We investigate the mechanism of the resonant X-ray scattering on the Ti $K$ edge region of YTiO$_3$ using the band structure calculation combined with the local density approximation. A large intensity is obtained for the orbital superlattice spots. The calculated spectra consist of several peaks as a function of photon energy in agreement with the recent experiments. Against a naive interpretation that directly relates the intensity to the orbitally polarized $3d$ states, the obtained large intensity arises from the distorted crystal structure, i.e., the tilt of the TiO$_6$ octahedra and the Jahn-Teller distortion, which considerably modifies the $4p$ states in the intermediate states of the dipolar process. This casts doubt on a prevailing assertion that the resonant x-ray scattering is a direct observation of the orbital order.

78.70.Ck, 71.20.Be, 71.30.+h

I. INTRODUCTION

Recently the resonant x-ray scattering spectroscopy has attracted much attention because this experimental method is considered as one of the most powerful tools which can directly observe the orbital order in the strongly correlated systems. A lot of experiments have already been carried out on the perovskite transition-metal compounds, e.g., V$_2$O$_3$, DyB$_2$C$_2$, and GdFeO$_3$ in which the scattering intensities were observed on the orbital superlattice spots, which are forbidden for usual x-ray scattering. Such anomalous x-ray scattering will simply be referred to as RXS. Despite much effort so far, how and to what extent the RXS spectra are reflecting the orbital order are still controversial, especially on the perovskite compounds, since the orbital order usually accompanies the Jahn–Teller distortion (JTD) and the GdFeO$_3$ type distortion, which can also gives rise to the RXS intensity.

The RXS spectra on YVO$_3$ have been observed for the pre $K$ edge and the main $K$ edge regions of V. The spectra consist of several peaks as a function of photon energy, and the shapes are different between the (100) and (011) reflections. Assuming that the scattering tensor is directly related to the orbital polarization of the $3d$ states, the authors argued that the azimuthal angle dependence of the spectra was consistent with the C-type orbital order in the low temperature phase. However, this assumption made there implies the dominance of the Coulomb effect, which is questionable. Recently the resonant x-ray scattering experiment has also been carried out on YTiO$_3$, and the RXS spectra have been observed with their shapes similar to those of YVO$_3$. In this paper, concentrating our attention on YTiO$_3$, we study the mechanism of the RXS spectra by carrying out a band structure calculation on the experimentally determined crystal structure.
FIG. 1. Sketch of the crystal structure of YTiO$_3$. The large spheres represent the oxygen ions, the small solid spheres the yttrium ions, and the octahedra the titanium ions. The arrows assigned to each Ti ion define the local $\xi\eta\zeta$ axes pointing to nearest neighbor oxygen sites.

The crystal structure of YTiO$_3$ is known to belong to the space group $Pbnm$, as shown in Fig. 1; four Ti ions are inequivalent in the unit cell. The Ti-O-Ti bond angles strongly deviate from 180° due to the tilt of the TiO$_6$ octahedra, and Ti-O bond lengths are different in TiO$_6$ octahedra due to the JTD. One of the $t_{2g}$ levels is occupied under the crystal field in the $d^1$ configuration of Ti$^{3+}$ ions, and since the $t_{2g}$ states are weakly hybridizing with O 2$p$ states, the JTD is smaller (~20%) than that on LaMnO$_3$. Note that the crystal structure of YVO$_3$ belongs to the same space group of $Pbnm$ with similar sizes of the tilt of VO$_6$ octahedra and the JTD.

We calculate the RXS spectra using the band calculation based on the local density approximation (LDA) together with the muffin-tin approximation. This approximate scheme leads to a metallic ground state for YTiO$_3$ with a very small orbital polarization. In spite of this shortcoming for the $3d$ bands, we expect that the $4p$ bands are well described in the present calculation, since they have energies ~15 eV higher than the $3d$ bands and thereby the details of the $3d$ bands are irrelevant. What is important, which will become clear, to make the $4p$ states different at different Ti sites is the O potential of neighboring sites. The $4p$ states are so extended in space that they are sensitively modified by hybridizing and interacting with the electronic states of neighboring ions. Actually, for LaMnO$_3$, it is known that the LDA+U method, which predicts an insulating ground state with large orbital polarization, gives the $4p$ bands and the RXS spectra nearly the same as those given by the LDA method, although the latter predicts a small band gap and a small orbital polarization.

