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Modeling and Simulation of Electron Spin Transport at LaAlO3/SrTiO3 Interface based Quantum Nanowire

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Abstract:

Interface between two band insulators LaAlO3 (LAO) and SrTiO3 (STO) forms a two dimensional electron gas (2DEG) owing to a polar discontinuity at the interface giving rise to an electrostatic potential. The LAO/STO is an excellent system to exhibit metal-insulator transition and the formation of 2DEG plays exciting role in the electron transport over the interface plane. Reports are made on some studies based on modeling and simulation of transport properties in 2DEG nanowire formed at atomically sharp LAO/STO (001) heterointerface considering the effect of Rashba spin orbit interaction (RSOI). It is observed that the conductance and the spin polarization may be controlled and manipulated by Rashba spin orbit interaction (RSOI). Rashba field modulated current peaks are also observed at definite values of electron energies signifying the effect of conductance quantization.

Keywords **— LAO/STO, Rashba, NEGF, Landauer-Buttiker, 2DEG, Band inversion**

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I. INTRODUCTION

Spin dependent transport in nanostructures manifests many interesting properties for application in spintronic devices. Coupled spin orbit dynamics of electrons in oxide interfaces, such as in LaAlO3/SrTiO3 (LAO/STO) system has widely been investigated [1-2] to explore possible spintronic applications. Successful growth technique of thin epitaxial films has made possible to form a confined two dimensional electron gas (2DEG) of high mobility [3] at the LAO/STO hetero-interface. These materials in contact with each other form an atomically sharp interface, where a polar charge discontinuity [3-4] is developed due to the mismatched electric boundary condition created by the dissimilar charges at the different atomic planes of the two materials in their (001) orientations. Along the orientation, with its alternating planes of AlO2- LaO+ / non-polar TiO2 interface leads to a macroscopic internal electric field in LAO giving rise to a diverging potential build-up with increasing film thickness of LAO. This so called polar catastrophe is resolved by consequent induced bending of LAO bands through electronic reconstruction over a critical length scale: at a critical thickness of LAO its valence O 2p bands reach the level of the STO Ti 3d conduction bands at the interface; this makes electrons to transfer from the charged surface AlO2- layer to the interface TiO2 charge-neutral layer. The transferred electrons through this reconstruction process occupy the Ti 3d conduction bands and form the 2 DES at the hetero-interface. These occupied conduction bands formed out of Ti(d) t2g states contribute to the electron transport at the LAO/STO heterointerface [5]. Density functional theory (DFT) calculation shows an increase of the interfacial charge density with increase in the number of LAO unit cells [6]. Increased charge transfer to the STO substrate for increasing film thickness of LAO is an

indication of insulator-to-metal transition of LAO/STO hetero-system with decreasing bandgap.

The conductive heterointerface of the LAO/STO system lacks an inversion centre and the broken structural inversion symmetry at the interface along the growth direction of the heterostructure causes the oblique orbital angular momentum and electric charge asymmetry to induce Rashba spin-orbit interaction (RSOI) resulting in splitting of the energy bands. The RSOI can be tuned by modulating the shape of the confining potential at the interface [7] and is applied in modern spintronic devices. The concept is used in the prediction of low consumption and fast switching spin_FET [8]. Its effect on the d-electrons in the t2g subband has been investigated in detail and predicted band inversion at the Γ point (zone centre) of Brillouin zone [1-2,9]. RSOI, a main ingredient of two dimensional topological insulators explains inversion of the parabolic profiles of conduction and valence bands and a consequent transition of metal to insulator.

State of art technology in manoeuvring the spin in nanostructures requires more theoretical understanding in physics and experimentation. Realization of long range spin transport is really a difficult task [10]. Only few reports on spin transport on 2DEG LAO/STO interface transport are available. Recently, an experimental demonstration of room temperature spin transport in the above system has successfully been made [10]. Only few literatures and reports on spin transport of the 2 DEG electrons at the LAO/STO interface are available.

