Strain effects on structural and magnetic properties of SrIrO$_3$/SrTiO$_3$ superlattice

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1. Introduction

Efficient means of controlling physical properties of materials, such as electronic and magnetic properties [1–3], with external stimuli is vital for functional devices [2–4]. One such interesting relation is the interplay between strain and magnetization. A stress/strain field can be used to control the magnetic properties of materials through magnetoelastic (ME) coupling [5–7]. For example, at low temperatures the magnetic moment in La$_{0.8}$Sr$_{0.2}$CoO$_3$ is slightly reduced with a tensile strain [6], and growing SrRuO$_3$ on a biaxially strained substrate leads to a decrease in the magnetic moment and Curie temperature [5]. Furthermore, if ferroelastic and ferromagnetic orders coexist in a single material, magnetic properties can be indirectly altered with an external strain. Such correlation between magnetic order and strain can create suitable conditions for assistive switching of magnetic orders in device applications [8–10]. Magnetoelastic coupling can also induce phase transitions in oxide compounds [9,11–15]. For instance, in perovskite oxide thin films, substantial strain could trigger a magnetic phase transition from ferromagnetic to antiferromagnetic coupling [16,17], which could be coupled with the tilting or rotation of the oxygen octahedra. Additionally, paraelectric SmFeO$_3$ could become ferroelectric using interfacial strain, and consequently become multiferroic materials [11]. Similar effect is observed for NaMnF$_3$ using epitaxial strain [9].

The ME coupling in complex oxides can be influenced by several factors, including structural distortions under strains, electronic interaction, and most importantly the spin-orbit coupling (SOC) [10,18–20]. In particular, 5$d$ transition metal oxides (TMO) receive increasing attentions due to the significant amplitude of the SOC [18–24]. For instance, SOC of Ir is about ~380 meV [21,25], which could exceed the correlation of 5$d$-electrons [26]. The large SOC in paramagnetic SrIrO$_3$ (SIO) can be used to tune the magnetic anisotropy of the neighboring manganite layer through proximity effect in manganite-iridate superlattice [20,27,28]. Therefore, it is possible to effectively manipulate the ME coupling through the strong SOC of 5$d$ orbital. Indeed, both theoretical and experimental studies of Sr$_2$IrO$_4$ have shown the existence of strong interplay among strain, octahedral rotation, and magnetic properties, suggesting that Sr$_2$IrO$_4$ possesses large ME coupling [23,29,30].

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structural distortions in oxide superlattices could be more sensitive to strain and an interesting effect can be found therein. Besides, the fundamental understanding of the interplay between strain and SOC is limited and it will be vital for controlling the ME coupling in materials.

In this study, we focus on the effects of strain, both tensile and compressive, on the structural and magnetic properties of SrIr-O$_3$-SrTiO$_3$ (SIO/STO), which consists of alternating single layer of SIO and STO. Crystal structures with different rotation patterns have been examined by first principle density functional theory (DFT) studies and compared with the results from x-ray diffraction measurements. Moreover, the most stable magnetic configuration of SIO/STO is identified using DFT and compared with experimental measurements. In addition, we have investigated the effects of epitaxial strain on the octahedral distortions, magnetic moments, and in-plane anisotropy. A systematic analysis on the correlation between octahedral rotation (tilting), magnetic structure, and Dzyaloshinskii-Moriya interaction is also presented.

