COLOURED INTERMETALICS

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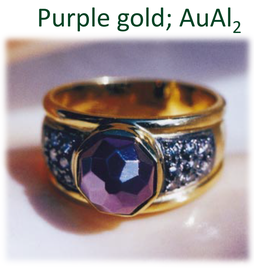
BACKGROUND

A fascinating fact is that the first interest of our ancestors to metals was not related to their superior mechanical properties, but the attractive look of shiny gold which has been exploited in jewelry for over 8000 years.

Colour in intermetallic solids is an unusual property, which if combined with a metallic luster can easily catch the eye. The colour of intermetallic compounds in most cases originates from the presence of a narrow band gap between conduction and valence bands. Typically researchers use the Zintl concept to target the band gap in metals, which works well for polar intermetallics.

Purple gold; $AuAl_2$



Blue gold; $AuGa_2$

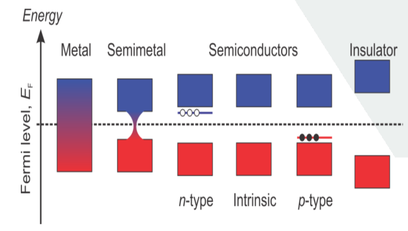
Yellow "Platigem" $PtAl_2$

AIMS AND OBJECTIVES

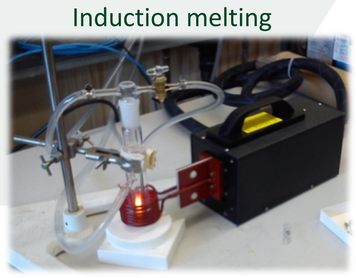
AIM: To develop cheaper, mechanically stable, safe intermetallic materials with band gap and the colour as intrinsic properties for energy conversion application.

OBJECTIVE: Exploring the possibilities of transition metals combined with *p*-block metalloids where the pseudogap at Fermi level is formed primarily due to the structure of intermetallic compound, rather than the combination of metals with a large difference in electronegativity (e.g., alkali metals with metalloids or 5*d*-elements). Within short span of time with the target of 100% yield, high frequency induction heating and arc melting technique is exploited.

Valence and conduction bands in materials



Induction melting



Arc melting

RESULTS

STRUCTURE:

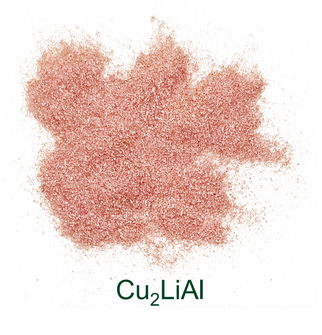
Cu_2LiAl, which is pink, gives a simple powder XRD pattern corresponding to a primitive cubic cell, similar to PdAl. Cu_2LiGa, which is yellow, clearly shows extra peaks corresponding to a doubling of the unit cell length, implying a superstructure. The sharp peaks indicate that both samples are highly crystalline. From the powder patterns alone, it can be inferred that Cu_2LiAl adopts the CsCl-type structure in which Li and Al are disordered within cubic sites, whereas Cu_2LiGa adopts the Cu_2MnAl- or Heusler-type structure in which Li and Ga atoms are in an ordered arrangement.

STRUCTURE AMBIGUITY:

Solid state ^7Li NMR spectroscopy was performed on these two compounds. In Cu_2LiGa, there is a single peak, consistent with one Li site, as expected. In Cu_2LiAl also, a single peak was observed, but there is an extra peak that might suggest some slight mixing with Cu. The other possibility is that there could be a Li-containing impurity phases, although the powder XRD seems to suggest only a single-phase sample.

