Cubic and tetragonal Heusler compounds

seminar

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Abstract

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In first part of the talk I will present an orbital coupling model for cubic full Heusler compounds that provides a unified set of rules that account for the chemical ordering, magnetic moment, and composition of the most promising candidates for half-metallicity. I will explain the origin and limitations of the rules. To the best of my knowledge all of the several dozen half-metallic Heusler compounds known in the literature that follow the Mt = Nt – 24 or Mt = Nt – 28 generalized Slater-Pauling behavior satisfy the derived half-metallicity rule. Calculations performed by using density functional theory confirm the validity of the orbital coupling model and derived rules for broad classes of Heusler compounds.

In second part of the talk I will describe the general mechanism of tetragonal distortion in Heusler compounds X2YZ. From 286 compounds studied using density-functional theory, 62% are found to be tetragonal. A shift of the DOS in the Y or Z series leads to an alternation of stable and nonstable cubic phases that depends on the value of the DOS at EF in the cubic phase. Groups of compounds with a large share of tetragonal distortions are identified and explained. Among 116 stable tetragonal compounds 10 compounds were found to have strong perpendicular magnetic anisotropy and are expected to have large tunneling magnetoresistance due to so-called 'Brillouin Zone spin filtering' effect.

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