### 2. Computational and experimental details

First principles density functional theory (DFT) calculations were performed using projector-augmented wave techniques in Vienna ab-initio Simulations Package (VASP) [31]. The Perdew Becke Ernzerhof (PBE) within the General Gradient Approximation (CGA) is used for the exchange and correlation interactions [32]. The Kohn–Sham wave function is described using plane wave basis set that are expanded to the cut-off energy of 550 eV. For proper description of the electron correlation we have included Hubbard correction to the 5d and 3d orbitals of Ir and Ti, respectively, using the Liechtenstein method [33,34]. The suitable values of U(J) are identified to be 2.2 (0.2) eV and 5(0.64) eV for Ir and Ti [35] d-bands, respectively. These parameters (U) ensure that the ground state of the SIO-STO superlattice remains an insulator within the investigated range of the strain up to 0.9% [36]. Firstly, the equilibrium structure of SIO/STO is obtained by fixing the in-plane pseudocubic lattice constant a and b to that of STO, i.e. 3.969 Å for PBE a=U, and optimized value of the in-plane lattice constant is compared with available results [35]. We define this in-plane lattice size as the zero-strain structure in our study, since all the reported experimental results are on samples grown on STO. For equilibrium structure of SIO/STO the c/a is found to be 1.0003, where c is the averaged out-of-plane pseudocubic lattice parameter of the two layers. The epitaxial strain effects are investigated by sequentially varying the in-plane lattice constants. Thereafter, the c/a is optimized for each value of strain. During these procedures, we have relaxed the structures until the force on each atom is less than 5 meV/Å. Due to the large SOC of 5d electrons of Ir, the magnetic properties are determined by including SOC in the calculation.

Analogous to the zero-strain reference structure of the calculation, the superlattice SIO/STO sample on commercial SrTiO$_3$ (001) substrate was fabricated by means of pulsed laser deposition technique [37]. The superlattice was grown epitaxially in layer-by-layer fashion and the thickness of the SIO/STO layer was precisely controlled. Synchrotron X-ray diffraction experiments were performed via the 33BM beamline and the 8IDB beamline at the Advanced Photon Source. Reciprocal space was defined based on a unit cell of a × a × 2c. To explore the magnetic anisotropy, in-plane and out-of-plane remnant magnetizations were measured in a superconducting quantum interference device. Before the measurement, the sample was first cooled down to 5 K under a 5 kOe magnetic field and the magnetic data was recorded during warming process without magnetic field on.

### 3. Result and discussion

#### 3.1. (a) Structural properties of SIO/STO

When both SIO and STO layers are monolayer-thick, the superlattice can be considered as a double perovskite Sr$_2$IrTiO$_6$ where the two B-sites alternate along the c-axis to form a supercell. As pointed out by Glazer, there are multiple structural distortions of perovskites from the pseudocubic structure when cations are displaced and the anion octahedron is tilted or rotated [38]. Bulk SIO and STO have octahedral rotation pattern C$^4$/C$^2$- and A$^4$C$^1$-, respectively [39,40]. The octahedral network of the Sr$_3$IrTiO$_6$ superstructure may adopt one of these two cases, or an intermediate one a-a$^1$. Previous studies on this superlattice have considered the situation of A$^4$C$^1$-, where c-axis is along the z-axis of the supercell [36,41]. In this case, the neighboring IrO$_6$ and TiO$_6$ rotations are out-of-phase, but all adjacent IrO$_6$ layers are in-phase with the planar oxygen ions remaining in the plane, in analogy to Sr$_3$IrO$_6$. However, if octahedral tilting occurs (i.e., a$^0$A$^0$C$^1$- → a$^1$A$^1$C$^1$-), the oxygen ions will move away from the plane of the B-sites, lowering the symmetry from tetragonal to monoclinic. Fig. 1 (c) and (d) show these two possible crystal structures of a-a$^1$C$^1$- and a-a$^1$C$^1$- (c$^1$) rotations. The difference between these two structures is that the two dissimilar octahedra (IrO$_6$ and TiO$_6$) are rotated about the z-axis of the supercell in-phase and out-of-phase, respectively. Therefore, for the SIO/STO superlattice it’s crucial to identify the proper rotation and tilting pattern of the oxygen octahedra in both theoretical and experimental studies before the electronic and magnetic properties are determined. From the DFT perspective, we evaluated three possible initial structure of SIO/STO at the zero-strain state, i.e. c$^1$-, c$^1$- and c$^0$ with different initial rotation and tilting angles and then relaxed the system. In all cases tested using DFT, we found that the SIO/STO superlattice relaxes to a c$^1$ rotational pattern with a small but finite a-a$^1$ tilting component as shown in Fig. 1 (b). Hence the in-plane oxygen ions will slightly shift (γ) upward or downward from their planar position.

