

Description for the general public

Over a hundred years ago, the German scientist Friedrich Heusler discovered CuMn_2Al – a ferromagnetic compound that does not contain any ferromagnetic elements. For a long time, physics textbooks have told us that besides iron, cobalt and nickel, ferromagnetism is only observed in the Heusler alloys.

The “Heusler family” contains as many as 1500 compounds, which are divided into two sub-classes: half-Heusler and full-Heusler compounds with, ATM or AT_2M stoichiometry respectively. In those formulas A is generally a transition metal from groups 3-5 or a lanthanide, metal T is a transition metal from groups 9-11 and M is a metal from the p – block or a metalloid (e.g. Sb, Bi).

A beautiful crystal structure for both classes is shown below. Atoms A and M build two interpenetrated, face-centered regular lattices that is nothing but a NaCl (rock salt) type structure. Atoms of the transition metal element T form a tetrahedron (a) or a cube (b) in the center of the unit cell.

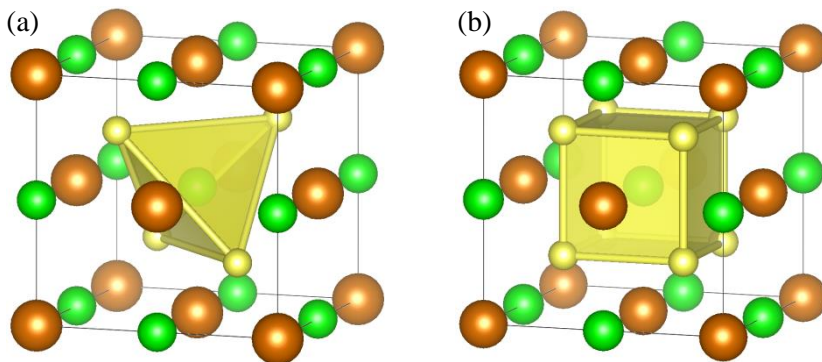


Figure 1. Crystal structure for: (a) half-Heusler MgNiSb and (b) full-Heusler MgNi_2Sb compounds. Orange and green balls represent Mg and Sb atoms, respectively. In the center of the unit cell there is a tetrahedron (a) or a cube (b) formed by Ni atoms (small yellow balls).

A wide variety of interesting properties have been found in this system such as magnetic and electrical transport properties, shape memory effects, semimetallic character, heavy fermion behavior, or half-metallic ferromagnetism behavior. Exotic semiconducting properties were discovered for the half-Heusler compounds with the number of valence electrons $N_{\text{el}} = 18$. The full-Heusler compounds are superconductors for $26 \leq N_{\text{el}} \leq 29$, with a maximum in T_c for $N_{\text{el}} = 27$. The coexistence of long-range magnetic ordering and superconductivity has been found in YbPd_2Sn and ErPd_2Sn .

The aim of this project is to synthesize new Heusler compounds with potentially interesting physical properties, such as superconductivity. It will be performed by careful choice of elements in order to get new full-Heusler type compounds with the number of valence electrons $N_{\text{el}} = 27$. In the same fashion, new half-Heusler semiconducting compounds will be synthesized with $N_{\text{el}} = 18$. We will work with alkaline earth metals, such as Mg or Ca, for which only few Heusler compounds have been reported or fully studied.

Polycrystalline samples of Heusler and half-Heusler alloys will be synthesized using a multistep solid-state reaction method employing pre-reacted binary precursors. TSb and TBi binaries will be obtained by annealing transition metal and metalloid powders pressed into pellets and sealed in evacuated silica glass ampoules. We will also study various phase diagrams, e.g. $\text{MgPd}_{2-x}\text{Sb}$ ($0 \leq x \leq 1$) tuning the system from MgPd_2Sb (superconductor) to MgPdSb (metal). Our studies will shed light on the nature of this intriguing family.

Samples will be analyzed by means of powder x-ray diffraction, magnetic susceptibility, electrical resistivity, magnetoresistance, the Hall effect and thermopower measurements. All measurements will be carried out by using a commercial Evercool II Physical Property Measurement System manufactured by Quantum Design.