We obtain the RXS spectra with sufficient intensities for YTiO$_3$. The obtained spectra as a function of photon energy resemble closely to the results of the experiment for the (100) and (011) reflections of YVO$_3$, and also to those of the recent experiment of YTiO$_3$. Since the muffin-tin approximation averages the Coulomb interaction between the $4p$ and the $3d$ states, the anisotropy of the Coulomb interaction is eliminated in the calculation of the RXS spectra. Therefore, the obtained RXS intensity arises from the distorted crystal structure. We may roughly estimate that the Coulomb effect is less than 1/4 of the JTD effect, since the Coulomb effect is evaluated as 1/100 smaller than the JTD effect in LaMnO$_3$. Note that the JTD effect cannot be distinguished from that of the tilt of the TiO$_6$ octahedra in the present calculation.

Such sensitivity of the $4p$ states to the electronic states at neighboring sites has already been recognized in the analysis of the magnetic circular dichroism of the $K$ edge absorption spectra on the ferromagnetic states of the transition metals and the analysis of the resonant x-ray magnetic scattering spectra on Co and NiO.

This paper is organized as follows. In the next section, we briefly discuss the band structure calculation on the ground state. In section 3 we outline the calculation procedure of RXS spectra and discuss the calculated results. The final section is devoted to concluding remarks.

II. CALCULATION OF THE GROUND STATE AND DENSITY OF STATES

![Graph showing the radial wave functions](image)

FIG. 2. The $4p$ wave functions of an atomic Ti$^{3+}$ ion, calculated within the Hartree-Fock approximation. Solid line and dashed line represent the radial wave functions $rR(r)$ without and with the core–hole potential. The arrows indicate the muffin-tin radius $r_{MT}$ of Ti site and the typical distance $d_{Ti-O}$ between Ti nucleus and O nucleus in YTiO$_3$.

First we examine the meaning of the atomic $4p$ states. Figure 2 shows the atomic $4p$ wave function for a Ti$^{3+}$ ion, calculated within the Hartree-Fock approximation.
The 4\(p\) wave function extends considerably in space so that a large part of the amplitude would lie on the neighboring oxygen sites or the interstitial region in solids. This situation is not changed in the presence of the core-hole potential, as shown by the broken line in the figure. Thus one may easily understand the sensitivity of the 4\(p\) states to electronic states at neighboring sites. The concept of the atomic 4\(p\) levels loses its clear meaning in solids, and the 4\(p\) states are to be treated as energy bands. Nevertheless, the \(p\) symmetric states (centered at a Ti site) above the Fermi energy are referred to the 4\(p\) states, since the atomic character is almost preserved inside the atomic sphere in the band structure calculation.

In the band structure calculation for YTiO\(_3\), we use the Korrinja–Kohn–Rostoker (KKR) method within the LDA scheme. We assume the crystal structure determined experimentally at room temperature in Ref.\(^{[25]}\), which is shown in Fig.\(^{[1]}\). As mentioned before, the crystal structure belongs to the space group \(Pbnm\)^\(^{[4]}\) the unit cell involves four Y ions, four Ti ions and 12 O ions. The four Ti sites are distinctive in terms of the orientation even though the orbital ordering does not occur. The large tilt of TiO\(_6\) octahedra makes the Ti-O-Ti bond angles strongly deviates from 180\(^0\) by as much as 35\(^0\). Each TiO\(_6\) octahedron also undergoes the JTD such that the direction \(\xi\) corresponds to the short bond, the \(\eta\) to the long bond, and the \(\zeta\) to the middle bond, where three arrows \(\xi\eta\zeta\) attached to each Ti ion are directed to neighboring oxygen sites and are almost orthogonal to each other. There exists an important symmetry that the configuration surrounding the Ti 1 site becomes coincident to that surrounding the Ti 2 site under the rotation of all positions of atoms by \(\pi\) around the line parallel to the \(x\) axis passing through the Ti 1 site. In the same way, the configuration surrounding the Ti 1 site becomes coincident to those surrounding the Ti 3 and the Ti 4 sites under the rotation of the atomic position by \(\pi\) around the line parallel to the \(y\) and the \(z\) axes, respectively, passing through the Ti 1 site.