X-ray diffraction patterns were correspondingly measured and analyzed to determine the structural parameters of the superlattice grown on STO substrate. The weak rotation/tilt diffraction peaks were accessed with the aid of Synchrotron X-ray beam. We performed a scan along the (0.5 1.5 L) truncation rod (Fig. 2), which covers various rotation peaks [37,38]. The relative ratios of integrated intensity of neighboring reflections were then extracted. We have observed both L-odd and even peaks characteristic of the c$^1$- and c$^1$- patterns of simple perovskite, respectively [38]. When considering the enlarged cell of the superstructure, both types of peaks could coexist due to the fact that the rotation magnitudes of IrO$_6$ and TiO$_6$ octahedra is expected to be different [38,42]. This magnitude difference would be the main cause for the L= odd peaks in the case of a c$^1$ pattern. Thus, they would be expectedly much weaker compared with the (0.5 1.5 even) peaks. However, we found that both (0.5 1.5 2n+1) (n = 1 and 2) peaks host stronger intensity than their L=2n counterparts. This observation strongly suggests a c$^1$ pattern in the present superlattice since an out-of-phase rotation relation would create an octahedral superstructure along the z-axis and dominate the structural factor at L = odd. To further verify this argument, we simulated the structural factors of these peaks of two lattice structures with opposite octahedral rotation, which are obtained from the aforementioned theoretical optimization. We found that indeed only the c$^1$-structure can produce much stronger L= odd peaks as compared with the L= even ones.

Experimentally, we also investigated the tilting pattern of the superlattice. Multiple (0.5 0.5 L) reflections corresponding to the out-of-phase a-a$^1$ tilting motion were observed, while no in-phase
A tilting peak has been found. These \((0.5\ 0.5\ \mathbf{L})\) reflections are significantly weaker than the \((0.5\ 1.5\ \mathbf{L})\) peaks, indicating the octahedral tilt angle is much smaller than the rotation angle. These observations are consistent with the DFT calculations in such a way that the ground state energy of the superlattices with a small \(a\)-\(a\) tilting component is always more stable than the untilted superlattices. Due to the strong coupling between lattice structure and various physical properties in iridates \([25]\), one may expect a significant difference between the superlattice and the bulk \(\text{Sr}_2\text{IrO}_4\), especially on the magnetic structure.

3.2. (B) The structural response to epitaxial strain

The \(\text{IrO}_6\) octahedra in the zero-strain structure of \(\text{SIO}/\text{STO}\) superlattice is rotated by \(14.2^\circ\) from the undistorted structure. Similarly, tensile strain suppresses the rotational angle of \(\text{TiO}_6\) octahedra by approximately the same order of magnitude like that of \(\text{IrO}_6\) as plotted in Fig. 3 (b). These findings on the equilibrium structure as well as the effects of strain reasonably agree with similar studies on Ir based oxide systems \([41,43]\). Particularly, our results on the variation of the rotational angle \(\text{IrO}_6\) caused by tensile (compressive) strains show the same trend as in Ref. \([43]\).

Previously, we have pointed out that the two octahedra rotate in an opposite way about the \(z\)-axis and there is a difference in the rotational angles of \(a\) and \(q\) (phase difference). Combining the effects of strain on both rotational angles \((a\) and \(q\)), we observe that the phase difference between \(\text{TiO}_6\) and \(\text{IrO}_6\) octahedra reduces (increases) because of higher tensile (compressive) strains. Additional distortion in \(\text{SIO}/\text{STO}\), induced by the epitaxial strain, is the tilting of \(\text{TiO}_6\) and \(\text{IrO}_6\) octahedra \((b)\). Unlike the rotational angles, the tilting angle increases with tensile strain, shown in Fig. 3 (c). Whereas, it decreases for compressive strain of \(0.9\%\) by about \(0.8^\circ\). These results indicate that the tilting angle is more susceptible to the epitaxial strain than the in-plane octahedra rotations. It is worthwhile to mention that we have found an increase in the tetragonality \((c/a)\) of \(\text{SIO}/\text{STO}\) as we introduce compressive strain. Hence, the out-of-plane (in-plane) Ir-O bond length becomes longer (shorter).

