

# Prediction of giant magnetostriction of a $\text{Fe}_{1-x}\text{Be}_x$ binary alloy

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Magnetostriction coefficients of some ordered BeFe alloys were investigated, using first principles calculation. The full-potential linearized augmented plane wave (FLAPW) method was employed within general gradient approximation for electron interactions. A giant magnetostriction coefficient ( $\sim 1160$  ppm) of a  $\text{Fe}_{0.875}\text{Be}_{0.125}$  alloy was predicted to be enhanced more than 50 times, compared to the calculated value (21ppm) of bulk Fe. We elucidated the origin of the giant magnetostriction coefficient of  $\text{Fe}_{0.875}\text{Be}_{0.125}$  with the change of its single particle energy spectra with at tetragonal distortion.