Topological Weyl semimetal CoSi thin films with spin Hall effect enhanced by *d-p* orbital hybridization

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Spin current generated by the spin Hall effect (SHE) provides a bright way to manipulate the magnetization orientation by spin-orbit torque (SOT) for energy-efficient spintronic devices. Recently, topological Weyl semimetals (WSMs) emerge as promising materials for efficient spin-current generation in SOT devices, due to their topological nature of the bulk band structures. A large intrinsic SHE has been predicted in the TaAs family of WSMs, arising from the interplay of the large spin Berry curvature near the Weyl nodes[1)]. The cobalt monosilicide CoSi is a newly discovered WSM with two types of chiral topological fermions at the band-crossing points near the Fermi level[2)-4)], while the spin transport properties in the CoSi films have not been investigated. In this work, a comprehensive study on the nanometer-scale CoSi thin films and their spin-transport properties is presented by combining experiments and first-principles calculations.

CoSi-based thin films and heterostructures were fabricated by the magnetron sputtering in a high-vacuum sputter chamber. The out-of-plane XRD measurement with Cu K_α radiation was used to characterize the crystalline structure. The morphology and surface structures were checked by atomic force microscopy and reflection high-energy electron diffraction, respectively. Then, the samples were microfabricated into Hall bar structures by conventional UV lithography and Ar ion milling. Electrical and magnetic transport properties were measured in a physical properties measurement system at room temperature. Regarding the first-principles calculations, the generalized gradient approximation using the full-potential linearized augmented plane-wave method was employed.

Polycrystalline CoSi films with the *B*20 crystal structure and the flat surface morphology were deposited on sapphire *c*-plane substrates. The SHE and SOT signals in the CoSi films were studied by spin Hall magnetoresistance and harmonic Hall measurements in multilayer stacks with the core structure of CoSi/CoFeB/MgO. The anti-damping like and field like spin Hall conductivities (SHCs) of the CoSi films are evaluated to be 60 $(\hbar/e)\Omega^{-1}\mathrm{cm}^{-1}$ and 95 $(\hbar/e)\Omega^{-1}\mathrm{cm}^{-1}$, respectively. The spin Hall efficiency of ~3.4% was obtained, which is appreciable in material systems without any heavy elements. From the first-principles calculations, it is found that the hybridization between *d-p* orbitals leads to a large enhancement of spin Berry curvature near the band crossings at the vicinity of the Fermi energy, making the dominating contribution to the SHC in the CoSi. The maximum SHC amplitudes of ~147 and ~119 $(\hbar/e)$ $\Omega^{-1}\mathrm{cm}^{-1}$ can be achieved when the Fermi energy shifts down to −0.16 and up to 0.24 eV, where correspond to dope of 0.51 holes and 0.28 electrons, respectively. Therefore, we suggest that the SHC of CoSi could be further improved by doping with other elements, such as Fe or Ni. This work indicates that the *d-p* orbital hybridization plays a significant role for spin-current generation in Weyl semimetals and will be beneficial for developing new topological materials with large SHE.

Reference

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