3.3. (C) Magnetic properties of equilibrium \(\text{SIO}/\text{STO}\) structure

The \(\text{IrO}_6\) octahedra in the zero-strain structure of \(\text{SIO}/\text{STO}\) superlattice is rotated by \(14.2^\circ\) from the undistorted structure. Likewise, a smaller in-plane rotation angle of \(4.25^\circ\) is found for \(\text{TiO}_6\) octahedra. Thereafter, the effects of epitaxial strain on octahedral rotation and tilting are studied and shown in Fig. 3. The variation of the rotational angle of \(\text{IrO}_6\) octahedra in \(\text{SIO}/\text{STO}\) as a function of strain is illustrated in Fig. 3 (a). When the tensile strain of \(0.9\%\) is introduced the rotational angle of \(\text{IrO}_6\) \((a)\) octahedra decreases by \(0.65^\circ\) as compared to the structure without strain. In contrast, compressive strain enhances the rotation of \(\text{IrO}_6\) octahedra. Additionally, tensile strain suppresses the rotational angle of \(\text{TiO}_6\) \((q)\) octahedra by approximately the same order of magnitude like that of \(\text{IrO}_6\) as plotted in Fig. 3 (b). These findings on the equilibrium structure as well as the effects of strain reasonably agree with similar studies on Ir based oxide systems \([41,43]\). Particularly, our results on the variation of the rotational angle \(\text{IrO}_6\) caused by tensile (compressive) strains show the same trend as in Ref. \([43]\).
from an enlarged magnetic supercell containing two structural supercells along z-axis. Our calculation shows that the Ir atoms couple ferromagnetically to the nearest neighbor in the adjacent SIO layer, which is consistent with previous studies [37]. Specifically, the energy difference between ferromagnetic and antiferromagnetic interlayer coupling is 6 meV per unit cell. Such a ferromagnetic interlayer coupling in the quasi-2D Ir sub-lattice align the canted moments of all the SIO layer, creating a spontaneous net magnetization of the entire superlattice.

In addition, we found a canted moment toward the out-of-plane direction — the $z$-axis, which is smaller than the in-plane component but not negligible. This can be attributed to the slight octahedra tilting, which cants the antiferromagnetic Ir moments toward the out-of-plane direction, resulting in a small out-of-plane net moment. To verify this effect, we measured the net magnetization of SIO/STO superlattice for both in-plane and out-of-plane configurations, as shown in Fig. 4. The in-plane component was attributed to the alignment of canted moments following octahedra rotation as discussed above [37]. The dominant in-plane magnetic response is also in accordance with the magnetic ordering found from DFT. A clear spontaneous out-of-plane net moment was indeed observed below the Neel transition. The magnetization is about one order of magnitude smaller than the in-plane one.

Fig. 4. Temperature dependences of in-plane and out-of-plane magnetizations.

3.4. (D) Coupling of strain with magnetization in SIO/STO

3.4.1. (D.1) Strain induced changes of the magnetic moments

The effects of strain on magnetic properties are shown in Fig. 5; we have plotted the $x$, $y$, and $z$ components of spin (circle) and orbital (square) moments of Ir atom in SIO/STO as function of strain. The spin and orbital moments for the stable and unstrained structure are also given in the figure, and the changes of the spin (orbital) moments are plotted. All components, except the $z$-component, of the spin and orbital moments have negative slope with respect to the strain. That means compressive strain increases the $x$ and $y$ components of the spin and orbital moments whereas tensile strain reduces these magnetic moments. For both canting moments, the strain-induced changes of the orbital moment, $x$ and $z$ components, are higher than the spin moments, suggesting that strain has a strong influence on the orbital moments via octahedral distortion.

