MAGNETIC STRUCTURE AT PEROVSKITE/ANTIPEROVSKITE INTERFACE

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ABSTRACT

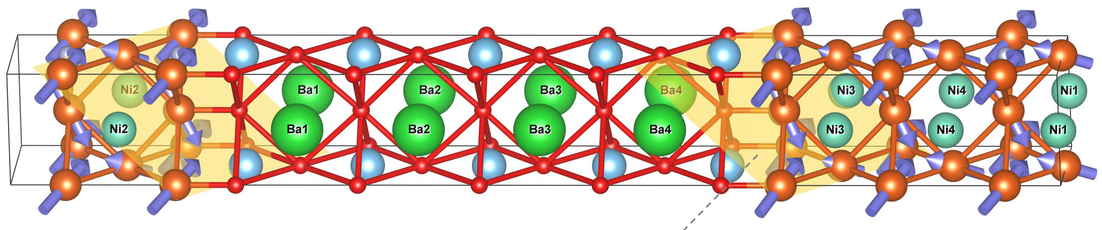
Mn-based antiperovskite nitrides with a formula unit $ANMn_3$ (A = Ga, Sn, In, Ni, Zn,…) show potential for a wide range of applications including spintronics [1,2,3] and solid-state cooling [4,5,6]. The functionality is mainly derived from the frustrated exchange interactions in the triangular antiferromagnetic (AF) structure and its response to symmetry lowering caused by biaxial strain [3,5] or by an adjacent layer with ferroelectric polarization [7].

Using density functional theory (DFT) and linear response approximation of the permittivity tensor as implemented in the VASP package we simulate the non-collinear magnetic structure in a thin film of $NiNMn_3$ and $SnNMn_3$ deposited on ferroelectric perovskite $BaTiO_3$. We find local deviations from the triangular magnetic order of the bulk system. Following predictions of magneto-optical Kerr effect (MOKE) in bulk antiperovskite nitrides [8], we simulate the MOKE spectra of bulk $NiNMn_3$ and $SnNMn_3$ assuming the magnetic structure obtained for the $A_3NiN/BaTiO_3$ bilayer earlier. Our results can be compared directly with measured MOKE data in order to identify the desirable magnetic structure in thin film samples.

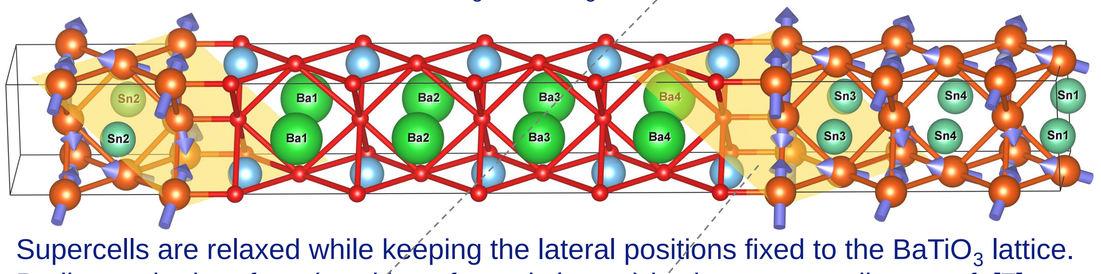
FRUSTRATED MAGNETIC MOMENTS AT INTREFACES

Frustration of Mn-Mn exchange interactions can be relieved by application of biaxial strain to bulk structure or by electric field at interfaces – both lower symmetry of the cubic lattice. We consider the following bilayers (periodic boundary conditions):

