Abstract

Structural, electronic and magnetic properties of the Heusler alloy Mn_2VIn have been investigated using the density functional theory and experimental techniques. Unlike many other Heusler compounds, Mn_2VIn is not predicted to be half-metallic at the optimized lattice constant, but is highly spin polarized at a slightly lower lattice constant. It however exhibits ferrimagnetic coupling between the Mn and V sublattices, as expected of Mn-based Heuslers. We have, then, synthesized the compound by arc melting and studied magnetic properties that are of interest fundamentally and for technological applications. The structural properties were determined using X-ray diffraction, revealing the presence of cubic and tetragonal phases in the sample. The chemical composition was determined using energy-dispersive X-ray spectroscopy together with the scanning electron microscope, and the magnetic properties were investigated by superconducting quantum interference device magnetometry. The alloy exhibits superparamagnetic spin blocking with a blocking temperature TB of 40 K.