The Ir atoms have net in-plane magnetic moment of 0.14 $\mu_B$, that are canted towards $x$-axis. When the compressive strain in SIO/STO reaches 0.9% the in-plane magnetic moment along $x$-axis (Fig. 5(a)) has been increased by 8.6%, as compared to the unstrained structure. The magnetic components in the $y$-direction show relatively moderate change with respect to strain. Interestingly, the largest strain-induced change of the magnetic moment is observed for out-of-plane ($z$) component by about 65%, though its zero-strain structure has the smallest magnetic moment of 0.025 $\mu_B$. These results indicate that the spin and orbital magnetic moments in SIO/STO are sensitive to strain and hence exhibit a significant magnetoelastic coupling. The effects are important for anticipating and tuning the magnetization of the superlattice on different substrates. The variations of the spin and orbital moments of Ir are attributed to the structural distortion in SIO/STO superlattice, and will be discussed in Section III (E).

3.5. (E) Analysis on correlation between structural distortions and magnetic properties

To correlate the structural changes and variation of magnetic properties as result of strain, we have performed a thorough analysis using multiple reference structures of SIO/STO. It is
worthwhile to point out that the strain introduces multiple structural distortions in these oxide superlattices. However, to our knowledge there is limited information on how the tilting or rotational angle relates to the magnetization of SIO/STO. The effective spin Hamiltonian for a square lattice of Ir $J_{eff} = \frac{1}{2}$ moments based on the dominant magnetic interactions is \[30\]:

$$H = JS_i^zS_j^z + J_xS_i^xS_j^x + \vec{D} \cdot \left[ S_i^x \times S_j^x \right]$$

(1)

where $J$, $J_z$ and $\vec{D}$ respectively are the isotropic Heisenberg exchange coupling, the symmetric anisotropy term and the Dzyaloshinskii-Moriya (DM) interaction \[44,45\], respectively. This model ignores corrections due to Hund’s coupling and only considers octahedral rotation in the absence of tilting. Under this model, the canting of the moments, without octahedral tilting, is attributed to the ratio of DM interaction and isotropic exchange couplings ($J$) \[30,44,45\]. DM interaction describes the anisotropic nature of magnetic interactions that basically originates from SOC and broken local inversion symmetry \[44,45\]. To investigate the implication of octahedral tilting to the change of the magnetization, we studied different reference structures that have no octahedral rotation and tilting. Basically, we began with a structure of SIO/STO with 180° bonds and increased the rotation or tilting angle linearly [see Fig. 6 (a)]. When all Ir-O-Ir bonds are straight, the magnetic interactions are only governed by Heisenberg exchange, whereas the DM interaction and the symmetric anisotropic exchange vanishes. As expected, in our DFT calculations we found an antiferromagnetic order, in which the magnetic moment of Ir is directed either along the y-axis or x-axis, as shown in Fig. 6 (a), since these two directions of magnetization are degenerate in such undistorted geometry.

Subsequently, the IrO$_6$ octahedra is rotated laterally to 14° without tilting angle, and the rotation of TiO$_6$ fixed to 0°. As shown in the exemplary magnetic structure of Fig. 6 (b), significant spin canting towards the x-axis (in-plane) is observed while the antiferromagnetic moments along the y-axis are only slightly changed. From these results one can see that an increment of the rotation of IrO$_6$ angle introduces a significant in-plane canting moment, which can be attributed to the DM interaction in Eq. (1).

Finally, a tilt angle of 2° is introduced without rotation and a relatively small spin canting of the Ir spin along the z-axis is observed without in-plane spin canting. Similar to the case of the octahedra rotation, the origin of such out-of-plane spin canting is related to the non-zero DM term introduced when tilting exists. In such superlattices, if the Sr ions are replaced with the smaller cations, which tends to off-center the oxygen ions further, we believe that the spin canting towards the z-axis can be enhanced.

Fig. 5. The variation of the magnetic moments ($\Delta M$) of Ir with respect to biaxial strain is plotted for (a) x, (b) y and (c) z components. The values of the spin and orbital moments for zero strain field are also given in units of Bohr Magneton. The change in the total magnetic moment is shown in (d).