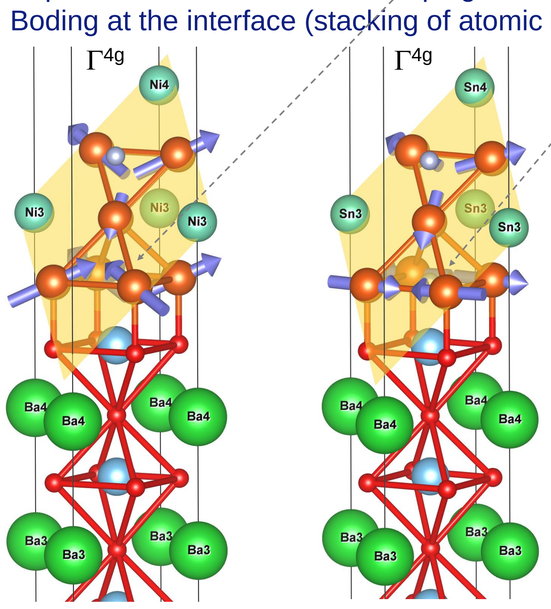
$NiNMn_3 / BaTiO_3$

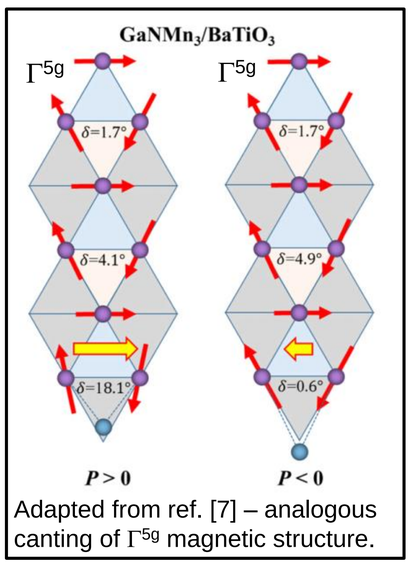


$SnNMn_3 / BaTiO_3$



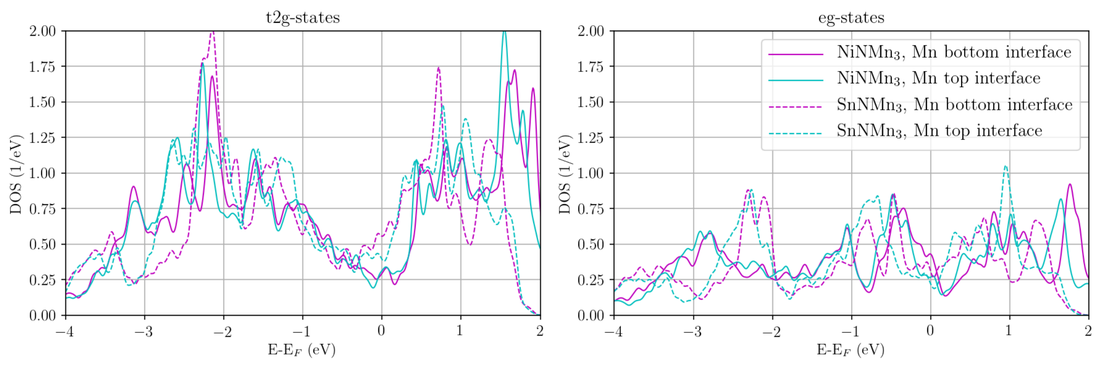
Supercells are relaxed while keeping the lateral positions fixed to the $BaTiO_3$ lattice. Boding at the interface (stacking of atomic layers) is chosen according to ref. [7].





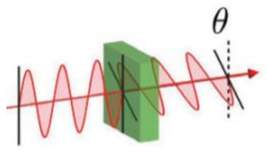
Adapted from ref. [7] – analogous canting of Γ^{5g} magnetic structure.

Note the significant canting at right interface in case of $SnNMn_3$ and significant change of size of the central Mn in case of $NiNMn_3$. This has impact on the density of states:



MAGNETO-OPTICAL KERR EFFECT IN BULK ANTIPEROVSKITES

We focus on the polar Kerr effect (rotation of the plane of linearly polarized light) caused by the reduction of symmetry of the paramagnetic state due to the magnetic ordering.
We calculate the Kerr angle from the dielectric tensor assuming the form below as in ref. [8]:



$$\theta + i\eta \approx \frac{-\varepsilon_{xy}}{(\varepsilon_0 - 1)\sqrt{\varepsilon_0}} \qquad \boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & 0 \\ -\varepsilon_{xy} & \varepsilon_{yy} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix}$$

