the system is not invariant under a lattice of translations [2]. Short peptides and other organic molecules yield numerous examples of molecular self-assembled systems. The host-guest alkane-urea inclusion compounds typically form such aperiodic crystals, and their structural instabilities have been extensively studied.[3,4 and herein ref.].

Here, we discuss very high resolution synchrotron diffraction studies of the structural instability in n-tetracosane/urea, a compound where competing forces maintains aperiodicity with a misfit parameter very close to a rational number at ambient conditions: γ= c_{host}./ c_{guest} $\cong$ 1/3 (0.337+/-0.002). Below phase transition, a complex crystallographic diffraction pattern is observed with a very dense set of superstructure Bragg peaks along the aperiodic direction (figure). These are interpreted as the appearance of a huge periodicity of about 460Å associated to the host guest intermodulation. Similar results will be discussed considering other compounds of this family.
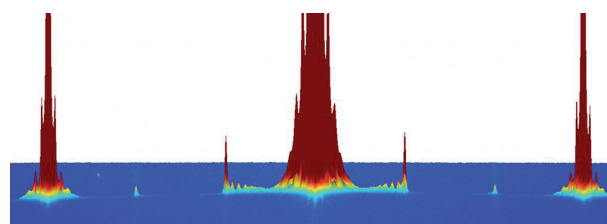
Tetracosane-urea superstructure line (90K) along the incommensurate channel direction in the q–range [-1.2, 1.2] in urea reciprocal units.

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On the criterion of modulated-structures formation for strain-induced-interacting vacancies in irradiated f.c.c. crystals.

O. V. Oliinyk, V. A. Tatarenko, *V. Kurdyumov Institute for Metal Physics, N.A.S.U., Kyyiv (Ukraine).* E-mail: neutrino@ukr.net

Within the crystals under irradiation, the modulated structures can be formed [1]. With decreasing temperature (T) or increasing concentration of defects (c), their interaction-caused drift begins to dominate their random motion, and the damping decrement becomes negative for every values of wave vector $\mathbf{k}$, which belongs to the sphere of a radius $k_0(T,c)$ about $\mathbf{k}=\mathbf{0}$, and the modulated structures appear. For $|\mathbf{k}|>k_0(T,c)$, the damping decrement is positive, and the modulated structures disappear [2].

A given paper is based on overrunning continuous approximation for the Fourier components, $\tilde{V}^{vv}(\mathbf{k})$, of the strain-induced vacancy–vacancy-interaction energies. Within the finite region near $_\mathbf{k}=\mathbf{0}$ [2, 3], the $\tilde{V}^{vv}(\mathbf{k})$ dependence is represented in a following form: $\tilde{V}^{vv}(\mathbf{k}) \cong A(\mathbf{n}) + B(\mathbf{n})|\mathbf{k}|^2 + Q$ ($\mathbf{n}=\mathbf{k}/|\mathbf{k}|$). Here, the well-known first term is based on long-wave-limit approximation [3], the second term is a correction to this approximation, and the third term is a gauge, which eliminates strain-induced self-action of vacancies.

The modulated structure can be formed along those crystallographic direction, which is parallel to $\mathbf{n}_c = \mathbf{k}_c/|\mathbf{k}_c|$ corresponding to the highest growth rate, and has the wave-vector with a magnitude $|\mathbf{k}_c| \cong \{-(A(\mathbf{n}_c)+Q+\tilde{\varphi}_{\text{el.chem}}(\mathbf{0})+k_BT/[c(1-c)])/[2(B(\mathbf{n}_c)+\gamma)]\}^{1/2}$; $\tilde{\varphi}_{\text{el.chem}}(\mathbf{k})$ is the Fourier component of energies of direct 'electrochemical' interaction between vacancies (v), c is their concentration, T is the temperature of a crystal, k_B is the Boltzmann constant. With the wave-length approximation, $\tilde{\varphi}_{\text{el.chem}}(\mathbf{k}) \cong \tilde{\varphi}_{\text{el.chem}}(\mathbf{0}) + \gamma|\mathbf{k}|^2$.

The approximated expansion coefficients for Fourier components of the strain-induced v–v-interaction energies are dependent on the elasticity moduli of f.c.c. crystals, C_{11}, C_{12}, C_{44}; *e.g.*, $A[100] = -9K^2(L^v)^2 a_0^3/(4C_{11})$ [2, 3], [2, 3], $B[100] \cong 9K^2 a_0^5 (L^v)^2 C_{44}/(32C_{11}^2)$, where $K=(C_{11}+2C_{12})/3$—the crystal-compression modulus, a_0—an f.c.c.-lattice parameter, L^v—the concentration coefficient of f.c.c.-lattice dilatation). As shown, the coefficient $B(\mathbf{n})$ is positive along all the high-symmetry [100], [110], [111], [½10] directions in reciprocal space for f.c.c. crystals with anisotropy factor $\xi \equiv (C_{11}-C_{12}-2C_{44})/C_{44} < 0$. If $\xi < 0$, $\tilde{V}^{vv}(\mathbf{k}_{\|\overline{XT}} \to \mathbf{0})$ has a one-sided minimum along the [100] direction, but it greater than $\tilde{V}^{vv}(\mathbf{0})$ as a result of the long-range character of strain-induced interaction. Besides, there are inequalities as follow: