Ab initio study of optical spectrum change at finite spin and lattice temperatures in ferromagnetic BCC Fe

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1. Introduction

A temperature change of optical spectrum has been popularly used to characterize various magnetic materials. Especially, the pump-probe magneto-optical spectrum measurements of ferromagnetic materials are utilized to investigate the (de)magnetization process and spin dynamics, and identify the precessional frequency with time-resolved experiment [1]. Concurrently, the computational approach with first-principles methods starts to study the lattice temperature effect on the optical spectrum of non-magnetic materials such as silicon through the perturbed lattice model through phonon dispersion [2]. To understand the temperature-related optical response in pump-probe measurement, it is essential to investigate how spin temperature affects the dielectric function of magnetic materials. In this study, we integrate first-principles density functional theory [3, 4] and atomistic spin dynamics [5] to simulate the optical spectrum of ferromagnetic BCC Fe at finite spin temperature using the analogous approach for lattice temperature [2].

2. Results

Three characteristic changes are predicted in the optical conductivity spectrum as a function of spin temperature. First, we found that the position of a peak near 3 eV shows a redshift as a function of temperature shown in Fig. 1 and 2. This behavior also appears with lattice temperature, but the shifting size of spin temperature is about four times larger than that of lattice temperature. This result can explain the large difference of the peak position between the calculated spectrum at 0 K and measurement at 300 K. Second, there is a large signal generation of optical conductivity from interband transitions below 2 eV. We identify that the physical origin of this phenomenon is induced by the large optical matrix elements change. However, this effect might not be measured in experiments due to the much larger change of intraband contributions. Lastly, we could reproduce the polar magneto-optical Kerr effect change at finite spin temperature, indicating the demagnetization of ferromagnetic BCC Fe. We expect that the proposed approach can be expanded to the other magnetic phases such as antiferromagnets or ferrimagnets and explains how spin temperature affects their optical properties.

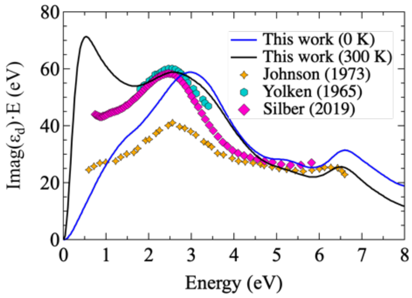

Fig. 1: Calculated optical conductivity of ferromagnetic BCC Fe at spin temperatures of 0 K and 300 K. Experiment works are shown in markers; Johnson [6], Yolken [7], Silber [8]

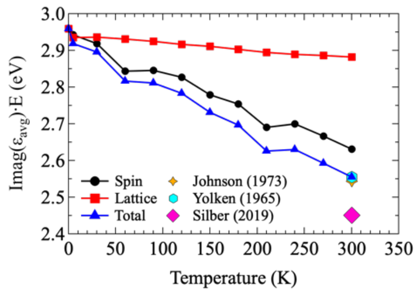

Fig. 2: The peak position change near 3 eV as a function of lattice and spin temperatures. Total change is a summation of individual spin and lattice temperature results

3. References

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