$$\varepsilon_0 = (\varepsilon_{xx} + \varepsilon_{yy})/2$$

SIMULATION METHOD

The imaginary part of the dielectric tensor are determined by a summation over empty states using the Projector-Augmented Wave method (PAW) and linear response theory [9]:

$$\varepsilon^{(2)}_{\alpha\beta}(\omega) = \frac{4\pi^2 e^2}{\Omega} \lim_{q\to 0} \frac{1}{q^2} \sum_{c,v,\mathbf{k}} 2w_{\mathbf{k}} \delta(\varepsilon_{c\mathbf{k}} - \varepsilon_{v\mathbf{k}} - \omega) \times \langle u_{c\mathbf{k}+\mathbf{e}_\alpha \mathbf{q}} | u_{v\mathbf{k}} \rangle \langle u_{c\mathbf{k}+\mathbf{e}_\beta \mathbf{q}} | u_{v\mathbf{k}} \rangle^*$$

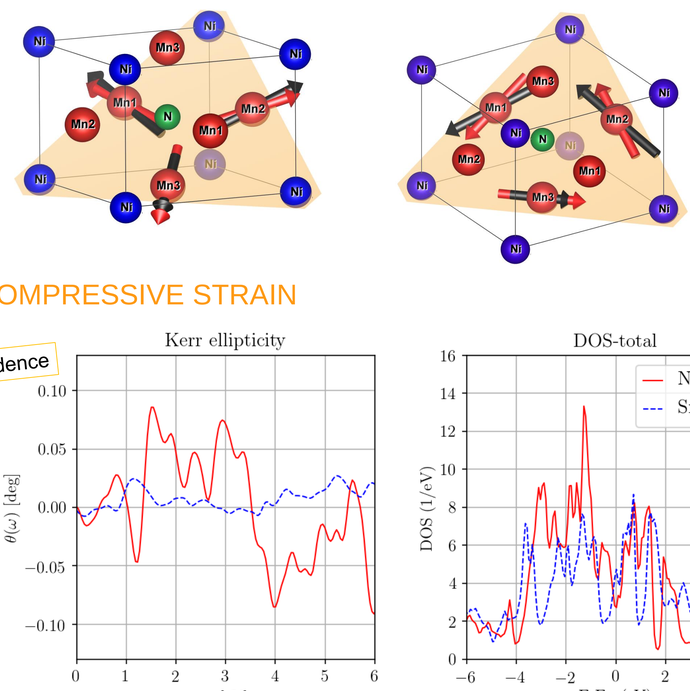
The real part of the dielectric tensor is obtained by Kramers-Kronig transformation:

$$\varepsilon^{(1)}_{\alpha\beta}(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\varepsilon^{(2)}_{\alpha\beta}(\omega')\omega'}{\omega'^2 - \omega^2 + i\eta} d\omega'$$

Spin-orbit coupling has to be included to obtain non-zero off-diagonal elements of the dielectric tensor. A large plane-wave energy cutoff of 500 eV and a Monkhorst-Pack k-point mesh of 20×20×20 were used in the PAW-PBE simulation [9].

MOKE spectrum vanishes in bulk $ANMn_3$ with the Γ^{5g} magnetic structure. In the interface study we assumed canted Γ^{4g} structure which gives finite MOKE. However, Γ^{5g} is the ground state of bulk $SnNMn_3$. The canting induced by biaxial strain is analogous to Γ^{4g} as shown below.

Tensor form of σ_{ij} obtained using bitbucket.org/zeleznyj/linear-response-symmetry (Jakub Železný)	Γ^{4g}	Γ^{5g}
Cubic lattice	$\begin{bmatrix} 0 & a & -a \\ -a & 0 & a \\ a & -a & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
Strained lattice (canting)	$\begin{bmatrix} 0 & a & -b \\ -a & 0 & b \\ b & -b & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & a \\ 0 & 0 & a \\ -a & -a & 0 \end{bmatrix}$



RESULTS FOR BULK WITH COMPRESSIVE STRAIN

$NiNMn_3$ and $SnNMn_3$ spectra differ significantly. The latter can be detected despite the Γ^{5g} representation when subject to strain and the incident beam is not normal to the surface.

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