In the present work, an attempt is made to study the electron transport of two dimensional d-orbital electrons in the LAO/STO (001) heterointerface nanowire (NWR) with and without the effect of RSOI. The work involves mathematical modeling and simulation and is based on the tight binding (TB) approach in the numerical computation.

The paper is organised as follows: in Section 2 theory and model, in Section 3 results and discussion and in Section 4 conclusion.

II. COMPUTATIONAL DETAILS

The underlying theory to frame the modeling and subsequent simulation of the work are given in separate subsections below.

A. Mathematical Modeling

Introducing the Rashba spin orbit interaction in the spinless Hamiltonian [11] of the tight binding approximation describing a two dimensional lattice of LAO/STO interface, we write down the total Hamiltonian [12] as

$$H=-t_1\sum_{n,\alpha} c^{+}_{n1\,n\alpha} c_{n2\,n\beta} - t_2\sum_{n,\beta} c^{+}_{n2\,n\beta} c_{n1\,n\alpha} + i\lambda_R \sum_{\langle i,j\rangle\alpha\beta} c^{+}_{i\alpha} \left(\sigma \times \hat{d}_{ij}\right)^{z}_{\alpha\beta} c_{j\beta} + h.c \quad (1)$$

$c_{i\alpha}^{+}$ ($c_{i\alpha}$) being the creation (annihilation) operator of electron with spin α at the site i, $\langle i,j\rangle$ being the summation over all pairs of nearest neighbour sites and σ being the Pauli's matrix vector. The first and second terms represent nearest neighbour intra-planar (x-y plane) hopping energy operators and the third term is the Rashba interaction energy operator. The unit crystal cells are labelled by n (= n1, n2 in the x and y directions) and α, β being the spins at the atom sites in the cell. For non-interacting systems in equilibrium, the non-equilibrium Green function (NEGF) formalism is equivalent substitute of Landauer-Buttiker (LB) formalism. Using the single particle Green function formalism, the total conductance (i.e., charge conductance) of two terminal device can be obtained within the LB framework as [13]

$$G(E)=\frac{e^2}{h}T_{pq}(E)=\frac{e^2}{h}Tr[\Gamma_p(E)G^{R}(E)\Gamma_q(E)G^{A}(E)] \quad (2)$$

where $\Gamma_{p(q)}=i[\Sigma^{R}_{p(q)}-\Sigma^{A}_{p(q)}]$ is the coupling matrix between the input (output) leads p(q) and the conductor, Σ s are the lead self energies and $G^{R(A)}$ being the Green retarded (advanced) function. Spin polarized conductance is given [14] by

$$G_m(E)=\frac{e^2}{h}Tr\left[\hat{\sigma}_m \Gamma_p(E)G^{R}(E)\Gamma_q(E)G^{A}(E)\right] \quad (3)$$

where $\hat{\sigma}_m$ is the Pauli matrix vector with m= x,y,z denoting the directions of spin polarisation **P.**

The magnitude of spin polarisation in any direction is given by

$$P_m(E) = G_m(E)/G(E) \quad (4)$$

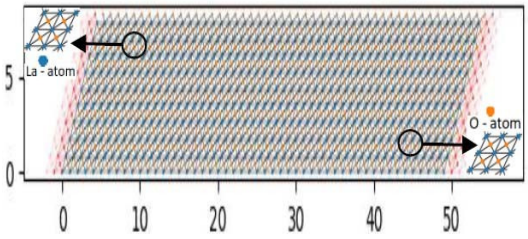

Fig.1(a)

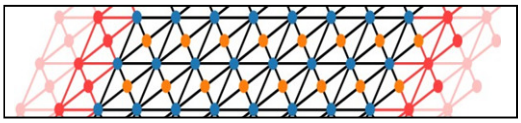

Fig.1(b)

Fig.1 Polyatomic rhombic structure of LAO/STO interface (fig 1(a) simulated structure; insets show locations of O and La atoms and fig 1(b) part of fig.1(a) zoomed).

