Spin transport electronics (spintronics) has recently become a very active research field in condensed matter and materials physics because of its potential applications in information storage and processing and other electronic technologies and also because of many fundamental questions on the physics of electron spin. Spin current generation is an important issue in the emerging spintronics. Recent proposals of the intrinsic spin Hall effect (SHE) are therefore remarkable. In the SHE, a transverse spin current is generated in response to an electric field in a metal with relativistic electron interaction (spin-orbit coupling). This effect was first considered to arise extrinsically, i.e., by impurity scattering. The scattering becomes spin-dependent in the presence of spin-orbit coupling (SOC), and this gives rise to the SHE. In the recent proposals, in contrast, the spin Hall effect can arise intrinsically in hole-doped (p-type) bulk semiconductors and also in electron-doped (n-type) semiconductor heterostructures due to intrinsic SOC in the band structure. The intrinsic SHE can be calculated and controlled, whereas the extrinsic SHE depends sensitively on details of the impurity scattering. Therefore, the intrinsic SHE is more important for applicational purposes, in comparison with the extrinsic SHE.

In semiconductors, there have been experimental reports on the SHE in n-type GaAs and p-type GaAs and n-type InGaN/GaN superlattices in recent years. These experimental results have been discussed theoretically, and it is now recognized that the SHE in n-type GaAs is due to the extrinsic mechanisms, i.e., skew scattering and side-jump contributions, while that in p-type GaAs is mainly caused by the intrinsic mechanism. This conclusion is supported by theoretical analysis of the impurity effect and vertex correction to SHE in the Rashba and Luttinger models. In p-GaAs the fourfold degeneracy at the Γ-point of the valence bands acts as the Yang-monopole, which enhances the SU(2) non-Abelian Berry curvature.

On the other hand, the SHE in metallic systems is currently attracting interest, stimulated by latest experimental reports on the SHE or inverse spin Hall effect (ISHE), i.e., the transverse voltage drop due to the spin current. This effect is due to the extrinsic mechanisms such as the skew scattering by the impurities in Au.

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On the other hand, the SHE in metallic systems is currently attracting interest, stimulated by latest experimental reports on the SHE or inverse spin Hall effect (ISHE), i.e., the transverse voltage drop due to the spin current. This effect is due to the extrinsic mechanisms such as the skew scattering by the impurities in Au.
Fermi energy and that the vertex correction due to impurity scattering vanishes, indicating that the large SHE observed experimentally in platinum\cite{10} is of intrinsic nature.

In this paper, we study the intrinsic SHE in Pd and Au metals with first-principles band structure calculations. The band structures of Pd and Au have been calculated using a fully relativistic extension \cite{11} of the all-electron linear muffin-tin orbital method \cite{20} based on the density functional theory with local density approximation \cite{21}. The experimental lattice constants for Pd and Au used are 3.89 and 4.08 Å, respectively. The basis functions used are s, p, d and f muffin-tin orbitals \cite{20}. In the self-consistent electronic structure calculations, 89 k-points in the fcc irreducible wedge (IW) of the BZ were used in the tetrahedron BZ integration. The SHC is evaluated by the Kubo formula, as described in Ref. \cite{22}. A fine mesh of 60288 k-points on a larger IW (three times the fcc IW) is used. These numbers correspond to the division of the ΓX line into 60 segments (see Fig. 1).

![Graph](image1)

**FIG. 1:** (color online) (a) Relativistic band structure and (b) spin Hall conductivity of fcc Pd. The zero energy and the dotted line is the Fermi level. The dashed curves in (a) are the scalar-relativistic band structure.

