Spin Hall effect originated from fractal surface

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Abstract

The spin Hall effect (SHE) has shown promising impact in the field of spintronics and magnonics from fundamental and practical points of view. This effect originates from several mechanisms of spin scatterers based on spin–orbit coupling (SOC) and also can be manipulated through the surface roughness. Here, the effect of correlated surface roughness on the SHE in metallic thin films with small SOC is investigated theoretically. Toward this, the self-affine fractal surface in the framework of the Born approximation is exploited. The surface roughness is described by the k-correlation model and is characterized by the roughness exponent $H$ ($0 \leq H \leq 1$), the in-plane correlation length $\xi$ and the rms roughness amplitude $\delta$. It is found that the spin Hall angle in metallic thin film increases by two orders of magnitude when $H$ decreases from $H = 1$ to $H = 0$. In addition, the source of SHE for surface roughness with Gaussian profile distribution function is found to be mainly the side jump scattering while that with a non-Gaussian profile suggests both of the side jump and skew scatterings are present. Our achievements address how details of the surface roughness profile can adjust the SHE in non-heavy metals.

Keywords: spin Hall effect, spintronic, spin–orbit coupling, surface

(Some figures may appear in colour only in the online journal)

1. Introduction

The spin Hall effect (SHE) and its inverse effect (ISHE) are a group of phenomena which stem from spin–orbit coupling (SOC) in non-magnetic metals [1]. The SHE via several mechanisms such as extrinsic, e.g. side jump and skew scattering, and intrinsic [2–8] converts an electrical current to a transverse spin current in non-magnetic layer without using magnetic field (ISHE acts in opposite way exactly). These two effects provide a possibility of detection and generation of spin current in non-magnetic materials [9–11] and have potential applications in novel spintronic devices [12], such as spin-Hall oscillators [13, 14], SHE transistors [15], spin photodetectors [16], spin thermoelectric converters [17, 18], spin Hall magnetic memories [19] and spin separators [20, 21]. In order to benefit from these effects, materials with large spin Hall angle (SHA), the conversion efficiency between spin and charge currents, are required. Heavy metals with intrinsically strong SOC are promising for a large SHA [11], e.g. Pt, Ir, Mo, as a limited list of materials for practical application in spintronic devices. Nonetheless, low-cost light metals show negligible SHE [9], thus introducing techniques to increase the SHE in light metals has made a great challenge.

During the first attempts, heavy metals impurity doping in light metals have found to be promising to achieve large SHA [22–25], e.g. Cu(Pt), Cu(Bi), Cu(Ir). Alternative suggestion was introduced in 2016 to use the surface oxidation to achieve a large SHA in light metals [26]. We note that, these are different to the known interfacial Rashba spin–orbit coupling effect to generate the SHA in metals [27, 28]. Interestingly, an uncorrelated surface roughness has been found as another possible way to produce a large SHA in light metals and it has been also shown that SHA can be enhanced by increasing root-mean-square (rms) roughness deviation or surface roughness fluctuation [29].

The surface roughness is known to be characterized and analyzed by atomic force microscopy (AFM) technique that results in surface topography images. However, these images
have shown that the roughness of the surface has correlated and has self-affine fractal structures [30] contrary to an uncorrelated surface roughness that seems to lack complete information. Moreover, the self-affine fractal surface is analytically characterized through the power-law correlation function, roughness exponent, correlation length, and surface roughness fluctuation [31]. To our knowledge, there is no theoretical study about the SHE originated from correlated and self-affine fractal surfaces. Hence, investigation of the SHE originated from correlated and fractal surface can be a valuable task. Results of this investigation are expected to provide further information in order to obtain an accurate SHA through engineering the surface roughness in metals.

The novelty of this paper is as follows: we present a theoretical description of the influence of self-affine surface roughness with power-law correlation function on SHA in metals with weak SOC (we focus on Cu thin film). To this end, the fractal surface roughness will be regarded as an effective impurity potential as a source of spin scattering [32] and the Fourier transformation of the correlation function of the surface roughness will be described by the k-correlation model [31, 33]. By introducing the SOC associated with effective impurity potential and in the framework of the second-order Born approximation, we determine the spin Hall conductivity (SHC) due to fractal surface roughness. It is also found that the roughness exponent and correlation length have major effects on the SHA and the surface roughness fluctuation has minor effect. Furthermore, the SHA can increase by two orders of magnitude through fractal surface roughness in Cu thin film.

