Electronic and Magnetic Properties of MnGe

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Abstract: We investigate the properties of MnGe in the B20 structure under pressure using density functional theory. We show that MnGe is magnetic at ambient pressure. Results for the electronic structure, density of states, and Fermi surface are presented for the zero pressure phase.

Keywords: Transition metal germanide, B20 structure, correlated electrons

1. Introduction

Strong electron-electron interactions are essential to producing the novel electronic properties needed for materials designed in next generation computing and energy storage and transmission. These interactions are responsible for novel magnetic behavior and high temperature superconductivity[1]. It has also been realized that the underlying atomic symmetry of the material strongly affects the kinds of novel magnetic or electronic order that may appear, as well as transitions between ordered phases[2, 3]. A common experimental approach is to find a class of materials of similar structure but different electron densities to probe the nature of the interactions. The variation in density is achieved by substitution of similar elements, which also allows a kind of "chemical pressure" to be applied since the lattice constant will also vary.

MnGe is representative of a class of transition metal (Mn, Fe, Co, Cr, Ru, Rh, Os, Ir) germanides and silicides that can all form in the B20 structure. The B20 structure is a cubic structure with a rather low internal symmetry, with 4 transition metals atoms occupying sites forming a tetrahedron aligned along the (111) direction, with the 4 nonmetals positioned on an tetrahedron inverted relative to the TM atoms. As a result, there is neither 4-fold rotation symmetry nor inversion symmetry in the lattice. The d-orbitals on the transition metal are localized, providing the strong interactions. This allows us to study the effect of chirality on the properties of materials, which is usually only studied in the context of organic molecules. The electronic density of states for these materials are all rather similar, and by chemical substitution at the transition metal or Ge/Si site, it is possible to vary the electron density and lattice constant in a controlled fashion.
In this work we will calculate the electronic properties of MnGe using a density functional approach. This is part of a computational-experimental collaboration with Dr. DiTusa's group as part of the LA-SiGMA program. While this method is a clear approximation in terms of the electron interactions in the strongly localized d-orbitals, it provides a very useful first

approximation to understanding the role the interactions play. By comparing these results with experiment, we can identify where the electronic interactions are significant and where they play a minor role. We will study this material in a variety of conditions, varying the lattice constant as might be accomplished with alloying to examine the possible ground states and provide a battery of quantities to be examined experimentally.

2. Calculations

We use the standard WIEN2K all-electron DFT package[4], which uses a LAPW basis including local orbitals. We have chosen for our study to use the Perdew-Wang GGA functional[5], which provides a significant improvement over LDA in terms of bond lengths and other properties. It is also considered to be a good choice for systems of moderate interaction. We used muffin tin radii of 2.34 $a.u.$ for Mn and 2.23 $a.u.$ for Ge. In the B20 structure (Wyckoff #198, $P2_13$), the atoms are at (u,u,u), $(½-u,1-u,½+u)$, $(1-u,½+u,½-u)$ and $(½+u,½-u,1-u)$, with $u=0.135$ for Mn and $u=0.842$ for Ge. These values are close to the experimental positions, but in our calculations we found the residual forces at these positions to be less than $0.01\,Ryd/au$. In the calculations, the plane wave cutoff $R*K_{max}$ was varied from 7.0 to 9.0 to ensure the basis set and energies had converged. For most of the calculations, we employed a grid of 19x19x19 k-points for Brilluoin zone integrations (340 points in the irreducible zone). For Fermi surface calculations we used a much denser 31x31x31 grid. While the observed ground state of this material is a helimagnet, the pitch of the helimagnetic order is much larger than the unit cell size, so we have done our magnetic calculations assuming a uniform ferromagnetic state[6, 7].

3. Results

In Figure 1 we show the total energy and total magnetic moment of possible magnetic and nonmagnetic ground states for a range of lattice constants. The experimental lattice constant is 4.795 Å. From the data we see that a magnetic ground state is preferred at the experimental lattice constant, and until the lattice constant is reduced to 4.46 Å. The calculated Bulk Modulus is $238\,GPa$.

