Searching for Novel Half and Full Heusler Alloys: Effect of substitution on Geometric and Electronic Structure

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Abstract

Full and half Heusler alloys are novel functional materials. These are important materials for topics of current research interest because mainly of many possible practical applications, primarily in the field of shape memory alloys (SMA) and spintronics. Out of all the full-Heusler alloys (FHA), only a few undergo the martensite transition. These alloys are prone to a cubic to tetragonal distortion when temperature is lowered and generally likely to exhibit the technologically important SMA property. These FHAs in general are found to be metallic in nature. On the other hand, it has been observed that there is another group of FHAs which are half-metallic-like in nature, with a much reduced density of states (DOS) at the Fermi level in case of one of the spin channels. These materials generally do not show the tendency of undergoing a tetragonal distortion. An application in the field of spintronics is a possibility for these materials. From both the points of view of fundamental understanding as well as technological application, it can be interesting to probe the similarities and differences in magnetic, bulk mechanical, and electronic properties of these two categories of materials. It will also be interesting to see if there is any novel FHA which has a tendency to undergo a tetragonal transition and at the same time possesses a high spin polarization at the Fermi level. We probe this on Ni and Co-based FHAs in the present work. While most of the FHAs shows a cubic or orthorhombic symmetry, there are many half Heusler alloys (HHA) which are found in a hexagonal symmetry in their ground state. While NiMnSb is a well-known half-metallic HHA with a cubic structure, NiMnGa exhibits a hexagonal symmetry and a metallic state in its ground state. In this work, we probe the effect of substitution on the ground state symmetry and the electronic structure of some Co, Ni and Pt-based HHAs. We probe here if there is any novel HHA which is a metal and exhibit a hexagonal symmetry at the same time.