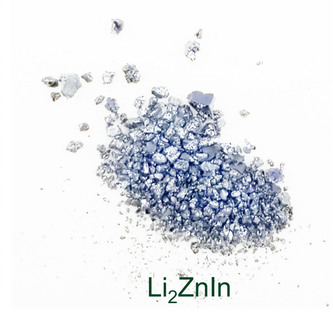
DIFFUSE REFLECTANCE SPECTRA:

Both Cu_2LiAl and Cu_2LiGa show absorption edges at around 2.7 eV, corresponding to a cutoff wavelength near blue. Their reflectance increases in the yellow and orange regions, accounting for the observed colours of these compounds. Although Cu_2LiGa is yellow-golden, similar to Au, its reflectance is quite a bit lower than gold. The absorption edge for Cu_2LiAl is sharper. Although the reflectance for both compounds appears to be low, we note that this is not too bad relative to other intermetallics, such as PdIn.

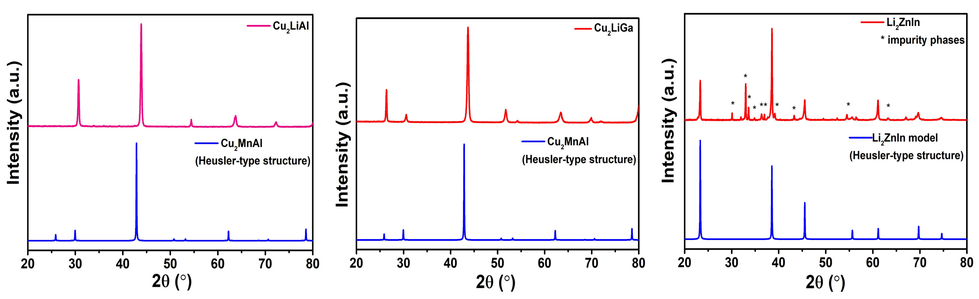


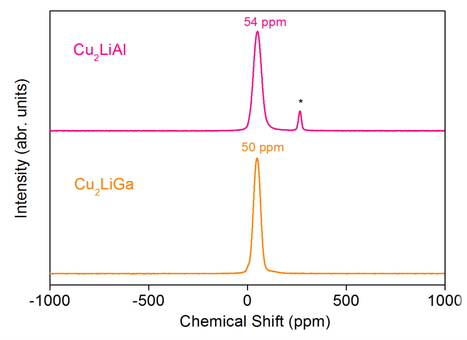
Cu_2LiAl

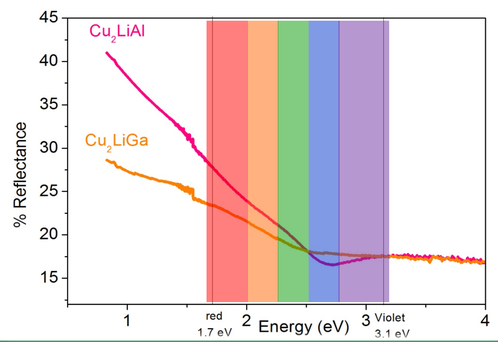
Cu_2LiGa



Li_2ZnIn







FUTURE DIRECTIONS

These phases containing transition metal and p-block metalloid can be potential candidates as unconventional semiconductors. Semiconductors have several applications related to their response to light and heat: solar energy and thermoelectric conversion (converting temperature gradient into electric potential). These sustainable technologies rely on the dependence of the electrical properties with temperature, which is different from metals because electrons are promoted across a gap, resulting in lower electrical resistance with higher temperature. Here is where we incorporate solid state chemistry in the doping strategy for tuning the band gap or structural optimization.

Interestingly, beside sustainable energy conversion, our materials can be used for jewelry applications.

FES PROJECT OVERVIEW

T12-P01 "High-throughput materials discovery through materials genomics"

Discovering better materials is essential for tackling the enormous challenges in developing new renewable energy sources. The experimental variables that must be considered to optimize a given property are too many and their relationships are too complex to allow anything but incremental improvements to be made. So how do we think "outside the box" to find entirely new materials? As part of the larger effort known as the "Materials Genome Initiative," approaches based on data-mining and materials informatics techniques can help screen new compounds with desired properties and features, at greatly accelerated rates, and provide insights into the design principles required to engineer improved materials. These tools will be used, in particular, to find better photovoltaics and catalysts for solar fuels.

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FUTURE ENERGY SYSTEMS

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