Moreover, we investigate the effects of Gaussian and non-Gaussian distribution functions of surface roughness in SHE and find that if the distribution function of surface roughness taken to be Gaussian, the side jump mechanism contributes to the SHE and the skew scattering does not have any contribution. Contrarily, in the case of non-Gaussian distribution function, the skew scattering can contribute in the SHE.

The rest of this paper is organized as follows. In section 2, a typical model is described for a self-affine fractal surface with power-law correlation function. In section 3, we present a theoretical description for a thin film with generalized correlated surface roughness and obtain the relaxation times using the transition probability. In section 4, we obtain the SHC and describe the influence of Gaussian and non-Gaussian roughness distribution functions on SHC. Finally some general results and discussions and conclusions are presented in section 5.

2. Self-affine fractal model

For a metal thin film with typical self-affine surface, in addition to the rms roughness deviation amplitude $\delta$, we considered the power-law correlation function, $C(r)$, described by a correlation length $\xi$, which demonstrates the average distance between valleys and peaks on the surface, and a local fractal dimension $d_f = 3 - H$. Here $H$ is the roughness exponent ($0 \leq H \leq 1$) and describes the degree of surface irregularity [31, 33].

$$C(r) = \begin{cases} A \left[1 - (r/\xi)^{2H}\right], & (r \ll \xi) \\ 0, & (r \gg \xi) \end{cases},$$

where $A = (\delta/t)^2$ is the dimensionless parameter and $t$ is the average thickness of the metal film. At short length scales ($r \ll \xi$) which the correlation function exhibits power-law behavior, large values of $H$ correspond to smoother surfaces, while small values of $H$ distinguish sharp points protruding or irregular surfaces. The Fourier transformation of the correlation function, $F[C(r)]$ in $k$ space, has the scaling behavior if $k\xi \gg 1$ and the white noise profile if $k\xi \ll 1$. We use $k$-correlation model, to satisfy these asymptotic limits, to describe the power spectrum of self-affine surface,

$$F[C(r)] = \frac{2\pi}{a_0^2} \frac{\xi^2 A}{(1 + ak^2\xi^2)^{1+H}}.$$

The normalization condition $\int_{-\infty}^{\infty} F[C(r)] d^2k = (2\pi/a_0)^2A$, gives the parameter $a_0$, where $a_0$ is the lattice constant, and $k_c = \pi/a_0$ represents the upper cutoff in the Fourier space.

3. Model

We consider a metal thin film ($M$) with rough surfaces. The film with dimensions $\Omega = A \times t$ is confined in the $z$ and extended in the $r = (x, y)$ direction, where $A$ represents the area of the metal film. The Hamiltonian for this system is given by,

