

DFT calculations of intrinsic properties of magnetically hard phase $L1_0$ FePt

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Due to its strong magnetocrystalline anisotropy, $L1_0$ FePt phase is considered a promising material for magnetic recording media and as a magnetically hard material that does not contain rare earth elements [1]. Although the magnetic properties of this phase have already been analyzed many times using density functional theory (DFT) [2], we decided to study it again using the full-potential local-orbital (FPLO) scheme [3]. In addition to determining the exact values of the magnetocrystalline anisotropy constants K_1 and K_2 , the magnetic moments, the Curie temperature, and the magnetostriction coefficient, we focused on investigating the dependence of the magnetocrystalline anisotropy energy (MAE) on the magnetic moment values, which was made possible by using the fully relativistic fixed spin moment method [3]. These calculations also allow us to understand the discrepancies between the results obtained previously for different exchange-correlation potentials. The obtained calculation results are in good agreement with the experimental results.

References:

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