Site preferences for La and Dy in $Nd_2Fe_{14}B$ Permanent magnet: A first principles study

Imran Khan* and Jisang Hong
Department of Physics, Pukyong National University, Busan 608-737, Korea

We studied the electronic structure and magnetic properties of pure, La and Dy substituted $Nd_2Fe_{14}B$ by using the full potential linearized augmented plane wave method. A DFT+U scheme was applied to treat the localized 4f electrons of Nd and Dy. To explore the magnetic ground state, we considered both ferromagnetic (FM) and antiferromagnetic (AFM) spin interaction between Fe and R (rare-earth) sub-lattice. The total energy calculation predicts that both La and Dy prefer 4f-site in $Nd_2Fe_{14}B$ on lower substitution, along with a negative value of substitution energy (-3.04 eV/atom) and (-4.04 eV/atom) respectively. The negative value of substitution energy shows that both La and Dy prefer to enter the $Nd_2Fe_{14}B$ phase on lower substitution. On increasing the substitution level La prefer g-site according to the total energy calculation but its substitution energy is positive (0.13 eV/atom), which shows that La don't prefer to enter $Nd_2Fe_{14}B$ phase rather it will be segregated at the grain boundaries. The calculated spin magnetic moments for different Fe and R sites were in good agreement with previously reported value. We found that for light rare-earth elements like Nd and La the spin and orbital magnetic moment was always anti-parallel. Overall, these findings will help for enhancing the magnetic properties of $Nd_2Fe_{14}B$ permanent magnet.