Theoretical limit of $(BH)_{max}$ for hexagonal strontium ferrite ($SrFe_{12}O_{19}$) permanent magnet

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The density functional theory (DFT) and generalized gradient approximation with Coulomb and exchange interaction effects (GGA+U) were used to calculate the electronic structure of hexagonal strontium ferrite ($SrFe_{12}O_{19}$). Since the calculated magnetic moments and energies are stable for U_{eff} = 7 eV, the exchange integrals were used to calculate the temperature dependence of magnetic moments $M(T)$ for the five sublattices (2a, 2b, 12k, 4f1, and 4f_2) based on the Brillouin functions. The $M(T)$ of the five sublattices are inter-related to the nearest neighbors, where the spins are mostly anti-ferromagnetically coupled. The sublattice $M(T)$ were used to obtain total $M(T)$, which is in good agreement with the experimental $M(T)$. The temperature dependence of maximum energy product ($(BH)_{max}(T)$) was then calculated using the calculated $M(T)$. The calculated $(BH)_{max}$ value of 5.9 MGOe at 300 K is higher than the experimental value of 4.8 MGOe at room temperature.