

# Oral Contributions

## [MS36] Twinning, polytypes and modular structures

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[MS36-01] New modular oxide structures through the use of lone pair cations as “chemical scissors” J.Hadermann, M. Batuk, D. Batuk, A.M. Abakumov

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Lone pair cations, such as Bi or Pb have a flexible coordination environment that enables them to operate as “chemical scissors”. Their flexibility reduces the strain that would otherwise be present at the interfaces separating structure modules. This was shown by Mayerova et al. to allow separating ionic and covalent parts. [1]. However, we have found that in complex oxides it also allows many other variants of interfaces, as for example to introduce crystallographic shear planes or (non)conservative twin planes in structures, enabling the synthesis of new structural families. As a first example, this concept allowed the introduction of crystallographic shear planes into the perovskite structure, a feat that was considered highly unlikely before. In turn this allowed the generation of a new anion deficient perovskite based homologous series  $A_nB_nO_{3n-2}$  ( $n = 4-6$ ). An interesting feature about this series is the magnetic frustration at the crystallographic shear plane separating the perovskite blocks, due to competing FM and AFM interactions. [2]

Also incommensurately modulated perovskites can be obtained, for example  $(Pb,Bi)_{1-x}Fe_{1+x}O_{3-y}$ . These arise by  $3+ 2+$  replacing Bi with Pb, which introduces an oxygen deficiency, which is then accommodated by periodically spaced CS planes to reduce the coordination of the A-cations at the interface. The flexible coordination  $3+ 2+$  environment of

Bi and Pb makes them ideally suited for these A cation positions. [3]

Another possibility was encountered in  $BiMnFe_2O_6$ . In this compound the  $Bi^{3+}$  induces the existence of a non-conservative twin plane. The result is a new structure type with hcp structured modules. [4]

[1] Z. Mayerova et al, *Angew. Chem.*, 2006, 45, 5602

[2] J. Hadermann et al. *Journal of Solid State Chemistry* 183, 2190–2195 (2010); S. Turner et al, *Applied Physics Letters* 101, 241910 (2012); E. Korneychik et al. *Journal of Solid State Chemistry* 184, 3150–3157 (2011); D. Batuk et al. *Inorganic chemistry* 50, 4978–86 (2011); A.M. Abakumov et al. *Inorganic chemistry* 49, 9508–16 (2010); I.V. Nikolaev et al. *Phys. Rev. B*, 78:2 (2008) p. 024426, 1-12; A.M. Abakumov et al. *Journal of the American Ceramic Society* 91,6 (2008) 1807–1813; J. Hadermann et al. *Solid State Sciences* 10, 4 (2008) 382-389; A.M. Abakumov et al. *Angewandte Chemie International Edition*, Volume 45, Issue 40 (2006) 6697-6700.

[3] W. Dachraoui et al.. *Chemistry of Materials* 24, 1378–1385 (2012), A.M. Abakumov et al. *Chemistry of Materials* 23, 255–265 (2011); C. Lepoittevin et al. *Inorganic chemistry* 48, 8257–62 (2009).

[4] Tao Yang et al. *Chemical Science* 1, 751 (2010).

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