MAGNETO-OPTICAL KERR EFFECT OF ANTIFERROMAGNETIC MATERIALS IN EXTERNAL MAGNETIC FIELDS

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EXECUTIVE SUMMARY

This work investigates the relationship between light and magnetically ordered materials, and particularly metallic antiferromagnets. Their weak response to applied external magnetic fields and terahertz frequency spin dynamics are interesting characteristics that make antiferromagnetic materials potential candidates for memory devices. In this context, the Magneto-Optical Kerr Effect (MOKE) is a useful phenomenon that provides information about magnetization through optical response; however, antiferromagnetic materials with a compensated spin configuration have no net magnetization. Based on the magnetic susceptibility, the spin response under applied fields can be predicted and related to tilted spin configurations that arise in external magnetic fields. MOKE signals are, hence, present for tilted spin configurations. In this project, we carried out first-principles calculations based on density functional theory to study MOKE and the magnetic susceptibility of antiferromagnetic materials. This will be useful guidance for experimentalists; e.g., to identify the wave length of maximum MOKE response in new materials.

RESEARCH CHALLENGE

Antiferromagnetic materials have interesting properties that can potentially lead to fast switching in future memory devices. Unlike ferromagnetic materials, they show a weak response to external magnetic fields, and do not show a magnetic field outside of the material due to spin compensation. However, this can become a double-edged sword. Due to the weak response under applied external fields, it is difficult to control the internal spin configuration. Spin compensation makes detecting the spin information of antiferromagnetic materials using optical measurements challenging. Measurements of optical response under external magnetic fields have been developed. However, it is still necessary to understand the fundamental behavior of antiferromagnetic materials better. In order to understand basic principles an experiment can benefit from theoretical guidance, e.g., to maximize the detected signal, in order to more easily measure the response.

METHODS & CODES

We used first-principles calculations based on density functional theory to understand the magnetic properties of antiferromagnetic materials using the Vienna Ab-Initio Simulation Package (VASP) [1]. Based on magnetic structures from neutron scattering, we performed structural relaxations in the presence of magnetism. We explicitly studied spin-tilted cases with noncollinear magnetism, based on a fully relativistic band structure and dielectric tensor [2]. MOKE signals were computed using the Kerr equation and the off-diagonal elements of the dielectric tensor. At the same time, we computed magnetic susceptibility from the relationship between total energies and net magnetic moments of spin-tilted magnetic unit cells. We further studied Néel temperatures based on magnon dispersion calculations using the spin spiral approximation and the frozen magnon model.

RESULTS & IMPACT

In this work, we used first-principles calculations to study magneto-optical properties of various antiferromagnetic metals. MOKE signals measured in experiment are usually small on the nanoradian scale, which is easily overwhelmed by noise. Since it is difficult to tune the laser system every time to find the optimal wavelength for excellent signal-to-noise ratios, first-principles calculations based on density functional theory can provide this information. In this project, wavelength-dependent MOKE spectra are computed for MnPt and Fe_2As. We find that MnPt shows a maximum Kerr rotation signal at 730 nm and Kerr ellipticity at 540 nm. For Fe_2As, Kerr rotation and ellipticity are maximized at 620 nm and 520 nm, respectively. These spectra give useful guidance to experimentalists, who seek it to find the wavelength that maximizes MOKE signals.

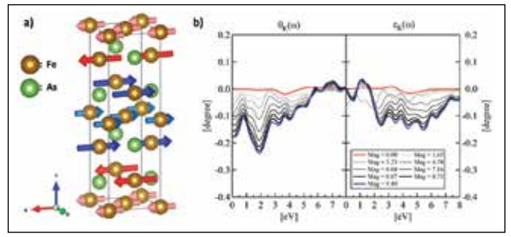

Figure 1: (a) Magnetic unit cell of Fe_2As, and (b) Wave-length dependence of MOKE signals under external magnetic fields. Kerr rotation (θ_K) and Kerr ellipticity (ε_K) are maximized at 2 eV (620 nm) and 2.4 eV (520 nm), respectively.

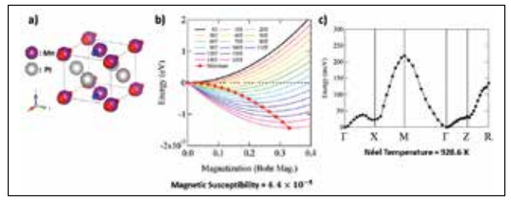

Figure 2: (a) Magnetic unit cell of MnPt; (b) magnetization and energy change of MnPt spin-tilted calculation for corresponding external magnetic fields. Red marker line in (b) presents ground states under corresponding fields and (c) magnon dispersion of MnPt.

At the same time, we also computed magnetic susceptibility, which can provide the spin response under applied external magnetic fields. For MnPt along the c-axis, which is perpendicular to the spin direction, computed magnetic susceptibility is $\chi=4.4\times10^{-4}$ which is close to $\chi=4.742\times10^{-4}$, as determined experimentally [3]. Based on this information, magnetic moments of spin-tilted magnetic-structure calculations can be converted to a response to external magnetic fields. Thus, MOKE signals under the applied field can be predicted.

In order to confirm the spin configuration stability at room temperature, we performed Néel temperature calculations. Through the mean-field approximation, the computed Néel temperature of MnPt is 928.6 K, while experimental measurement of MnPt finds 953 K [3]. The results of magnetic susceptibility and Néel temperature calculations illustrate that this first-principles computational approach can provide reasonable predictions for magnetic properties of antiferromagnetic materials. Thus, our calculations are helpful guidance to understand the behavior of antiferromagnetic materials and to develop advanced magnetic devices. For this work, we acknowledge funding through the Illinois Materials Research Science and Engineering Center, which is supported by the National Science Foundation MRSEC program under NSF Award Number DMR-1720633.

WHY BLUE WATERS

Even though first-principles calculations are a great opportunity to thoroughly investigate antiferromagnetic materials, optical and magnetic calculations still require significant computational resources. Unlike nonrelativistic cases, a fully relativistic band structure and its dielectric function calculation with magnetism are demanding processes. Spin-tilted calculations are challenging because noncollinear calculations need more computational resources than collinear calculations. In addition, these require more computational resources because magnetic unit cells of antiferromagnets are usually larger than chemical unit cells. Magnon dispersion calculations for Néel temperatures also require dense Brillouin zone sampling to achieve convergence to an appropriate accuracy. In order to address those challenges, Blue Waters is well suited due to its fast communication and large amount of memory per node. Thus, Blue Waters provides a unique chance to unveil the unknown properties of antiferromagnetic materials.