$$\mathcal{H} = \frac{p^2}{2m} + uc + u_I + u_R + u_{R_0}.$$

The first term is the kinetic energy with momentum operator $p$ and electron mass $m$. $uc = u_+ \Theta (-z - t) + u_- \Theta (z)$ is the confining potential of $M$, where $u_+$ ($u_-$) is the height of the potential barrier at $z = 0$ ($-t$) and $\Theta (z)$ is a Heaviside step function. $u_I = \sum_{i=1}^{n_{imp}} \delta_B (r - r_i) \delta (z - z_i)$ is the bulk impurity potential with impurity concentration $n_{imp} = N_i/\Omega$, where $N_i$, $n_{imp}$, $k_p$ and $\delta_B$ are the number of impurities, the magnitude of the scattering, the Fermi wave vector and the Dirac delta function, respectively, and $r_i$ and $z_i$ represent the position of $i$th impurity. $u_R = \lambda_r (2mc + z\partial_z mc)$ describes the surface roughness potential with dilation length $\lambda_r = \ln (t/r(r))$ [32], where $t(r)$ represents the thickness of $M$ in $r = (x, y)$. We first assume that the surface roughness profile follows a Gaussian distribution, therefore the volume of the original film with surface roughness remains unchanged after dilation transformation, hence the thickness ensemble average, $\langle \rangle_{ave}$, over roughness profile becomes $\langle t(r) \rangle_{ave} = 1$, thus $\langle \lambda_r \rangle_{ave} = 0$. Furthermore, in this work we have considered the surface roughness is correlated and to be isotropic, therefore the correlation function $C(r = |r' - r|) = \langle \lambda_{r'} \lambda_r \rangle_{ave}$, and its Fourier transformation, $\langle \lambda_{k_f} \rangle_{ave}$, defined by equations (1) and (2). The last term in equation (3) is the spin–orbit
interaction potential due to the correlated surface roughness, $u_R^0 = \eta \sigma \nabla u_R \times (\hat{q} \times \hat{h})$, where $\eta$, $\sigma = (\sigma_1, \sigma_2, \sigma_3)$, and $h$ are the SOC parameter, the Pauli spin operator and the reduced Planck constant, respectively.

We treat $u_t$, $u_R$ and $u_R^0$ as a perturbation in $\mathcal{H}_0 = \left(p^2/2m \right) + u_t$, and take the limit $u_\pm \to \infty$ for simplicity. We obtain the eigenenergies and eigenstates of $\mathcal{H}_0$ for spins with $s = \pm |\hat{z}|$ and in-plane wave vector $k$ and a transverse channel index $n$,

$$E_{kn} = \frac{\hbar^2 k^2}{2m} + E_0 n^2,$$

$$|kn\rangle = \sqrt{\frac{2}{\Omega}} \sin \left[ k_n (z) \right] \exp (i k.r) |s\rangle,$$

where $E_0 = \hbar^2 \pi^2 / 2m r^2$, $k_n = n \pi / l$, and $|s\rangle$ is the eigenspin state with $\sigma |s\rangle = s |s\rangle$.

The three last terms in equation (3) can lead to the transition probability between the unperturbed eigenstates. The transition probability is provided by Fermi’s golden rule,

$$P (|kn\rangle \to |k'n'\rangle) = \frac{2\pi}{\hbar} \left| \langle T_{k'n'} | kn \rangle \right|^2 \times \delta (E_{k'n'} - E_{kn}),$$

where $T_{k'n'}|kn\rangle \equiv \langle k'n'|T|kn\rangle$ describes the scattering matrix element and includes the scattering potential $u_t, u_R$ and $u_R^0$, we find the $T$ matrix element up to second-order by Born approximation [32],

$$T_{k'n'}|kn\rangle = \delta_{kn} \left[ u_{p_{k'n'}} + u_{g_{k'n'}} \right] + \frac{\hbar}{4}\int \sum_{k'n''} \frac{|u_{p_{k'n''}} u_{p_{k'n'}} + u_{g_{k'n''}} u_{g_{k'n'}}|}{E_{k'n'} - E_{kn} + i\epsilon},$$

$$|k'n'\rangle = \frac{|kn\rangle}{\lambda_{k'n'}},$$

where $\delta$ is Kronecker delta, $\epsilon$ is a positive infinitesimal, $\sigma_{k'n'} = \{ s' \sigma | s \}$, $F_{m'}(q) = 2 \sum_{n_{m'}=1}^{N} \sin \left[ k_0 (z_n) \right] \sin \left[ k_0 (z_{n'}) \right] \exp (i q.r)$, and $\lambda_{kn}$ is the Fourier component of $\lambda$ with the wave vector $q = k-k'$. After averaging over impurity positions and surface roughness profile, we find that the scattering probability have two terms, symmetric and asymmetric. We obtain the charge and spin relaxation time via symmetric parts of probability $P_{sym}$,

$$\frac{1}{\tau} = \sum_{k'n'} P_{sym} (|kn\rangle \to |k'n'\rangle) (1 - \delta_{k'n')},$$

with

$$\frac{1}{\tau} = \frac{1}{\tau_0} + \frac{1}{\tau'} (1 + 2\eta^2),$$

where $\tau_0$ is the intrinsic SHC. Because of considering $\mathcal{H}_0$ for spins with $s = \pm |\hat{z}|$ and in-plane wave vector $k$ and a transverse channel index $n$,