To obtain total spin current $I_q^{s\alpha}$ in the leadq of two terminal device driven by a voltage bias we use the LB formula obtained in the NEGF formalism [13] and therefore write,

$$I_q^{s\alpha} = \frac{1}{e}\int_{-\infty}^{+\infty} G_m(E)\{f_p(E)-f_q(E)\}dE \quad (5)$$

The spin current is constructed from the spin resolved charge currents I_q^{σ} where $\sigma=\uparrow,\downarrow$ is the spin quantisation axis chosen along e_α.

B. Simulation

The NEGF formalism is employed to obtain the transport parameters within the Landauer-Buttiker scattering/transmission formalism [13] For simulation purpose, we use the simulator Kwant, a python based package built on the framework of tight binding (TB) Hamiltonian [15].

The structural geometry of the interface is polyatomic rhombic [11]. Central portion (the extended region, marked blue) of the diagram is the "system" representing the two dimensional scattering region of the LAO/STO interface and the red portions at the two ends are the two periodic semi-infinite ballistic "leads" carrying the incident input wave and the scattered output wave, terminating at the two reservoirs, source and drain respectively [13]. The source bound lead and the drain bound lead are at different potentials. The leads are represented by a linear chain of atoms of one or more orbitals. Interaction between the inter-atom or intra-atom orbitals are given by the hopping matrix elements. Nature and number of these hopping elements in intra-rhombohedral or inter-rhombohedral atomic structure in LAO/STO interface influence the band structure of the LAO/STO based nanowire. Tight binding approach is employed because the system is defined so as to interact only with the nearest neighbors. This allows one to deal with the Hamiltonian of the system in a convenient and solvable way. The "orange" and "blue" dots in the rhombic structure (fig.1b), part of fig.1a zoomed for clear visibility, are the oxygen (O) atoms and lanthanum (La) atoms respectively. Length and width of the system considered for the transport are taken to be 50 atoms long and 10 atoms wide respectively. Such a small width is taken to take care of coherent length scale to maintain the quantum transport.

A conducting interface can be obtained by depositing four or more unit cells on a TiO2 terminated (001) STO crystal, where a SrO terminated crystal leads to an insulating surface [3]. Controlled thickness of LAO is assumed to be grown epitaxially on the substrate STO such that the LAO/STO interface conduction electrons in the NWR may exhibit initially a metallic character. The ordinary band insulting material STO now behaves as a topological insulator in the LAO/STO system under this structural composition. Band overlapping between valence band of LAO with the Ti 3d conduction band of STO occurs at this interface due to the reason explained earlier.

III. RESULTS AND DISCUSSION

The quantum transport is studied on the (001) directed crystallographic orientation of the LAO/STO interface. Initially the existence of both the crystal inversion symmetry and time reversal

symmetry in the bulk STO make its band spin-degenerate. At

LAO/STO interface, however, the crystal inversion symmetry is broken and causes a triangular potential profile, owing to the reason of polar catastrophe, to appear at the interface. This produces an internal electric field perpendicular to the interface. Resulting Rashba field potential now plays a role to lift this degeneracy. As a result, inversion in the parabola profiles of both the conduction and valence band sets in at and near the r point [fig.2]. This is depicted by the reversal in the directions of the curvatures of the two bands. The energy dispersion plot is given in the direction of kx=0 and the r point corresponds to the point of zero momentum.

