Research Group for Condensed Matter Theory

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The internal degrees of freedom of electron (spin, charge and orbital) and the electrons correlation are the keys for new functional materials. Our study has been focused on new principle in condensed matter physics and new function of devices. In particular, the energy efficiency is our major concern. In this fiscal year, we have clarified the origin of phonon Hall effect, by which a heat current carried by phonons is changed under a magnetic field [1]. Another interesting phenomenon is the spin Hall effect (SHE), by which the charge current is converted into the spin current and vice versa. Using the density functional theory and the quantum Monte Carlo method, we have shown that the SEH is enhanced due to the electrons correlation, in particular on a surface [2]. Another correlation effect on the SHE appears in its sign [3]. Detail of the latter case is explained in the highlights.

Control of heat by magnet

Heat diffuses from hotter to colder regions and, in general, its direction cannot be changed externally (Fig. 1 left). If a heat current can be controlled by design, energy efficiency will be improved dramatically. In an insulator, heat is carried by lattice vibrations, which have neither charge nor spin. Nevertheless, it was reported that a heat current in the insulator, terbium-gallium-garnet, was bended by a magnetic field at low temperatures (Fig. 1 right). This is called phonon Hall effect [4, 5]. We find that this phenomenon originates from a resonant scattering of phonons at Tb ions. A key interaction is a coupling between the quadrupole moment of Tb ions and the lattice strain. The transverse component of the heat current is induced by this interaction with a quasi-doublet state of Tb ions, which is split by an applied magnetic field. The obtained magnitude of the effect is in agreement with experiments, and furthermore, we predict that the magnitude of the effect grows significantly with temperature. In this study, the Tb ion plays an important role to obtain this phenomenon. If the same scattering mechanism can be implanted by artificially creating nano-structures in some materials, i.e., meta-material, the control of heat by a magnet would be realized at higher temperatures and will contribute to the energy efficiency. Finally, it is noted that the mechanism similar to that considered here will be also valid for the Hall effect of light.

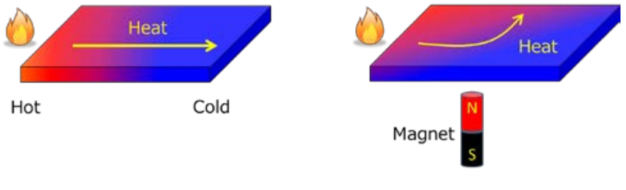

Fig. 1 The heat flow from the high temperature to the low temperature sides (left). Usually, heat dissipates from hotter to colder regions. By the phonon Hall effect, however, the heat flow is changed under a magnetic field as shown schematically in the right.

Enhanced spin Hall effect by electrons correlation

The spin Seebeck effect is a completely new principle of thermopower generation using a simple device structure, i.e., a metal on a ferromagnet. It is natural to hope to enhance its figure of merit. From a viewpoint of material science, the key factor is the SHE, especially, the ratio of an induced spin current to the input charge current (Fig. 2). It is called spin Hall angle (SHA). So far, the SHA was about several percent at most even in a heavy element such as Pt. However, Niimi et al. has reported that Cu doped with a few percent of Bi shows 24% of the SHA at low temperatures [6]. Considering the spin-dependent scattering of electrons (skew scattering) due to the spin-orbit interaction at Bi impurities with 6p orbitals (See Fig. 2), we find that the SHA can be dramatically enhanced by Bi impurities on Cu surface combined with the electrons correlation effect. The mechanisms of this enhancement are two-fold. One is that the localized impurity state on surface has a decreased hybridization and is combined with Coulomb correlation effect. The other comes from the low-dimensional state of conduction electrons on surface, which results in a further enhancement of skew scattering by impurities. The character of materials is captured by the density functional theory and the correlation effects such as quantum fluctuation are taken into calculation by the quantum Monte Carlo method. Our method is applied to another case, e.g., Ir doped Cu, in which electronic correlation is crucial to find the sign of the SHE [3]. In addition, we clarify that the apparent discrepancy between the experiment and previous theories about sign of SHA in CuBi simply came from a confusion of definitions, i.e., resistivity-based or conductivity-based.

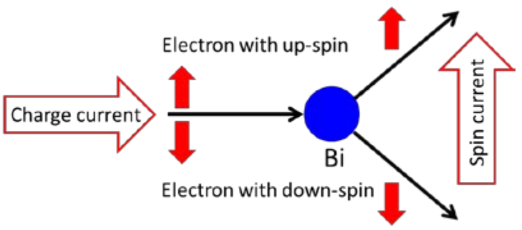

Fig. 2 Schematic figure of spin Hall effect. By the spin-dependent scattering of electrons (skew scattering), the charge current is converted into the spin current, which is the flow of magnetism (spin). The spin-orbit interaction at Bi is the key factor of the skew scattering.

References

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