As regards the magnetism, the system undergoes a ferromagnetic transition below the Curie temperature \(T_C = 29\text{K}\)\(^{[26]}\). Neglecting the spin-orbit coupling, we obtain a ferromagnetic ground state with the magnetic moment 0.95\(\mu_B\) per Ti\(^{3+}\) site (0.68\(\mu_B\) inside the muffin–tin sphere of Ti\(^{3+}\) site), consistent with the previous calculations\(^{[25]}\). This value is a little larger than the experimental value 0.84\(\mu_B\)\(^{[24]}\). The orbital polarization is underestimated to be very small. The ground state is obtained as a metal, although it is experimentally a semiconductor. The LDA is known to have a tendency to wrongly predicting a metallic ground state. We think these shortcomings for the 3\(d\) states have only minor effects on the 4\(p\) states, since they have high energy (\(~\sim 15\) eV above the Fermi level).

![Diagram of DOS](image_url)

**FIG. 3.** The DOS projected onto the \(s\), \(p\) and \(d\) symmetric states inside the muffin–tin sphere of a Ti site. The origin of energy is at the Fermi level. The \(d\) DOS is overwhelming the \(s\) and \(p\) DOS’s. The inset shows the magnified DOS projected onto the \(p\) symmetric states.

Figure\(^{[2]}\) shows the density of states projected onto the \(s\), \(p\), and \(d\) symmetric states inside the muffin–tin sphere of a Ti site. Around 7 eV below the Fermi level, the 3\(d\) states form bonding states with the 2\(p\) states of the neighboring O ions. Around the Fermi level, the 3\(d\) states are highly concentrating in a form of antibonding states with the O 2\(p\) states. In high energy region, a broad band appears, to which the \(s\), \(p\) and \(d\) symmetric states equally contribute. The \(p\) DOS in this energy region is much smaller than the \(d\) DOS near the Fermi level, as expected from the character of the atomic 4\(p\) wave function that extends considerably in the interstitial region. The \(p\) DOS is enlarged in the inset. It has two peaks. Note that the \(p\) DOS is roughly proportional to the \(K\) edge absorption spectrum, if the effect of the core hole potential is neglected in the final states. This final state interaction may enhance the peak of the low energy side in the \(p\) DOS. In any event, the two-peak structure corresponds well to the absorption spectrum of YVO\(_3\)\(^{[2]}\).

**III. CALCULATION OF RXS SPECTRA**

**A. Formulation**

In the resonant process around the Ti \(K\) edge region, the 1\(s\) core electron is virtually excited to the 4\(p\) states. Therefore the RXS spectra directly reflect the 4\(p\) states at the scattering center. We specifically calculate the RXS intensities for the (100), (001) and (011) reflections.

We choose the \(x\), \(y\) and \(z\) axes such that they are parallel to the crystal \(a\), \(b\), and \(c\) axes, respectively. With respect to these axes, we define the 1\(s\)-4\(p\) dipole transition density matrix \(r_{mn}(\varepsilon)\) at the Ti \(k\) site in the unit cell as
\[ \tau_{mn}(\varepsilon) = \sum_{b,k} \int r^2 dr r'^2 dr' [R^*_k(r) R_{1s}(r)] \phi_{b,k}(r) \phi_{b,k}(r') \delta(\varepsilon - \varepsilon_{b,k}), \]  

where \( \phi_{b,k} \) represents the wave function with the band index \( b \), wave-vector \( k \) and energy \( \varepsilon_{b,k} \). The \( P_m \) is a projection operator which projects the wave function \( \phi_{b,k} \) onto the \( m \) component of the \( p \) symmetric part around the \( Ti \) site, and \( R_{1s} \) represents the Ti 1s wave function. This matrix is obtained from the KKR Green’s function \( g^{(k)}_{mn}(r, r'; \varepsilon) \) by the equation

\[ \tau_{mn}(\varepsilon) = -\frac{1}{\pi} \text{Im} \int r^2 dr r'^2 dr' g^{(k)}_{mn}(r, r'; \varepsilon) R_{1s}(r) R_{1s}(r'). \]  

