MS26 Incommensurate modulated and composite phases

Chairs: Michal Dusek, Artem Abakumov

MS26-O1 Incommensurate charge order and charge-density waves

Sander van Smaalen[1]

1. University of Bayreuth, Laboratory of Crystallography

email: smash@uni-bayreuth.de

Charge order is an important phenomenon in functional materials. For example, in doped manganites, Mn^{3+}/Mn^{4+} charge order is intimately connected with the colossal magnetoresistance effect [1]. In magnetite (Fe_3O_4), low-temperature Fe^{2+}/Fe^{3+} charge order has been shown to involve a pattern of trimerons Fe^{3+}—Fe^{2+}—Fe^{3+} and isolated Fe^{2+} in a supercell of the cubic spinel structure type of magnetite [2]. Several types of interactions may drive a material into the charge-order state. On the other hand, a charge-density wave (CDW) was originally believed to occur exclusively by the Peierls mechanism in so-called quasi-one-dimensional (1D) electronic crystals containing weakly interacting metallic chains. Nesting by a single **q** vector of flat, co-planar portions of the Fermi surface drive the system into a charge-modulated state with wave vector **q**, which is generally incommensurate to the crystal lattice [3]. The CDW is intrinsically coupled to a periodic lattice distortion (PLD) of the same period, which can easily be measured by diffraction techniques. This simple interpretation of the CDW state has recently been questioned, and the role of electron-phonon interactions has been stressed. Alternative mechanisms will be required for so-called strongly coupled CDW systems, which lack an obvious anisotropy of their metallic electrical conductivity, like $RNiC_2$, $R_5Ir_4Si_{10}$, $R_2Ir_3Si_5$ and CuV_2S_4 (R = rare earth element) [4,5]. Here, I will discuss the crystallography of charge-ordered and CDW systems, with particular emphasis on the consequences of aperiodic crystal structures for understanding the ordered states.

Literature

[1] C. Sen, G. Alvarez & E. Dagotto, Phys. Rev. Lett. **98,** 127202 (2007). Competing Ferromagnetic and Charge-Ordered States in Models for Manganites: The Origin of the Colossal Magnetoresistance Effect.

[2] M. S. Senn, J. P. Wright & J. P. Attfield, Nature **481**, 173 (2012). Charge order and three-site distortions in the Verwey structure of magnetite.

[3] S. van Smaalen, Acta Cryst. A **61**, 51-61 (2005). The Peierls transition in low-dimensional electronic crystals.

[4] A. Wölfel, Liang Li, S. Shimomura, H. Onodera & S. van Smaalen, Phys. Rev. B 82, 054120 (2010). Commensurate charge-density wave with frustrated interchain coupling in $SmNiC_2$.

[5] S. Kawaguchi, H. Ishibashi, N. Tsuji, J. Kim, K. Kato, M. Takata & Y. Kubota, J. Phys. Soc. Jpn **82**, 064603 (2013). Structural Properties in Incommensurately Modulated Spinel Compound CuV_2S_4.

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