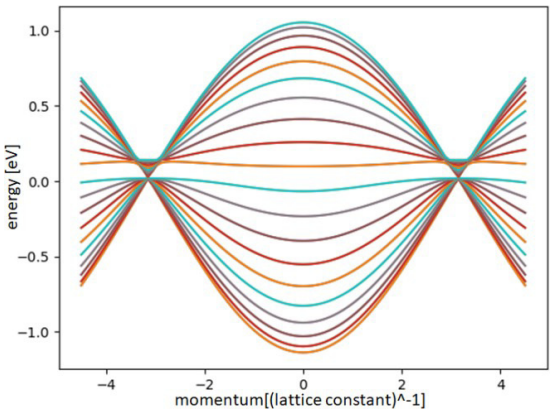

Fig.2 Inverted structure of the conduction and valence bands at the LAO/STO interface.

To explain this band inversion mechanism, we look first at the initial state of the metallic conductivity of LAO/STO interface [3]. This is a result of overlapping of the LAO valence band with the Ti(d) t2g conduction band of STO at the interface with gapless energy spectrum.

Let us now consider the Rashba spin splitting of the orbitals in the interface layer at the r point [16]. All the 3d conduction bands of STO exhibit a parabola like (concavity upwards) behavior near the r point and are degenerate at that point in absence of spin orbit interaction. The O 2p valence band of LAO is also parabolic with concavity downwards. The density functional theory calculation shows that in n-type LAO/STO bilayers, the top of the valence band surface AlO2 layers crosses the Fermi level at a critical thickness of LAO. This causes electron transfer from LAO to Ti-3d bands of the interface STO unit cells. This is recognized as conduction and valence bands overlapping with two crossing k-points at two sides of the r point with no bandgap. When the spin orbit coupling (SOC) is taken into account a gap opens at the crossing points and separated and distinct conduction and valence bands appear. This has contributions from the band that made the valence band originally and vice versa. This creates convex hump in the Ti 3d conduction band and concave dip in the LAO valence band at the LAO/STO interface [fig.2].

Electron energies in this figure and in all other subsequent figures are given with reference to the Fermi level (set to 0 value, shown by horizontal line at energy=0). Above this line, all levels are unfilled and below it all are filled because the temperature is assumed to be low. This fact is cosidered in the Kwant code [15] taking the electron distribution to be highly degenerate.

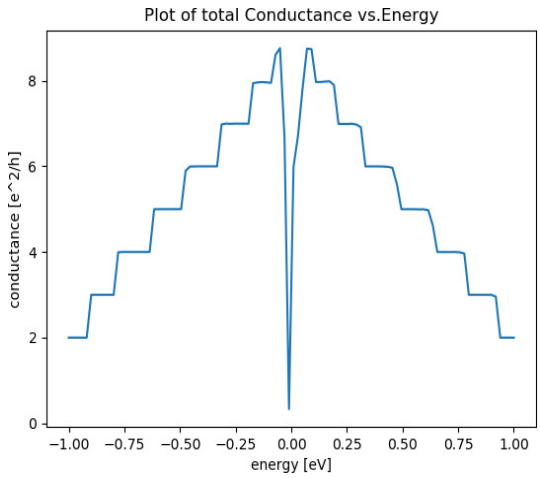

Fig.3 Plot of total conductance of the 2D LAO/STO interface as a function of energy.

The region of inversion is restricted to k values within the first Brillouin zone. Total conductance of the 2D LAO-STO interface is plotted in fig.3 as a function of energy using eqn.(2).

For energies below the Fermi level in the conduction band, the total conductance by the

occupied electrons is seen to increase in gradual steps with energy while that for electrons above the Fermi level decreases with increasing energies. This is because higher the energies higher is the number of conducting channels below the Fermi but is not so above the Fermi. A sharp dip in the conductance is observed at the Fermi level. It signifies the fact that a sharp transition of the electron population takes place just below and immediately above the Fermi energy. Gradual depopulation of the step-like energy levels above the Fermi results in such a corresponding decrease of the conductance.

The spin conductance with and without RSOI is plotted in figs.4 as a function of energy using eqn.3. The nature of conductance with varying energy without any RSOI (fig.4a) shows that the conductance is insignificant throughout the energy range except at and very close to the Fermi level. The merged energy bands in absence of the spin orbit interaction is not split-off.

