Magnetically induced variations in phonon frequencies

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1. 서론

The fundamental physics of metallic magnetism has not been satisfactorily understood as yet and continues to be a highly active field of research both theoretically and experimentally. On the theoretical side, recent efforts have been focused on the correct description of observed quantities

such as Curie temperature and magnon spectra, while experimental studies show the large variety and complexity of materials whose magnetic properties can be investigated with today's techniques. Manganites, ruthenates, and even high T_C superconductors are a few examples. However, all these studies are mainly focused on the electronic and charge degrees of freedom; although an important constituent of solids, the phononic one has not been seriously taken into account in magnetism research.

2. 계산방법

In this work, we present results of a systematic first-principles study of the phonon dispersions of fcc Ni with variation of its magnetic moment. To this end, we used a combined density-functional perturbation theory (DFPT) as implemented with full-potential linearized augmented plane wave (FLAPW) method and fixed spin moment (FSM) approach. Nickel is selected because it is one of the ferromagnetic elements with a simple lattice and electronic structure, which alleviates the computational workload in phonon calculations and simplifies the interpretation of the results obtained.

3. 계산결과 및 고찰

Our first-principles calculations reveal that due to the interplay between the electronic screening and the magnetostriction, the phonon frequencies of Ni show an appreciable change as its magnetic moment varies: the frequencies increase with the magnetic moment near the Brillouin zone center, whereas the situation becomes reversed near the zone boundary.

4. 결론

We note that just as the magnetization affects the phonon frequency, the magnetization can be affected by phononic contributions as derived by Kim, which implies that the phonons and magnetization need to be determined in a self-consistent way. Thus, the present work is expected to stimulate more investigations in these directions as well.

5. 참고문헌

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