Co_2MnGe-Cr Multilayers: Cr as an Antiferromagnetic Half-Metal

M. Williams[1], M. Chshiev[2], C.A. Culbert[2], W.H. Butler[2]

[1]University of Maryland Eastern Shore, [2]MINT Center, The University of Alabama

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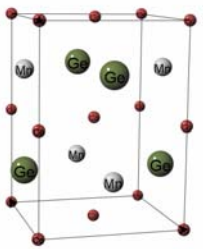
Abstract

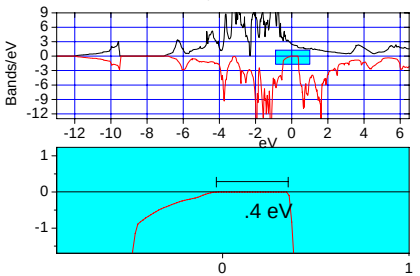
Full Heusler alloys of composition X_2YZ and structure type $L2_1$ have aroused considerable interest for application as electrodes for readers in future hard disk drives because many of them are half-metals. The X and Y elements are typically transition metals, the Z element is typically a non-transition metal. The structure of these alloys can be viewed as a variant of bcc in which (100) atomic layers of X alternate with layers of YZ. As part of a study of possible spacer layers for Heusler alloys, we have investigated the Heusler alloy Co_2MnGe with Cr spacer layers by calculating the electronic and magnetic structure of supercells consisting of five (four) atomic (100) layers (2 atoms per layer) of Co_2MnGe alternating with one (two) atomic layers of Chromium. The calculations used the VASP code with PAW pseudopotentials and the generalized gradient approximation to DFT.

Co_2MnGe

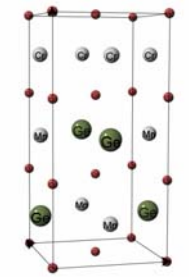


By itself, Co_2MnGe is already a half-metallic ferromagnet, having a gap at the Fermi energy of approximately 0.4 electron volts.

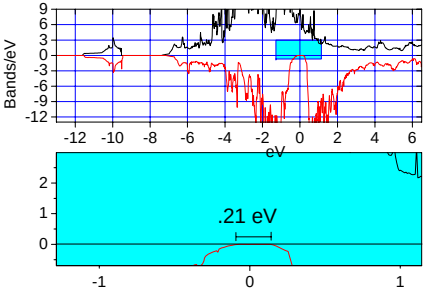
Density of States



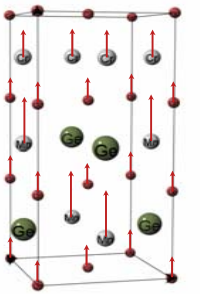
Five layers of Co_2MnGe alternating with 1 layer of Chromium between Cobalt



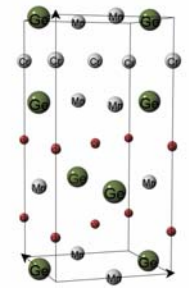
A single layer of Chromium between Cobalt layers decreases the length of the energy gap from that of the pure Heusler



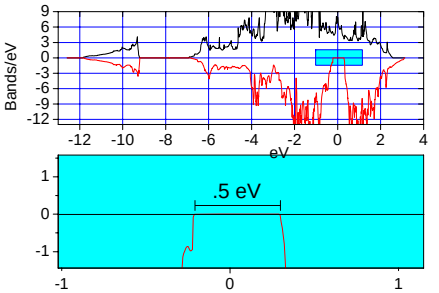
When adjacent to Cobalt, the magnetic moments of the Chromium atoms align parallel to those in the Heusler



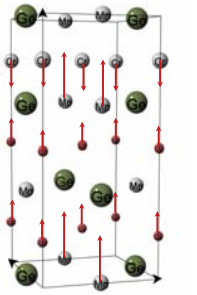
Five layers of Co_2MnGe alternating with 1 layer of Chromium between GeMn



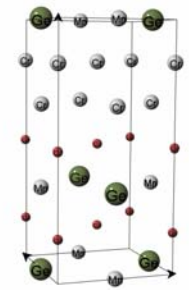
A single layer of Chromium between Germanium & Manganese layers increases the length of the energy gap from that of the pure Heusler



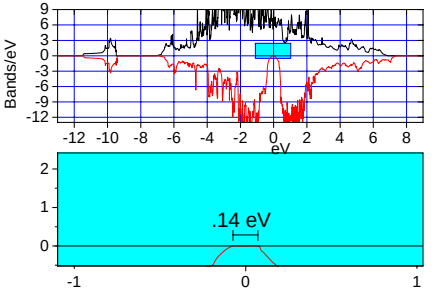
When adjacent to GeMn, the magnetic moments of the Chromium atoms align anti-parallel to those in the Heusler



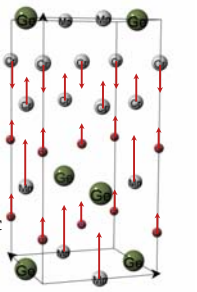
Four layers of Co_2MnGe alternating with 2 layers of Chromium



Two layers of Chromium decreases the length of the energy gap from that of the pure Heusler



When adjacent to both Co and GeMn, the Chromium layers are anti-parallel to each other, forming an antiferromagnetic half-metal



For more information contact:
Christopher Culbert
cculbert@mint.ua.edu