First principles study of magnetic properties of Zn-Sn substituted M-type Sr-hexaferrite

SEONG-GON KIM, LAALITHA LIYANAGE, Department of physics and astronomy, Mississippi state university, JEFF HOUZE, None, SUNGHO KIM, Center for advanced vehicular systems, Mississippi state university — Site occupancy and magnetic properties of Zn-Sn substituted M-type Sr-hexaferrite SrFe$_{12-x}$(Zn$_{0.5}$Sn$_{0.5}$)$_x$O$_{19}$ with $x = 1$ were studied using density functional theory and generalized gradient approximation (GGA). Using the GGA+U method the description of strongly correlated 3$d$ electrons of Fe was improved. Our results show that Zn and Sn atoms prefer to occupy 4$f_1$ and 4$f_2$ sites respectively. Favorable Zn-Sn substituted configurations show an increase in saturation of magnetization ($M_s$), and a decrease in magnetic anisotropy energy (MAE), over the pure M-type Sr-hexaferrite ($x = 0$). Experimental observations agree with the decrease of MAE and the increase of $M_s$ for Zn-Sn substituted Sr-hexaferrite.

Laalitha Liyanage
Department of physics and astronomy, Mississippi state university

Date submitted: 11 Nov 2011