Structural, magnetic and transport properties of $Fe_2Cr_{0.5}Ti_{0.5}X$ (X = Al, Ga, In) Heusler alloys

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Half-metallic materials demonstrating 100% spin polarization at the Fermi level are the key ingredient for spintronic applications. Theoretical calculations [1] have pointed out that X_2YZ Heusler alloys obeying the Slater-Pauling rule, which states that the number of valence electrons N_V determines the total magnetic moment M_t as $M_t = N_V - 24$, can demonstrate well-defined half-metallic properties. This approach implies that the Heusler compounds with N_V = 24 should have zero net magnetic moment. Considering Fe_2-based Heusler alloys, this rule is valid for Fe_2VAl, which is a well-known thermoelectic materials. In order to extend this approach for another representatives of the Fe_2-based Heusler alloys, we performed theoretical and experimental study of $Fe_2Cr_{0.5}Ti_{0.5}X$ (X = Al, Ga, In) alloys, which satisfy the N_V = 24 condition.

Results of our first-principles calculations indicated that, indeed, the electronic structure of the $Fe_2Cr_{0.5}Ti_{0.5}X$ Heusler alloys resembles the electronic structure of a gapless semiconductor with zero net magnetic moment. Experimentally studied magnetic properties of these alloys confirmed the absence of a long-range magnetic ordering down to 4.2 K, which is in a sharp contrast with the well-defined ferromagnetism of the parent Fe_2CrX compounds, whose Curie temperature T_C exceeds 300 K [2]. However, a deviation of the inverse magnetic susceptibility curve of the studied $Fe_2Cr_{0.5}Ti_{0.5}X$ alloys from the Curie-Weiss law suggests that short-range magnetic correlations make a significant contribution to magnetic properties of these compounds. Hence, it can be concluded that the degree of the $L2_1$ superstructural ordering can strongly modify magnetic properties of the $Fe_2Cr_{0.5}Ti_{0.5}X$ Heusler alloys.

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