Multiferroics

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March 13, 2008
Outline

1. Introduction
2. Ferroelectricity
3. Ferromagnetism
4. Multiferroics
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 possess 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

- 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 possess spin.
- E.g. Fe, Co, Ni, MnSb, MnAs.
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 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$_3$.

<table>
<thead>
<tr>
<th>Material</th>
<th>$\nu$ (cm$^{-1}$)</th>
<th>Bi</th>
<th>Mn</th>
<th>Oz</th>
<th>Ox</th>
<th>Oy</th>
</tr>
</thead>
<tbody>
<tr>
<td>BiMnO$_3$</td>
<td>72.39i</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>-1/\sqrt{2}</td>
<td>1/\sqrt{2}</td>
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<tr>
<td>BiMnO$_3$</td>
<td>98.20i</td>
<td>-0.43</td>
<td>0.09</td>
<td>0.16</td>
<td>0.62</td>
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<tr>
<td>LaMnO$_3$</td>
<td>49.04i</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>-1/\sqrt{2}</td>
<td>1/\sqrt{2}</td>
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<tr>
<td>LaMnO$_3$</td>
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<td>-0.59</td>
<td>0.22</td>
<td>0.21</td>
<td>0.53</td>
<td>0.53</td>
</tr>
</tbody>
</table>
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.