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Magnetic anisotropy modified by strain effects in $Y_2Fe_{14}B$[1]

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In exhibiting the coercivity of permanent magnets, magnetocrystalline anisotropy plays an important role. Since itinerant magnetic states are responsible to direct interactions among magnetic sites, d states are expected to be sensitive to lattice strain. In this work, we report strain effects on magnetic properties theoretically studied by first-principles calculations for $Y_2Fe_{14}B$, where Y is a prototypical f^0 rare-earth element [1]. To analyze the local magnetic anisotropy, we developed a method to decompose the magnetic-anisotropy energy into contribution from each atomic site as well as from couplings among specific atomic orbitals, where the sum rule is satisfied by including indirect off-site contributions in the second-order perturbation. The OpenMX code is used for first-principles calculations. The lattice constants of $Y_2Fe_{14}B$ are changed from the equilibrium values independently, where we found the uniform compression enhances the perpendicular magnetic anisotropy. Our magnetic-anisotropy decomposition identified dominant magnetic site and orbital couplings. Our method will enable us to study the anisotropy at microstructure interfaces. [1] Z. Torbatian, T. Ozaki, S. Tsuneyuki, and Y. Gohda, Appl. Phys. Lett. 104, 242403 (2014).

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