This leads to conclude that the spin polarization, on an average, is finite but small in that range and accordingly the spin conductance is also finite and small. This may possibly be due to the reason that the spin flip scattering of the conduction electrons by magnetic impurity (developed magnetic dipoles) at the LAO/STO heterointerface causes spin polarization of the Fermi electrons [17].

Plot of spin polarized conductance with varying energy in presence of the RSOI is depicted in fig.4(b). Effect on the spin conductance for two different strengths (λ_R) of Rashba interaction is demonstrated in the same figure by superposition of the two corresponding plots. Different values of Rashba coefficients may be possible to obtain by modulating the number of unit cell thickness of the interfacial layer of the heterojunction plane of LAO/STO system [18]..

In the work, two nominal values of Rashba coefficients are taken as 0.019 eV.A0 and 0.25 eV.A0. The spin conductance for small Rashba field exhibits relatively large amplitude fluctuations close to the Fermi level and decays appreciably away from it. The spin dephasing directly depends upon the orientations of spin with reference to the in plane or perpendicular plane of the 2D interface well. Dominant spin dephasing/relaxation of the 2D interface electrons is due to the momentum dependent effective magnetic field (Rashba effect) arising out of the structure inversion asymmetry [19]. Also, the Larmor precession frequency of the spin axis increases with this effective magnetic field and, in turn, with the strength of Rashba effect. Average Larmor frequency of the electrons within a short range of energies centered around the Fermi level is assumed to be such as to make the momentum relaxation time of the scattered electrons very small while the spin dephasing time to be correspondingly high.

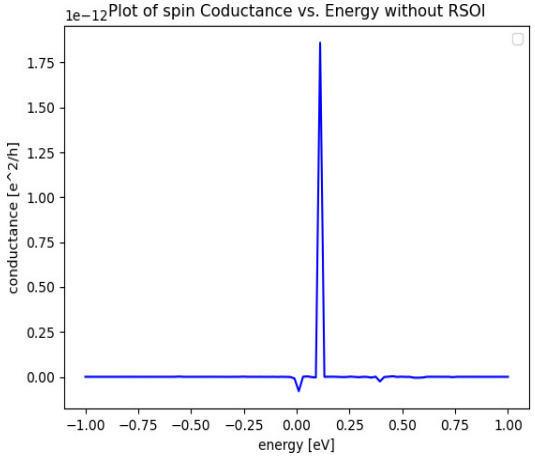

Fig 4(a)

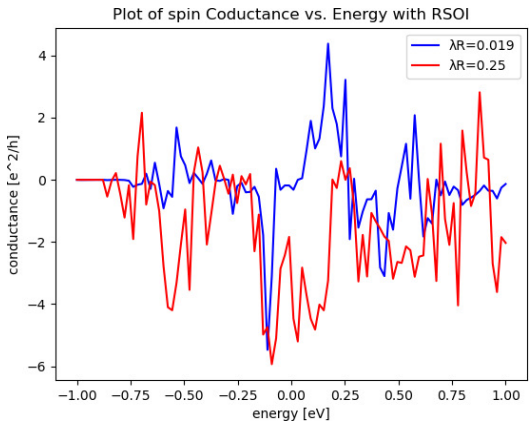

Fig 4(b)

Fig.4 Plot of spin polarized conductance of the 2D LAO/STO interface as a function of energy (fig 4(a) without RSOI and fig 4(b) with RSOI).

A close look to the plots in fig.4 clearly shows decaying fluctuations of conductance all over the energy range under consideration except in a short range around the Fermi level. This range increases with increasing strength of Rashba field obeying the principle of spin dephasing/relaxation explained above.

