Peculiarities of magnetic properties and electronic structure in Mn_2YAl (Y = Ti, V, Cr, Mn, Fe, Co, Ni) Heusler compounds

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Some Heusler alloys demonstrate properties of half-metallic ferromagnets (HMFs) [1] and spin gapless semiconductors (SGSs) [2]. These two classes have a significant difference: there is no energy gap near the Fermi level for the spin up current carriers in HMF, whereas in SGS the gap is being zero. However, the electronic band structure is the same in HMF and SGS for spin down: both the materials have a gap [1,2]. Since in X_2YZ Heusler compounds Y-elements are 3d-transition metals [3], it is of great interest to follow experimentally the changes in the electronic and magnetic properties of the Mn_2YAl Heusler alloys system, when varying Y in the sequence Ti, V, Cr, Mn, Fe, Co, Ni. The main purpose is to compare the results obtained from the electronic band structure calculations and investigate a possible proximity to HMF- and/or SGS-states in the Mn_2YAl system. An elemental analysis was carried out by using a FEI Company Quanta 200 scanning electron microscope equipped with an EDAX X-ray microanalysis unit. The temperature dependences of the electrical resistivity were obtained in a wide temperature range from 4.2 to 1000 K. The field dependences of the magnetization were measured in the fields up to 50 kOe at $T = 4.2$ K. The calculations of the electronic structure and magnetic properties of Mn_2YAl were performed in generalized gradient approximation within the Quantum-Espresso software package [4]. As a result, the experimental study showed a good agreement with the electronic band structure calculation. The energy gap parameters and the current carrier spin polarization vary significantly depending on the number of valence electrons, which is reflected in the change of their electrical and magnetic characteristics. Some features in the electronic and magnetic properties of Mn_2YAl Heusler alloys may indicate conditions close to the HMF or SGS states. A high degree of charge carriers spin polarization makes it possible to use these materials in the development of spintronic devices.

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