References

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Principal Publication and Authors

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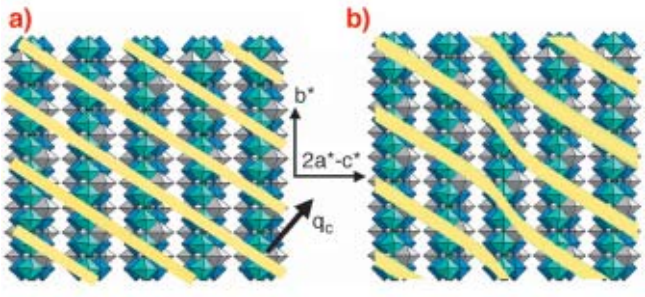

Fig. 121: Schematic representation of the Blue bronze CDW in the (2a*-c* ; b*) plane in a) a defect-free crystal and b) a crystal with a screw-like dislocation line running along b* in the middle of the figure. Only Mo octahedra are represented. Yellow lines represent the constant phase wave front of the CDW. Note that this dislocation does not introduce any dilatation or compression of the CDW along b*.

Evidence of Topological Defects in an Electronic Crystal

Electron confinement, for example along chains of atoms, give rise to original phenomena. These effects are observed in charge-density wave (CDW) materials. Upon cooling, these materials exhibit a modulation of the electron density along the chains and become insulating. Moreover, under a large enough electric field, a strong decrease of the resistivity is observed. This phenomena, still under debate, is generally interpreted as being caused by a collective "sliding" of the CDW as a whole [1].

This CDW can be considered as an electronic crystal, ordered in the three directions of space. In particular, its wave number along the chain is equal to twice the momentum of the fastest electrons of the system: $2k_F$. Like a crystal, this electronic system is elastic and can exhibit dislocations. Predicted theoretically for 25 years [2], such topological defects are thought to play an essential role in the behaviour of the CDW under electric field. In a similar way dislocations in metals explain metal plasticity.

The direct observation of CDW dislocations has never been achieved. Our recent experiment on the ID20 beamline has shown that coherent X-ray diffraction measurements are very sensitive to such topological defects. In the model system called "blue bronze" (a molybdenium oxide of formula $K_{0.3}MoO_3$), the structure of a CDW dislocation imbedded in the bulk has been studied. The interference fringes of the **Figure 122b** are interpreted as originating from the presence of a screw dislocation running along the chain axis. Since the one-dimensional CDW wave vector q_c is not parallel to the chains axis, this topological defect corresponds to a mixed dislocation (between screw and edge), running along the chains direction (see in **Figure 121b**). Remarkably, this dislocation introduces no energy expensive compression or dilatation of the CDW along the chains, but involves only shears: due to the charged character of the CDW, this is expected to cost less energy than an edge dislocation.

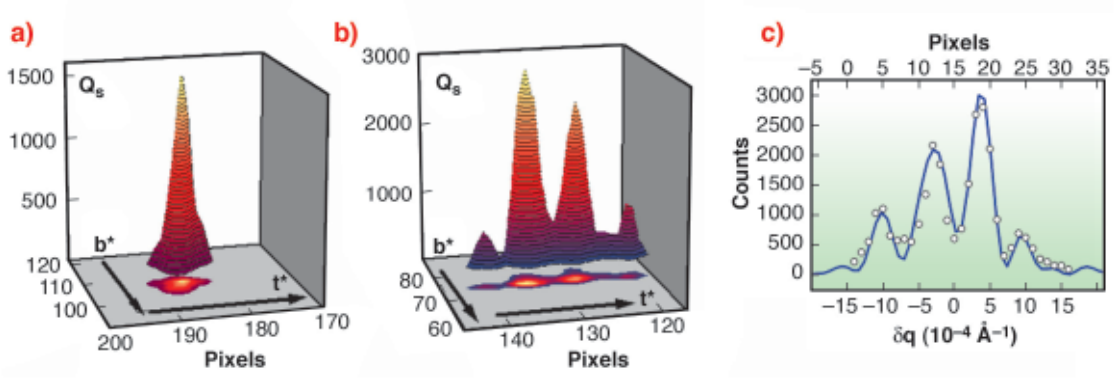

Fig. 122: 2D diffraction patterns of the $Q_s = (5,-1,-3)+q_c$ satellite reflection corresponding to a) **Figure 121a** and b) **Figure 121b**, at T = 75 K. c) Fit of the t*-scan of b) using the Fourier transform of the screw like dislocation shown in **Figure 121b**.