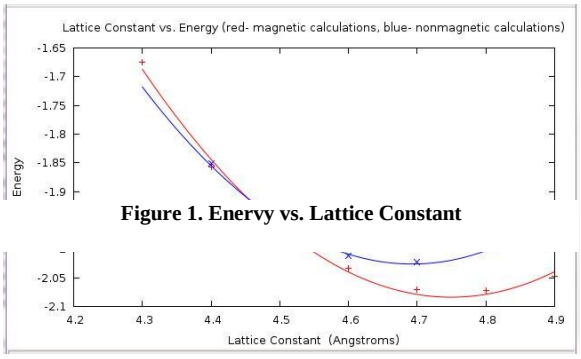

Figure 1. Enervy vs. Lattice Constant

In all of these B20 materials, the states within 5 eV of the Fermi energy are predominately derived from the Mn d-orbitals. We show in Figure 2 the total DOS for the magnetic ground state with its contributions from Mn and Ge separately delineated. While the shape of the density of states is different in the nonmagnetic case, the DOS character remains the same. One notable feature that also shows up in both the magnetic and nonmagnetic DOS is the appearance of pseudogaps in the density of states (here at about 2 eV above the Fermi level). These features, resulting from d-band splitting by the low symmetry of the crystal field, are seen in almost all DOS of these TM silicides and germanides.

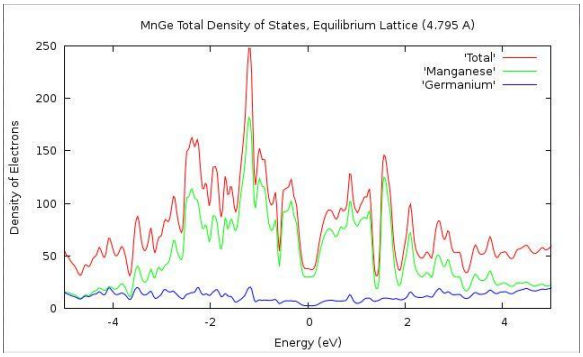

Figure 2. DOS contributions of Mn and Ge to the total

We conclude with a presentation of the electronic bands and Fermi surface sheets at the equilibrium lattice constant. The band structure is shown in Figure 3 for the two spin orientations.

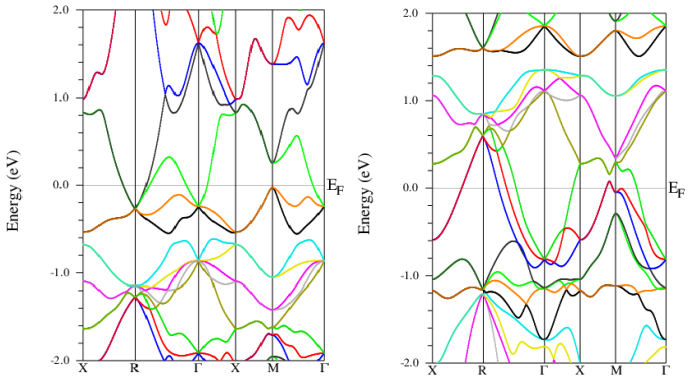

Figure 3. (a) Up spin, left, and (b) down spin, right, bands at the equilibrium lattice spacing

The two spin up bands give pockets of electrons, one centered at Γ and two centered at R. The pockets are not very spherical, having a significant octahedral distortion which is not surprising given the low site symmetry in this structure. These are shown in Figures 4(a) and 4(b) below. The three spin down bands give rise to a hole-like spherical pocket around R, shown in Fig 4(c), and two extended surfaces, shown in Figures 4(d) and 4(e).

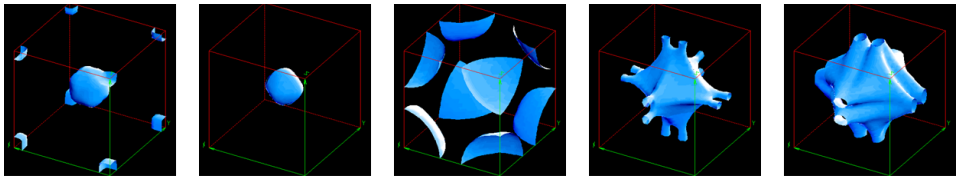

Figure 4. Fermi surface sheets at the equilibrium lattice constant. (a) and (b) show up spin states, producing 2 electron pockets at Γ and one at R, (c) is a spin down spherical hole pocket around R, and (d) and (e) are down spin bands giving rise to open surfaces.

4. Conclusion

We have calculated the electronic properties of MnGe using a GGA functional for a number of lattice constants. We observe a magnetic ground state at the experimental lattice constant.. The bands and Fermi surfaces at the equilibrium lattice constant are also shown. We will present additional data on a low moment state coming from the lattice under pressure, and calculations of the optical conductivity and Kerr effect in a later publication.

5. Acknowledgments

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6. References

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