Fig. 6. Structural distortion of IrO$_6$ octahedra and the respective magnetic moments. (a) The octahedra have no tilting and rotation. The structures with only lateral rotation (b) and tilting angle (c) of IrO$_6$ are shown. The $xy$ direction in (c) depicts the crystallographic [110] direction. In all cases SIO/STO has in-plane antiferromagnetic order and the evolution of the spin and orbital moments for the Ir atoms are shown.
Thereafter, an out-of-plane spin moment could be induced. Besides, we have shown earlier that the out-of-plane magnetic moment is highly sensitive to epitaxial strain. Overall, the increase in the tilt angle as a function of tensile strain is accompanied by a non-zero DM interaction, leading to an increase in the out-of-plane magnetization. This implies that octahedra tilting has significant impact on the out-of-plane spin canting.

3.5.1. (E1) Effect of strain on the in-plane anisotropy

For all the calculated structures, we found that the antiferromagnetic Ir moments prefer to be aligned within the xy-plane of the out-of-plane one, which can be attributed to the easy-plane anisotropy from the Hund’s coupling [46]. In addition, when a finite octahedral tilt exists, the antiferromagnetic moments tend to align along the y-axis in the plane. To investigate the in-plane anisotropy, we have explored possible magnetic configurations and investigated the relative stabilities of competing antiferromagnetic configurations. Particularly, we have performed calculations aligning the antiferromagnetic Ir moments along the two in-plane magnetization axes, x’ and y’ shown in Fig. 7 below, and evaluated their energy differences to capture the change of the in-plane anisotropy as a function of strain. The x’ and y’ directions, that are slightly rotated clockwise from the crystal coordinates x and y, represent the local coordinates of the Ir moments (inset of Fig. 7). Fig. 7 shows the variation of the energy difference between two in-plane directions of magnetization as a function of the strain. For all cases, the most stable antiferromagnetic order of SIO/STO occurs when the Ir moments are counter-aligned along the y’-axis. To account the small energy differences of the in-plane anisotropy we performed the calculation with much denser k-point meshes of 9 × 9 × 6 and larger energy cutoff (600 eV), and similar setting has been used to calculate magnetic anisotropy energy [47,48]. At zero strain, the in-plane anisotropy is found to be 7.4 × 10^{-2} meV/Ir atom. A tensile strain of 0.9% increases the in-plane anisotropy by 0.02 meV per Ir atom, as shown in Fig. 7. The energy levels of the two directions of magnetization are expected to be identical in highly symmetrical tetragonal structure without octahedral tilt [49]. The removal of the degeneracy between the two axes can be related to the fact that the octahedral tilting which effectively reduces the in-plane symmetry of SIO/STO. Therefore, tensile strain which increases the tilt (Fig. 3) tends to favor larger in-plane anisotropy. The main contribution to the in-plane anisotropy might come from additional anisotropic exchanges, caused by the tilting distortion, and is expected to be minimized by reducing the tilting angle.

4. Summary

We have found that the SIO/STO superlattice possesses an a’c rotation pattern from DFT simulations, which is in good agreement with the experimental results of synchrotron X-ray diffraction. The magnetic ground state of the SIO/STO is found to be antiferromagnetic with small in-plane canting. The response of structural distortions and magnetization in SIO/STO to epitaxial strain has been systematically studied. Compressive/tensile strains increase/decrease the rotational angles of the octahedra, whereas the opposite effect is observed for tilting angle. Moreover, we have shown that strain can induce more spin canting and in-plane anisotropy, which are found related with octahedral rotation and tilting, respectively. These changes have been discussed and correlated with the DM interaction within the distorted structures of SIO/STO. Practically one can infer the behavior of SIO/STO on different substrates from these results. In addition, our study provides insights on how structural and magnetic properties of complex oxides are influenced by epitaxial strains, which provides a route to control magnetic order through strain engineering.

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