First-principles study of magnetic anisotropy in $\text{Y}_2\text{Fe}_{14}\text{B}$

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Since yttrium is a prototypical $f^0$ element, $\text{Y}_2\text{Fe}_{14}\text{B}$ is suitable to study the effects of itinerant d electrons in permanent magnetic materials. In contrast with localized f electrons, d electrons are expected to be sensitive to lattice strain due to their itinerant nature. In this work, we have investigated the magnetic anisotropy energy (MAE) and the magnetic moment of $\text{Y}_2\text{Fe}_{14}\text{B}$ on the basis of density functional theory by using localized pseudoatomic orbitals. The calculated MAE (2.5 meV) of $\text{Y}_2\text{Fe}_{14}\text{B}$ is within the same order with underestimating experimental results [1]; this underestimation is a systematic error consistent with other first-principles works. We have found the MAE is significantly enhanced upon compression of the lattice. The density of states (DOS) becomes broader with compressing the lattice; the DOS around the Fermi energy becomes considerably larger compared with the case with the equilibrium lattice constants for both majority and minority spins as seen in Fig.1. By analyzing the origin of the MAE using the matrix elements in the second-order perturbation theory [2], couplings among occupied and unoccupied states of 3d$^{x^2-y^2}$ and 3d$_{xy}$ components of Fe are identified to have most significant contributions in enhancing the perpendicular anisotropy found (Fig.2).


Figure 1: The DOS for $\text{Y}_2\text{Fe}_{14}\text{B}$ with equilibrium (shade) and uniformly compressed (3%, solid lines) lattice constants.

Figure 2: The local DOS for compressed $\text{Y}_2\text{Fe}_{14}\text{B}$, which is decomposed to $d^{x^2-y^2}$ and $d_{xy}$ components of Fe 3d orbitals.