Fig. 1 shows the relativistic band structure of Pd, and also the SHC ($\sigma_{xy}$) as a function of $E_F$. Clearly, the SHC peaks just below at the true Fermi level (0 eV), with a large value of $\sim$1400 ($h/e$)(Ωcm)$^{-1}$. This large value of the SHC is smaller than that of Pt \cite{13}. Nonetheless, it is still orders of magnitude larger than the corresponding value in p-type semiconductors Si, Ge, GaAs and AlAs \cite{22,23}. Note that the SHC in Pd decreases monotonically as the $E_F$ is artificially raised and becomes rather small above 3.0 eV. When the $E_F$ is artificially lowered, the SHC first peaks just below the $E_F$ (-0.3 eV), then decreases considerably, and changes its sign at $-1.2$ eV. As the $E_F$ is further lowered, the SHC increases in magnitude again, and becomes peaked at $-3.0$ eV with a large value of $-2600$ ($h/e$)(Ωcm)$^{-1}$. The SHC decreases again when the $E_F$ is further lowered, and finally becomes very small below $-5.0$ eV. Note that the bands below $-5.5$ eV and also above 0.5 eV are predominantly of 5s character and the effect of the SOC is small.

![Graph](image2)

**FIG. 2:** (color online) (a) Relativistic band structure and (b) spin Hall conductivity of fcc Au. The zero energy and the dotted line is the Fermi level.

We notice that a peak in the SHC appears at the double degeneracies on the L and X points near $E_F$ in the scalar-relativistic band structure (i.e., without the SOC) while the other peak at $-3.0$ eV occurs near the double degeneracies at the L and Γ points (see Fig. 1). The double degeneracy (bands 5 and 6) at L is made mostly of $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ ($z'$: threefold axis), being consistent with the point group $D_{3d}$ at L. The double degeneracy (bands 4 and 5) at X consists mainly of $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ ($z'$: fourfold axis), being consistent with the point group $D_{4h}$. These double degeneracies are lifted by the SOC, with a rather large spin-orbit splitting. As in Pt, the large SHC in Pd may be attributed to these double degeneracies.\cite{14}

The relativistic band structure of Au, and also the SHC ($\sigma_{xy}$) as a function of $E_F$ are displayed in Fig. 2. It is clear that both the shape and amplitude of the SHC versus $E_F$ curve (Fig. 2b) of Au are very similar to that of Pd (Fig. 1b) and Pt \cite{13}. This is because the band structure of Au (Fig. 2a) is rather similar to that of Pd (Fig. 1a) and Pt \cite{13}. However, because Au has an extra valence electron and hence its d-band is completely filled, the $E_F$ falls in the broad 6s6p band where the SOC is relatively small. As a result, the SHC in Au is relatively small at low temperatures [$\sigma_{xy}(T = 0K) \approx 400(h/e)(Ωcm)^{-1}$], being consistent with the previous $ab\ initio$ calculation \cite{22}. Nonetheless, it is a few times larger than the SHC in semiconductors \cite{22,23}.

The SHC can be written in terms of Berry curvature
The spin current operator increases steadily with temperature to reach a value of room relevant to the SHC there. Nevertheless, the SHC at room temperature is in fact larger than the intrinsic SHC in Au at room temperature. This rather strong temperature dependence is also due to the near degeneracy of the Berry curvature for the n-th band, and it is enhanced when other bands come close in energy (i.e. near degeneracy).

The SHC in Au and Pd calculated as a function of temperature using Eq. (1) is shown in Fig. 3. Fig. 3 shows that the SHC in Pd decreases substantially as the temperature (T) is raised above 100 K, although it increases with temperature below 100 K. This rather strong temperature dependence is also due to the near degeneracies since the small energy scale is relevant to the SHC there. Nevertheless, the SHC at room T [\sigma_{xy}(T = 300K) = 350(h/e)(\Omega cm)^{-1}] is still rather large. Interestingly, in contrast, the SHC in Au increases steadily with temperature to reach a value of 750 (h/e)(\Omega cm)^{-1}. This is because the E\textsubscript{F} cuts across the broad 6s6p band in Au. As a result, the intrinsic SHC in Au at room temperature is in fact larger than that of Au and Pt.

