

Abstract of Presentation

Note: This paper should be typed in “Times New Roman” of 12pt.

Semiconducting and half metallic Heusler compounds for multifunctional applications

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Abstract :

Silicon is still the most important semiconductor for various applications such as electronic devices and solar cells. Binary semiconductors YZ such as GaN and GaAs are alternative materials because it is possible to tune their properties by choosing different element combinations. Recently, ternary and quaternary semiconducting materials have been designed for more complex applications. Ternary semiconductors derived from the ZnS structure exhibit the chalcopyrite structure type or C1b structure type, the so called half-Heusler structure. The former is a superstructure of the ZnS structure, whereas the C1b structure can be understood as “filled” ZnS structure type [1]. Instead of a few possible binary combinations crystallizing in the ZnS structure type more than 250, mainly semiconducting, compounds are known to crystallize in the C1b structure type.

Half-Heusler compounds XYZ have attracted attention as potential candidates for thermoelectric applications [2]. Favorable for thermoelectric applications are semiconductors with a small band gap. Similar to the binary semiconductors, the band gap depends on the electronegativity difference of the elements, which build the diamond-like substructure (van Vlechten). Complex C1b compounds such as TiNiSn phases are promising n-type thermoelectrical materials illustrated by exceptionally large figure of merit, $ZT \sim 1.5$ at high temperatures [2]. Doped TiCoSb, a p-type material, exhibits a large thermopower of $S = -400 \mu\text{V/K}$ at 300 K.

Heusler compounds X_2YZ were discussed mainly in the context of materials for spintronics and magnetic shape memory alloys [3]. Magnetic Half Heusler and Heusler compounds can be half metallic ferromagnets. Half metallic ferromagnets behave like metals with respect to the electrons of one spin direction and like semiconductors with respect to the electrons of the other spin direction. The tremendous progress of Heusler compounds for spintronics was based on the discovery of large negative magnetoresistance (MR) for $\text{Co}_2\text{Cr}_{0.6}\text{Fe}_{0.4}\text{Al}$ [4] and the general success of tunnel junctions. High Curie temperatures were found in Co_2 -Heusler compounds with values up to 1120 K in Co_2FeSi [5]. Ferrimagnetic Heusler compounds are candidates for spin torque application, because of their low magnetic moments despite their high Curie temperatures [6].

The potential for application of these ternary compounds as multifunctional materials on a basis of a rational design will be discussed

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