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Effect of Structural Disorder on Magnetic Properties of MnCrVAl

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Atomic disorder induced modification of magnetization in MnCrVAl

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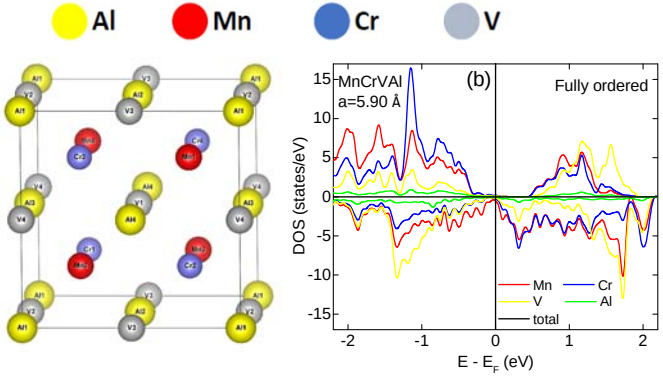
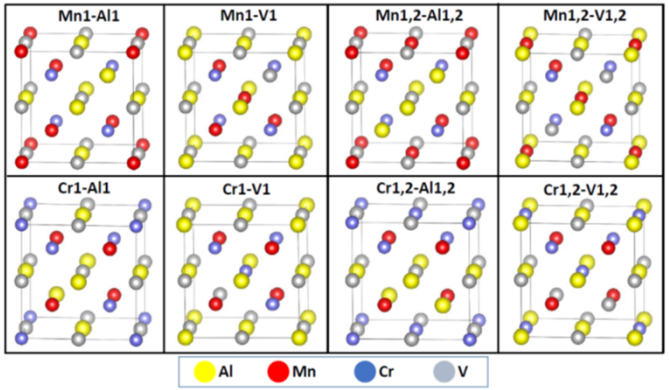
Motivation and Methods

- ✓ 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



Atomic disorder



Various crystal structures of disordered MnCrVAl.

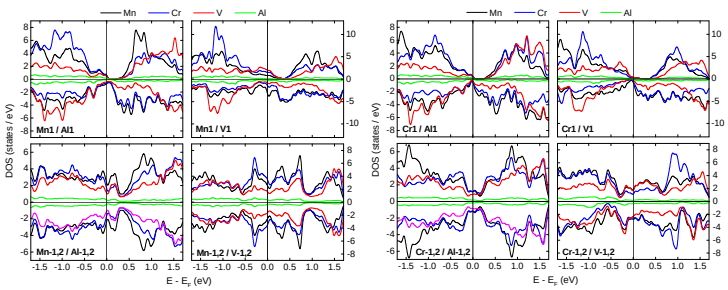
Calculated magnetic moments

	Lattice (a/b/c)	Mn1	Mn2,3,4	Cr1	Cr2,3,4	V1	V2,3,4	Al1	Al2,3,4	Total
Ideal	5.90/5.90/5.90	1.776	1.776	2.077	2.077	-0.943	-0.943	-0.007	-0.007	11.610
Mn1-Al1	5.88/5.88/5.88	-1.741	1.632	1.189	1.716	-1.007	-0.864	-0.018	-0.012	5.840
Mn1-V1	5.91/5.91/5.91	-2.204	1.950	2.021	1.975	0.961	-0.901	-0.003	0.010	9.880
Mn2-Al2	5.84/5.77/5.84	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Mn2-V2	6.04/5.73/5.73	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Cr1-Al1	5.87/5.875.87	1.122	1.694	-1.359	1.600	-1.077	-0.837	-0.030	-0.013	5.99
Cr1-V1	5.90/5.87/5.87	1.911	1.836	-1.303	2.105	1.558	-0.891	-0.005	0.008	11.34
Cr2-Al2	5.78/5.78/5.91	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Cr2-V2	5.91/5.90/5.91	-0.522	1.558	-0.528	-0.528	-0.357	-0.523	0.005	0.010	
			1.558		1.691		-0.329		0.010	1.88
			-1.530		1.691		-0.329		0.005	

Calculated magnetic moments (in units of μ_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 μ_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.

✓ P. Kharel, J. Herran, P. Lukashev, Y. Jin, J. Waybright, S. Gilbert, B. Staten, P. Gray, S. Valloppilly, Y. Huh, and D. J. Sellmyer, AIP Advances **7**, 056402 (2017).