Effect of Structural Disorder on Magnetic Properties of MnCrVAl

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Atomic disorder induced modification of magnetization in MnCrVAl

Motivation and Methods

✓ Research on magnetic materials for potential applications in spin-based electronics is one of the most active fields of current study in both academia and industry.
✓ High degree of spin polarization in electron transport – wanted in spintronics.
✓ Spintronics – an emerging technology utilizing a spin degree of freedom in electronic devices.
✓ There are various mechanisms which could potentially alter the degree of transport spin polarization, such as mechanical strain, structural disorder, temperature, termination surface/interface in thin film multilayer geometry, etc.
✓ The main purpose of this work is to investigate effect of atomic disorder on magnetic properties of MnCrVAl, a material which recently attracted attention as a potential spin-gapless semiconductor.
✓ Spin-gapless semiconductors are recently discovered materials which are characterized by a zero band gap in one spin channel and by a finite band gap in the other channel.
✓ Here, we employ density functional calculations to explore effect of atomic disorder on magnetic properties of Heusler compound, MnCrVAl.
✓ Vienna Ab Initio Simulation Package (VASP).
✓ Computations performed at the Department of Physics computing facilities (20-node Beowulf cluster), UNI.

Crystal and electronic structure of MnCrVAl

Various crystal structures of disordered MnCrVAl.

Calculated magnetic moments

<table>
<thead>
<tr>
<th>Lattice (a/b/c)</th>
<th>Mn1</th>
<th>Mn2,3,4</th>
<th>Cr1</th>
<th>Cr2,3,4</th>
<th>V1</th>
<th>V2,3,4</th>
<th>Al1</th>
<th>Al2,3,4</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ideal</td>
<td>5.90/5.90/5.90</td>
<td>1.776</td>
<td>1.776</td>
<td>2.077</td>
<td>-0.943</td>
<td>-0.943</td>
<td>-0.007</td>
<td>-0.007</td>
<td>11.610</td>
</tr>
<tr>
<td>Mn1-A11</td>
<td>5.88/5.85/5.88</td>
<td>-1.741</td>
<td>1.632</td>
<td>1.189</td>
<td>1.716</td>
<td>-1.007</td>
<td>-0.864</td>
<td>-0.018</td>
<td>-0.012</td>
</tr>
<tr>
<td>Mn1-V1</td>
<td>5.91/5.91/5.91</td>
<td>-2.204</td>
<td>1.950</td>
<td>2.021</td>
<td>1.975</td>
<td>0.961</td>
<td>-0.901</td>
<td>-0.003</td>
<td>0.010</td>
</tr>
<tr>
<td>Mn2-A21</td>
<td>5.84/5.77/5.84</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>Mn2-V2</td>
<td>6.04/5.73/5.73</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>Cr1-Al1</td>
<td>5.87/5.87/5.87</td>
<td>1.122</td>
<td>1.694</td>
<td>-1.359</td>
<td>1.600</td>
<td>-1.077</td>
<td>-0.837</td>
<td>-0.030</td>
<td>-0.013</td>
</tr>
<tr>
<td>Cr1-V1</td>
<td>5.90/5.87/5.87</td>
<td>1.911</td>
<td>1.836</td>
<td>-1.303</td>
<td>2.105</td>
<td>1.558</td>
<td>-0.891</td>
<td>-0.005</td>
<td>0.008</td>
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<tr>
<td>Cr2-Al2</td>
<td>5.78/5.78/5.91</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>Cr2-V2</td>
<td>5.91/5.90/5.91</td>
<td>-0.522</td>
<td>1.558</td>
<td>-0.528</td>
<td>-0.528</td>
<td>-0.357</td>
<td>-0.523</td>
<td>0.005</td>
<td>0.010</td>
</tr>
</tbody>
</table>

Calculated magnetic moments (in units of $\mu_B$) and lattice constant (in Å) of MnCrVAl in ordered and disordered states.
✓ In completely ordered structure, MnCrVAl exhibits net magnetic moment of ~3.0 $\mu_B$/f.u.
✓ Recent experimental work showed that MnCrVAl samples demonstrate close to zero net magnetization.
✓ XRD measurements indicated a significant degree of atomic disorder in the samples
✓ Magnetization quenching is induced by atomic disorder.

Electronic structure

✓ Spin- and atom- resolved densities of states (DOS).
✓ Spin-flip transition if 25% Mn/Cr atoms interchanged with V/Al.
✓ Paramagnetic transition if 50% Mn/Cr atoms interchanged with V/Al.
✓ Cr1-Al1 disorder results in nearly half-metallic transition.
✓ Paramagnetic transition accompanied by tetragonal distortion.

Summary

✓ We analyzed physical mechanism of magnetization reduction in MnCrVAl: potential spin-gapless semiconductor.
✓ Various atomic disorder schemes are studied.
✓ Depending on the degree of disorder, exchanging of atomic positions between Mn / Cr with V / Al results in either reduced total magnetization due to spin flip, or in ferrimagnetic – paramagnetic transition.
✓ In certain disordered structures the spin polarization of MnCrVAl significantly increases, almost reaching the half-metallic state.
✓ Exchange of atomic positions of Mn with Cr, and V with Al has no significant effect on electronic and magnetic properties of MnCrVAl.
✓ These findings may have important contribution to understanding the role of atomic disorder on magnetic properties of materials with potential applications in spin-based electronics.