Excitingly, giant spin Hall effect at room temperature has been recently observed in a multi-terminal device with a Au Hall cross and an FePt perpendicular spin injector.\textsuperscript{24} The measured \sigma_{xy} \approx 10^3 (h/e)(\Omega cm)^{-1} is orders of magnitude larger than the intrinsic SHC in bulk Au reported above. This obviously indicates that the SHC due to intrinsic SOC in the band structure of pure Au is not the dominant mechanism in the Au/FePt system. Indeed, the authors of Ref.\textsuperscript{24} attributed the giant SHE to the extrinsic mechanism of the skew scattering by impurities in Au. Nonetheless, its microscopic origin remains a puzzle and is currently under intensive investigation.\textsuperscript{25}

The author thanks N. Nagaosa, S. Murakami, T.-W. Chen and S. Maekawa for stimulating discussions and collaboration on spin Hall effect in metals. The author also thanks National Science Council of Taiwan for support, and also NCHC of Taiwan for the CPU time.

FIG. 3: (color online) Temperature-dependence of the spin Hall conductivity \(\sigma_{xy}\) in Pd and Au metals.

\[
\sigma_{xy}(k) = \frac{e}{h} \sum_{m} \Omega_m^z(k) = \frac{e}{h} \sum_{m} J_{m} \Omega_m^z(k),
\]

where the spin current operator \(J_{m}^z = \frac{1}{2}\{s_z, v_m\}\), with spin \(s_z\) given by \(s_z = \frac{\hbar}{2}\beta \Sigma_z\) (\(\Sigma_z\): 4 \times 4 Dirac matrices)\textsuperscript{22}. \(J_{m}\) is the Fermi distribution function for the n-th band at k. \(\Omega_m^z\) can be regarded as an analogue of the Berry curvature for the n-th band, and it is enhanced when other bands come close in energy (i.e. near degeneracy). The SHC for Pd and Au calculated as a function of temperature using Eq.(1) is shown in Fig. 3. This figure shows that the SHC in Pd decreases substantially as the temperature (T) is raised above 100 K, although it increases with temperature below 100 K. This rather strong temperature dependence is also due to the near degeneracies since the small energy scale is relevant to the SHC there. Nevertheless, the SHC at room T [\sigma_{xy}(T = 300K) = 350(h/e)(\Omega cm)^{-1}] is still rather large. Interestingly, in contrast, the SHC in Au increases steadily with temperature to reach a value of 750 (h/e)(\Omega cm)^{-1}. This is because the E\textsubscript{F} cuts across the broad 6s6p band in Au. As a result, the intrinsic SHC in Au at room temperature is in fact larger than that of Au and Pt.

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\[
\sigma_{xy}(k) = \frac{2\text{Im}\{\langle \mathbf{k}|j_{m}^z|\mathbf{k}'\rangle\langle \mathbf{k}'|\mathbf{v}_m|\mathbf{k}\rangle\}}{(\epsilon_k - \epsilon_{k'})^2}, \tag{1}
\]

where the spin current operator \(j_{m}^z = \frac{1}{2}\{s_z, v_m\}\), with spin \(s_z\) given by \(s_z = \frac{\hbar}{2}\beta \Sigma_z\) (\(\Sigma_z\): 4 \times 4 Dirac matrices)\textsuperscript{22}. \(J_{m}\) is the Fermi distribution function for the n-th band at k. \(\Omega_m^z\) can be regarded as an analogue of the Berry curvature for the n-th band, and it is enhanced when other bands come close in energy (i.e. near degeneracy). The SHC for Pd and Au calculated as a function of temperature using Eq.(1) is shown in Fig. 3. Fig. 3 shows that the SHC in Pd decreases substantially as the temperature (T) is raised above 100 K, although it increases with temperature below 100 K. This rather strong temperature dependence is also due to the near degeneracies since the small energy scale is relevant to the SHC there. Nevertheless, the SHC at room T [\sigma_{xy}(T = 300K) = 350(h/e)(\Omega cm)^{-1}] is still rather large. Interestingly, in contrast, the SHC in Au increases steadily with temperature to reach a value of 750 (h/e)(\Omega cm)^{-1}. This is because the E\textsubscript{F} cuts across the broad 6s6p band in Au. As a result, the intrinsic SHC in Au at room temperature is in fact larger than that of Au and Pt.