Effect of composition on the structural and magnetic properties of SiFeMn-based alloys

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One of the modern materials that have proven to be a suitable candidate for the construction of devices used in the field of spintronics is the Heusler alloy. The conventional formula for ternary full-Heusler alloys is usually written as X_2YZ, where X and Y are transition metals or lanthanides, and Z is an element from the p-block [1]. However, recent research [2] suggests that Heusler alloys with the formula Z_2XY could also exist. The investigation focused on the analysis of the Si_2FeMn alloy, which corresponds to the newly proposed formula Z_2XY, with the aim of comparing its structural and magnetic properties to those of the Mn_2FeSi alloy [3], representing the standard X_2YZ formula. X-ray diffraction analysis revealed that the Heusler crystal structure, belonging to space group F-43m (No. 216), occurs in Mn_2FeSi, whereas Si_2FeMn forms a different cubic structure assigned to space group P213 (No. 198). The lattice parameter of Si_2FeMn was determined to be 0.452 nm. Scanning electron microscopy confirmed the presence of two phases in both alloys: a dominant phase, with an elemental ratio corresponding to the required stoichiometry and forming the main matrix, and a minor phase consisting of sparsely distributed Mn-rich precipitates. Magnetic properties of Si_2FeMn were measured using a vibrating sample magnetometer and a physical property measurement system. Similar to Mn_2FeSi, hysteresis loops at room temperature and thermomagnetic scans between 300-550 K indicate paramagnetic behavior. Differences in magnetic behavior between the alloys become apparent only at low temperatures. While the thermomagnetic curve of Mn_2FeSi upon cooling to 5 K reveals a coexistence of ferromagnetic and antiferromagnetic transitions [3], Si_2FeMn retains a paramagnetic profile. Only at very low temperatures, around 5 K, a slight reversal appears in the magnetic hysteresis loops of Si_2FeMn, suggesting the onset of ferromagnetism. Experimental results are complemented by theoretical calculations based on density functional theory.

References:

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