Figure 1. Spin Hall resistivity $\rho_{SH} = \sigma_{SH}/\sigma_0$ as a function of resistivity $\rho = \rho/N$, for $l = 10$ nm, $\xi = 1$ nm, $H = 0.5$, $\delta = 5 a_0$, $\eta = 0.5$, $\tau = 2 \times 10^{-15}$ s, $k_F = 3.6 \times 10^{-16}$ m$^{-1}$, and $E_F = 7$ eV.

1. Spin Hall conductivity

The SHE originates from the side jump effect, skew scattering and intrinsic mechanism due to the anomalous velocity, the asymmetric scattering of spin induced by the SOC and the band structure properties, respectively. Hence, the SHC, $\sigma_{SH}$, in thin metal films is given by, $\sigma_{SH} = (\alpha_{side} + \alpha_{skew})$ $\sigma_N + \sigma_{int}$. Here, $\alpha_{side}$ and $\alpha_{skew}$ are the SHA due to the side jump and the skew scattering, respectively. Moreover, $\sigma_N$ is the in-plane conductivity and $\sigma_{int}$ is the intrinsic SHC. Because of considering a thin film with a weak SOC such as Cu, the intrinsic SHC becomes negligible and $\sigma_{int}$ $\approx$ 0 [9, 10]. We assume that an in-plane electric field $E \hat{e}$ is applied along the $M$, where $\hat{e}$ is an unit vector along the electric field $E$. The in-plane longitudinal charge conductivity is obtained from the Boltzmann equation [32] as $J = \sigma_N E = (2\epsilon/\Omega) \sum_{kns}(h/e/m) g_{ksn}$, where $\epsilon$ is the electron charge and $g_{ksn} = -e\tau (h/m) \delta (E_{ksn} - E_F) E \hat{e} \cdot \hat{k}$.

4. Spin Hall conductivity
\[ \delta = a_0, 5a_0, 10a_0 \text{ with } H = 0.7 \text{ and } \xi = 1 \text{ nm}. \]

(d) SHA as a function of surface roughness \( \delta / a_0 \) for three cases of \( t = 1 \text{ nm}, 2 \text{ nm}, 3 \text{ nm} \) with \( H = 0.8 \) and \( \xi = 1 \text{ nm} \). (d) SHA as a function of surface roughness \( \delta / a_0 \) for three cases of \( t = 1 \text{ nm}, 2 \text{ nm}, 3 \text{ nm} \) with \( H = 0.8 \) and \( \xi = 1 \text{ nm} \). (d) SHA as a function of surface roughness \( \delta / a_0 \) for three cases of \( t = 1 \text{ nm}, 2 \text{ nm}, 3 \text{ nm} \) with \( H = 0.8 \) and \( \xi = 1 \text{ nm} \).}

5. Results and discussions

The relation between the spin Hall resistivity and the longitudinal resistivity in bulk SHE is \( \rho_{SH} = \rho + \rho_s^2 \) [10], where the linear term is due to skew scattering and the quadratic term occur as the consequence of side jump mechanism. Also the spin Hall resistivity, \( \rho_{SH} \), due to correlated surface roughness is given by, \( \sigma_{SH} \), equation (14) dividing by \( \sigma^2 \). We show in figure 1 the plot of \( \rho_{SH} \) as a function of \( \rho \) in the unit of \( \rho_0 = 1 / \sigma_0 \) and find that the slope of a power-law fit becomes 2, i.e. \( \rho_{SH} \sim \rho^2 \), which related to the side jump term and this is consistent with our result. So our first result shows that a metal thin film with surface roughness can convert a longitudinal charge conductivity to a perpendicular SHC. Here, the main mechanism in a surface roughness with Gaussian profile is the side jump and the skew scattering does not have any...
contribution in SHC. Contrarily, for a non-Gaussian profile, the skew scattering can contribute in the SHC because of \((\langle u_R \rangle)\) and \(\langle u_R^2 \rangle \neq 0\).

