First principles calculations of magneto-optical conductivity in heavy metals

Mie Univ.[1], Osaka Electro-Communication Univ.[2], °(M1) T. Shiraki[1], A.-M. Pradipto[1], T. Akiyama[1], T. Ito[1], S. Nagai[1], T. Koshikawa[2], and K. Nakamura[1]

E-mail: 419M610@m.mie-u.ac.jp

An interest of spin-polarized electrons playing a central role in spintronics has been growing in optoelectronic applications using circularly polarized light. At an earlier stage in this field, an attention was paid to a spin-polarized electron emission from semiconductor heterostructures,[1] e.g., by using a strained GaAs thin-layer that leads to exited electrons with highly spin-polarization as much as 86%.[2] It is however demanded more efficient materials for the photo-spin current conversion in the applications. Although first-principles calculation is known to be an effective tool to search such materials, there is no report available. In the present work, the magneto-optical conductivity to spin currents for 5*d* heavy metals, as well as GaAs, were investigated in order to search the material candidates. Self-consistent calculations were carried out by using full-potential linearized augmented plane-wave method[3] based on the generalized gradient approximation, and the conductivity coefficients as a function of photo energy were evaluated on the basis of Kubo-formula in the linear response theory by using the calculated eigenvectors. For GaAs, we observe the off-diagonal component of the magneto-optical conductivity, reflecting the excited spin-polarized electrons by circularly polarized light even though the spin-orbit-coupling (SOC) of GaAs is weak, which agrees with experiments. For 5*d* heavy metals, we find that the intensity significantly increases due to the large SOC, for example, for Pt the intensity ranging from 1 eV to 2 eV of photo energy increases by one order of magnitude compared to that of GaAs. More details including the mechanism will be presented.

[1] D. T. Pierce *et. al*., Phys. Rev. B **13**, 5484 (1976)

[2] T. Nakanishi *et. al*., Phys. Letters A**158, 345 (**1991).

[3] K. Nakamura *et. al*., Phys. Rev. B **67**, 14405 (2003)