Multiferroics

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March 13, 2008

Outline

What are multiferroics?

- Materials that manifest both ferroelectricity and ferromagnetism.
- ???

What are ferroelectrics?

- Materials that show instantaneous electric dipole moment.
- Used in capacitors and computer memories.
- Derives from the fact that electrons posses charge.
- E.g. perovskite structured oxides such as $PbTiO_3$ and $BaTiO_3$.

Perovskite Structure

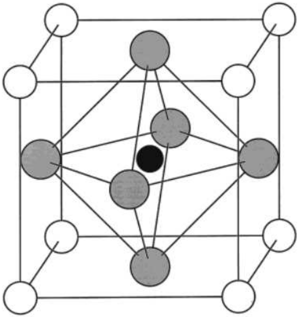

Figure: Cubic perovskite structure. The white circles at the corners represent A, grey circles represent O and black circle represents B.

Ferroelectricity

- Above T_c: a normal dielectric. Below T_c: spontaneous polarization.
- Below T_c there is a structural distortion which moves cation B slightly away from the center of the octahedral cage.
- There is competition between Coulomb repulsion between atoms and bonding consideration due to hybridization of orbitals.
- At high temperatures, the Coulomb repulsion dominates.
- Below the transition temperature, forces associated with stabilization of polarized bonding dominate.

What are ferromagnets?

- Materials that possess instantaneous dipole magnetic moment.
- The usual magnets. Also used in computer memories.
- Derives from the fact that electrons posses spin.
- E.g. Fe, Co, Ni, MnSb, MnAs.

Ferromagnetism

- Above T_c the dipole moments of atoms are arranged haphazardly.
- Below T_c the dipole moments of atoms arrange themselves in the same direction causing spontaneous magnetism.
- The dipole moment in the atom is caused by the spin of electrons in partially filled orbitals.

Curie-Weiss theory of ferromagnetism

- Exchange energy favours electrons with parallel spins.
- Above T_c, thermal energy is larger than exchange energy.
- Explains ferromagnetism in most materials but fails to predict correct magnetic moment per atom.
- Also incorrectly predicts magnetic moment in each atom to be the same in both ferromagnetic and paramagnetic case.

Stoner theory of ferromagnetism

- The difference between adjacent band energies compete with exchange energy.
- Exchange energy favours one band to be occupied with electrons of only one type of spin.

Stoner theory of ferromagnetism

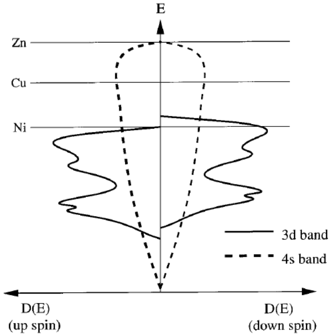

Figure: 3d and 4s up- and down-spin densities of states in some transition metals

Multiferroics

- Materials that show both spontaneous electric dipole moment and magnetic dipole moment.
- Could be used in multistate data storage or novel memory media which allows simultaneous reading and writing of data.
- Unfortunately very few multiferroic materials.
- E.g. $BiFeO_3$, $Pb(Fe_{\frac{1}{2}}Nb_{\frac{1}{2}})O_3$, $YbMnO_3$, etc.

Limiting factors in simultaneous existence of ferroelectricity and ferromagnetism

- *Symmetry* There are thirteen point groups that allow both ferroelectricity and ferromagnetism.
- *Electrical Properties* Ferroelectric materials must be insulators. Ferromagnets are are often metallic.
- *Chemistry* Ferroelectric materials have ions in a d^0 state. Ferromagnets have partially filled d orbitals.

Why so few multiferroics?

- Insulators vs. metallic
- d orbital status
- Perhaps ions with partially filled d orbitals are simply too large to move away?

Multiferroic $BiMnO_3$

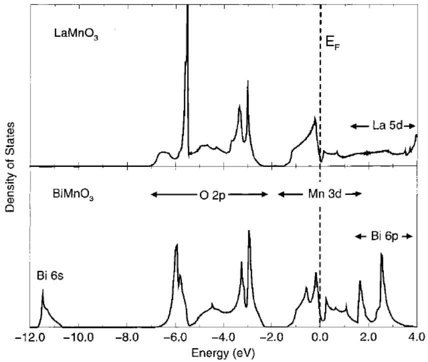

Figure: Density of states for cubic paramagnetic $LaMnO_3$ and $BiMnO_3$.

Multiferroic $BiMnO_3$

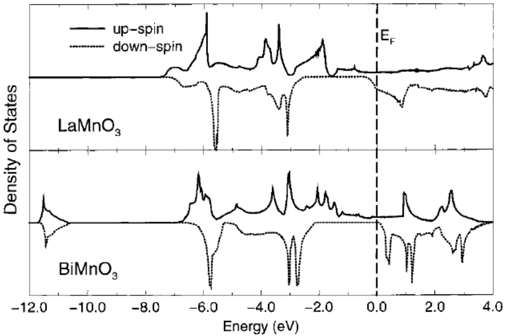

Figure: Density of states for cubic ferromagnetic $LaMnO_3$ and $BiMnO_3$.

Multiferroic $BiMnO_3$

Table: Eigenvectors and eigenvalues of the dynamical matrix that correspond to the unstable phonon modes in cubic paramagnetic $BiMnO_3$ and $LaMnO_3$.

Material	ν (cm^{-1})	Bi	Mn	Oz	Ox	Oy
$BiMnO_3$	$72.39i$	0.0	0.0	0.0	$-1/\sqrt{2}$	$1/\sqrt{2}$
$BiMnO_3$	$98.20i$	-0.43	0.09	0.16	0.62	0.62
$LaMnO_3$	$49.04i$	0.0	0.0	0.0	$-1/\sqrt{2}$	$1/\sqrt{2}$
$LaMnO_3$	$44.69i$	-0.59	0.22	0.21	0.53	0.53

Conclusions

- Multiferroics are materials that show spontaneous electric and magnetic polarization.
- The scarcity can be explained by the fact ferroelectricity and ferromagnetism compete with each other.
- In some materials these competing factors can be balanced such that it shows both electric and magnetic properties.