The SHA is given by \(\sigma_{SH}\) divided by \(\sigma_N\). In figures 2(a)-(d), we show the effects of the roughness exponent \(H\), the correlation length \(\xi\), the thin film thickness \(t\), and the the rms roughness deviation \(\delta\) on SHA. In a thinner and a rougher film, the SHA is larger and considerably influenced at large correlation lengths by the roughness exponent \(H\). It shows that the SHA can increase by two orders of magnitude, i.e. SHA% ∼ O(0.1), when the roughness exponent varies from \(H = 1\) to \(H = 0\) in Cu thin film, that is comparable with the bulk of heavy metals such as Pt. As shown in figures 2(a) and (b), the SHA in large scale correlation lengths is enhanced by (i) decreasing correlation length \(\xi\) and (ii) decreasing roughness exponent \(H\). In small scale correlation length, the situation is reversed because in this range the Fourier transform of correlation function has the white noise profile equations (1) and (2). We have also found that in correlation lengths comparable with the lattice constants, \(\xi \sim 0.1\) nm, the SHA is strongly dependent upon the roughness exponent figure 2(b). In addition, we have demonstrated that if the surface is self-affine, major interplay of the SHA of surface roughness occurs for \(H\) and \(\xi\) and the parameter \(\delta\) has a minor effect (especially in thicker films), see figures 2(c) and (d).

The generation of SOC due to the electrons scattering from fractal surface is the main physical reason of these results. When the electrons with velocity \(p/m\) pass through the field, \((\nabla u_R)\), generated via the roughness effects, they feel an effective magnetic field \(B_{eff} \sim \nabla u_R \times (ip/\hbar)\). This effective magnetic field can couple the spin of electrons to the orbital movements, \(\langle u_R^2 \rangle\) in equation (3). Thus, the effective magnetic field and as a result the SHA can be enhanced by increasing of \(u_R\). Therefore, any mechanisms that increases the scattering of electrons from the fractal surface can be effective in increasing the SHC and SHA such as decreasing the correlation length and the roughness exponent.

Based on experimental reports, the SHA increases by increasing the surface roughness in thin films [36, 37] which seems to agree with our aforementioned argument. Based on our results proposed in this paper the SHA due to fractal surface roughness is obtained in thin metal films. This can approach better to any experiments as the AFM information suggests that surfaces are correlated and have self-affine structure and other parameters such as the correlation length \(\xi\) and the roughness exponent \(H\) can contribute in the SHE. Furthermore we show that, in figure 2(c), the SHA increases with decreasing the metal film thickness \(t\), opposite to the SHA in bulk heavy metals or in heavy metals impurity doped thin films. This characteristic makes it possible to distinguish the fractal surface roughness origin of the spin Hall effect experimentally.

In conclusion, we study the contribution of correlated surface roughness and the fractality effects on the spin Hall effect of metallic thin films with self-affine correlation as a more realistic model. In the group of three surface roughness

parameters \((\delta, \xi, H)\), major interplay of the roughness effect occurs for \(H\) and \(\xi\). The parameter \(\delta\) has a minor contribution (especially in thicker films). The roughness exponent \(H\) has a powerful impact on the spin Hall angle mainly for relatively large correlation lengths that can increase the spin Hall angle for Cu thin film two order of magnitude. The spin Hall angle due to fractal roughness scattering increases with decreasing the correlation length and roughness exponent, and the film thickness in large scale, whereas the situation is reversed in small scale. Moreover, two different surface roughness distributions, namely the Gaussian and the non-Gaussian profile, have been examined. It is shown that for the Gaussian profile the only side jump mechanism will contribute on the spin Hall effect, while for the non-Gaussian one both side jump and skew scattering mechanisms play roles. Results reveal additional contribution from statistical information at surface of thin films which have important effects on the spin Hall effect. It is interesting to explore the contribution of non-Gaussianity and multifractality nature in overall behavior of SHE, and we will address them in future.

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