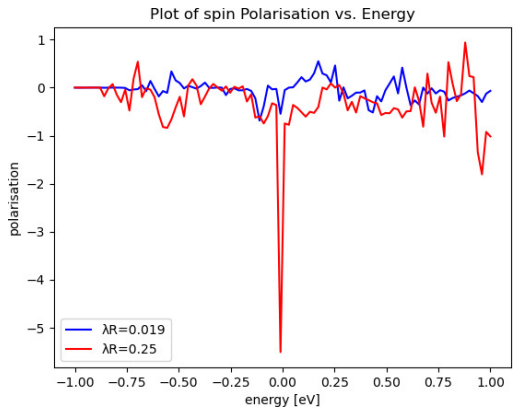

Fig.5 Plot of spin polarization of the 2D LAO/STO interface electrons as a function of energy.

A plot of the spin polarization with energy is given in fig.5 using eqn.(4). Net spin polarization value of conductance reflects a numerical measure of the difference between the positive and negative peak values of the conductance. It is also to be remarked here that the conductance fluctuation is a direct mapping of the fluctuation of spin polarization which is evident from the corresponding figures. This entire observation implies that a net spin polarization may occur if

$$P_{m\uparrow\uparrow}(E) \neq P_{m\downarrow\downarrow}(E)$$

and hence

$$G_{m\uparrow\uparrow}(E) \neq G_{m\downarrow\downarrow}(E)$$

It may further be concluded from fig.5 that the spin polarization and hence the spin conductance are substantially affected by strong Rashba interaction while they are not so for weak ones.

Study on the spin polarized transport is also made to investigate the effect of Rashba coupling strength on the current dependency on electron energy in the LAO/STO interface NWR (fig.6).

For stronger Rashba interaction, the increasing effect on current-voltage relation in the wire is prominent. This result is in conformity with the observation on the nature of variation of the spin resolved conductance with energy shown in fig.4b. Higher conductance is observed because of strong RSOI and this naturally results in higher current. The current shows peaks at definite values of energies for which the discretized conductance is substantially large. The insignificant current contributed by electrons above the Fermi level is justified because of the scanty electron population above the Fermi. It is also observed that the current is affected prominently at stronger RSOI and thus can be controlled by the Rashba field.

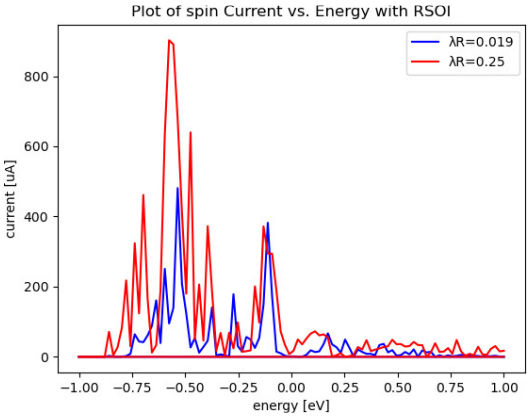

Fig.6 Plot of spin polarized current of the 2D LAO/STO interface NWR a function of electron energy.

All the observations made in the plots given in figs. (4b) through fig. 6 may be shown to be in conformity with the nature of the inverted band depicted in fig. 2: with decrease in momentum the electron energy increases and vice-versa. This, in turn, corresponds to the decrease of RSOI with increase of energy and vice-versa. The increase of spin polarization and hence the spin conductance and the spin current with increase of the Rashba interaction, which in turn, with decrease of electron energy is clearly indicated in the above plots. The variations are strengthened with the strength of RSOI.

IV. CONCLUSION

In the present work, spin polarized electron transport in the 2DEG nanowire formed at the (001) oriented LAO/STO heterointerface is examined through NEGF calculations. Band merging of the STO Ti 3d conduction bands with the O 2p valence band of LAO of at least a critical thickness without any spin orbit interaction shows in simulation a band separation with a gap in between under spin orbit interaction. The band inversion, a key ingredient of topological insulating material, is discussed based on the concept in [16]. Simulated study gives clear signature of the formation of 2DEG at the interface of the perovskite oxide system and its electron transport is observed to be controlled by the Rashba field.

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