Beyond CDW systems, this study shows that coherent X-ray diffraction is well suited to probe any phase field deformation in the bulk, in nearly perfect lattices.

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D. Le Bolloc'h (a), S. Ravy (b), J. Dumas (c), J. Marcus (c), F. Livet (d), C. Detlefs (e), F. Yakhou (e), and L. Paolasini (e), *Phys. Rev. Lett.* **95,** 116401 (2005).

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The Mysteries of Low-temperature Ground States of Actinide Oxides Resolved by Synchrotron Experiments

The discovery at the ESRF in 2002 [1] of quadrupole ordering in neptunium dioxide opened a new chapter in the understanding of the low-temperature ground states of actinide oxides. We concentrate in this report on the solid solutions $(U_{1-x}Np_x)O_2$, all with the simple cubic CaF_2 crystal structure and which have been studied for many years. The phenomena found at 25 K in NpO_2 (x = 1) is that the 5*f* charge distribution develops an anisotropic component that exhibits long-range ordering at T_o = 25 K. This is known as the ordering of the charge quadrupoles.

The experiments, carried out on beamline ID20, consist of tuning the photon energy to the actinide *M* absorption edge (at which photon energy core 3*d* electrons are promoted to the partially occupied 5*f* valence states), and then, once the repeat (wavevector) of the anisotropic charge distribution is known, one measures the azimuthal distribution of the scattered resonant X-ray intensity. This intensity distribution is related to the symmetry of the 5*f* anisotropic charge. The experiments were performed on single crystals prepared and mounted at the Institute of Transuranium Elements in Karlsruhe, Germany.

NpO_2 has pure quadrupole ordering, with no measurable dipole moment. In 2003 experiments were performed on a single crystal with x = 0.25 [2]. Dipole ordering was found on both the U and Np ions, and quadrupolar ordering was also found associated with both ions. However, these were different from those in pure NpO_2. Whereas a longitudinal configuration was found for x = 1 (NpO_2), the x = 0.25 sample was found to have a transverse configuration. The difference between these configurations is shown in **Figure 123**.

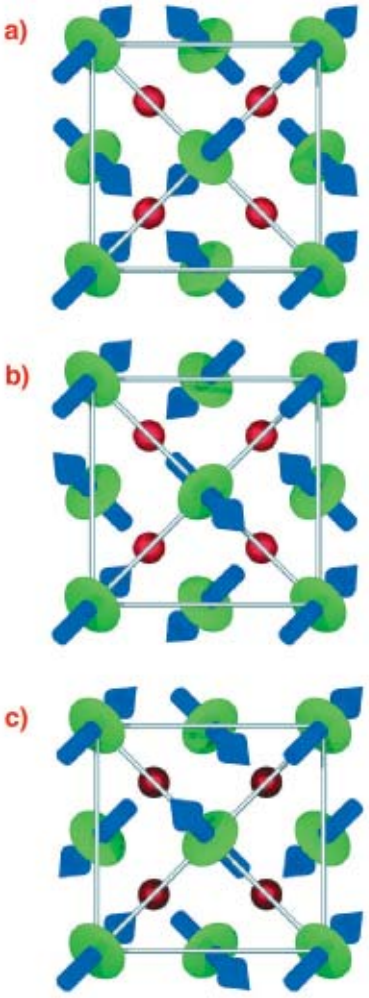

Fig. 123: Schematic representation of triple-*k* magnetic and electric-quadrupole ordering within the *a*-*b* plane for the single longitudinal (a) and two transverse (b,c) modes. The magnetic (dipole) moments are represented by blue arrows whereas the electric-quadrupole moments are shown as the green ellipsoids. The red spheres represent oxygen atoms.

The understanding of these different configurations then allowed an experiment to be performed in 2004 on a single crystal of UO_2 (x = 0). The azimuthal dependence of the intensity from the (112) reflection in UO_2 is shown in **Figure 124**, together with the predictions for a transverse configuration. Shown also in **Figure 124** is the temperature dependence of both the magnetic dipole, electric-quadrupole and the internal distortion of the oxygen cage. The complication in UO_2 is that both dipole ordering and an internal distortion of the oxygen atoms due to the quadrupole ordering are present; these have contrived to make it difficult to observe the quadrupole ordering in UO_2 directly, although such ordering was predicted almost 40 years ago [3], and the oxygen displacements reported 30 years ago [4].

These experiments also suggest a qualitative explanation of the unusual behaviour [5] of the mixed oxides with 0.40 < x < 0.80. In this region there is