The evolution of high-pressure phases in near half-metallic Heusler alloys

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Intermetallic ternary full Heusler alloys are considered good candidates for spintronic applications[1]. Their suitability for spin-injection and spin-currents is defined by metallic and semiconducting behaviours of the majority and minority spins respectively. These compounds have a generic formula X2YZ (where X, Y= transition metals and Z is a group III or IV element) and crystallize in a cubic L21 crystal structure with space group Fm3m. The underlying reasons that establish half-metallicity in select Heuslers have long been debated.

One of the open questions is concerning whether magnetism in ternary Heusler alloys could be playing a crucial role in their half-metallic behaviour. The magnetism in such systems often arises from an imbalance between the majority and minority spin populations at particular atomic sites. Thus, fully localized magnetic moments can appear despite the presence of completely itinerant electrons [2]. Similar to magnetism, half-metallic behaviour in Heuslers may also have its origins in spin disproportionation, which influences the conduction gap at the Fermi level.

In this work, we present recent experimental measurements on several Heusler alloys which have been chosen due to strongly competing magnetic interactions, making them easily tuneable by factors such as magnetic field, chemical doping, strain and pressure [2],[3],[4]. Multiple physical properties probes - such as electrical resistivity, thermal transport and magnetization are used together with in-depth analysis to ascertain the nature of the high pressure ground state in these materials in search of a true halfmetal. An example of the significant pressure-induced changes in one such system - Pd2MnIn is shown in Fig 1a & 1b.

The results reveal that the intermetallic ternary full Heusler alloys, such as Pd2MnIn, are extremely sensitive to pressure and strain, easily tuning between competing ground states with changes in the lattice.

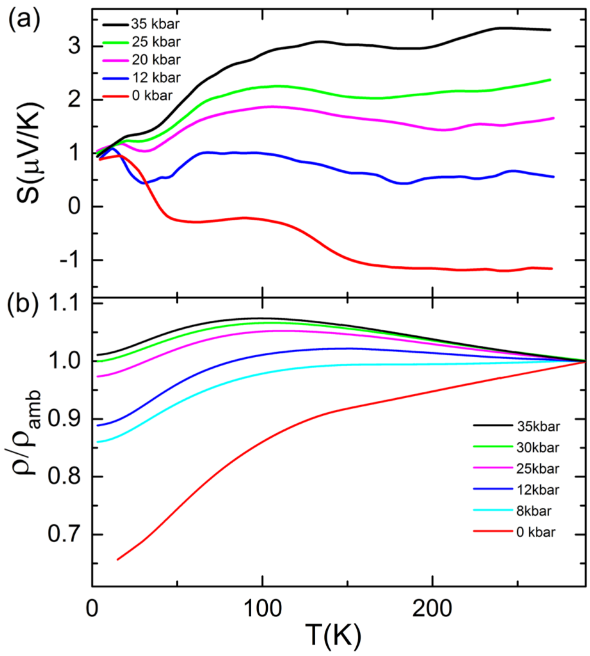

Figure 1. Thermopower (a) and electrical resistivity (b) in Pd2MnIn Heusler.

[1] T. Graf et al, *Prog. Solid State Chem.* 2011, **39,** 1-50.
[2] J. Kubler et al, *Phys. Rev. B.* 1983, **28,** 1745-1755.
[3] C.M. Hurd et al, *Phys. Rev. B.* 1982, **26,** 701-709.
[4] S. Pramanick et al, J. *Phys. Condens. Matter.* 2018, **30,** 405803.