Numerically this 1s–4p transition density matrix is roughly proportional to the 4p density matrix \( \rho_{mn}(\varepsilon) = -\frac{1}{\pi} \text{Im} \int_0^{\infty} r^2 dr g^{(k)}_{mn}(r, r; \varepsilon) \) with \( r_{MT} \) being the muffin-tin radius. Assuming that photons are linearly polarized, we have the scattering amplitude at the \( Ti \) k site as

\[ f^{(k)}(\omega) = \frac{A}{4} \int d\varepsilon \sum_{m,n=x,y,z} E^{\text{out}}_m \frac{\tau_{mn}(\varepsilon)}{\omega - \varepsilon + \varepsilon_{1s} + i\Gamma} E^{\text{in}}_n, \]  

where \( A \) is a numerical constant, \( E^{\text{in}}_m \) and \( E^{\text{out}}_n \) are the \( m \) and \( n \) components of polarization of the incident and the emitted photons, respectively. In the denominator, \( \omega \) is the photon energy, and \( \varepsilon_{1s} \) is the energy of the 1s state. The \( \Gamma \) describes the broadening due to the core-hole lifetime, which are assumed \( \Gamma = 1 \) eV. The effect of the core-hole potential is neglected in the intermediate states. We think this effect on the RXS intensity is small, since the core hole potential is spherically symmetric, and it affects merely the diagonal elements of the density matrix which are irrelevant to the RXS intensity. The integration in terms of \( \varepsilon \) is performed from the Fermi energy to 60 eV above it.

It is obvious that the transition density matrix \( \tau_{mn}^{(k)} \) becomes symmetric with neglecting the spin–orbit interaction. Using \( a, b, c, \alpha, \beta \) and \( \gamma \), functions of \( \varepsilon \), the matrix at the Ti 1 site can be represented as

\[ \tau^{(1)} = \begin{pmatrix} a & \alpha & \gamma \\ \alpha & b & \beta \\ \gamma & \beta & c \end{pmatrix}, \]  

Due to the crystal symmetry mentioned before, the transition density matrices \( \tau^{(2)}, \tau^{(3)} \) and \( \tau^{(4)} \) at the Ti 2, Ti 3, and Ti 4 sites are represented as

\[ \tau^{(2)} = \begin{pmatrix} a & -\alpha & -\gamma \\ -\alpha & b & \beta \\ -\gamma & \beta & c \end{pmatrix}, \]

\[ \tau^{(3)} = \begin{pmatrix} a & -\alpha & \gamma \\ -\alpha & b & -\beta \\ \gamma & -\beta & c \end{pmatrix}, \]

\[ \tau^{(4)} = \begin{pmatrix} a & \alpha & -\gamma \\ \alpha & b & -\beta \\ -\gamma & -\beta & c \end{pmatrix}. \]

Using these representations, the scattering amplitudes are expressed in simple forms. For the (100) reflection, we have

\[ f^{(100)}(\omega) = f^{(1)}(\omega) - f^{(2)}(\omega) - f^{(3)}(\omega) + f^{(4)}(\omega) = A(E^{\text{out}}_y E^{\text{in}}_x + E^{\text{out}}_y E^{\text{in}}_x) \int d\varepsilon \frac{\alpha(\varepsilon)}{\omega - \varepsilon + \varepsilon_{1s} + i\Gamma}. \]

In the similar way, we have the scattering amplitude for the (001) and (011) reflections as

\[ f^{(001)}(\omega) = A(E^{\text{out}}_x E^{\text{in}}_y + E^{\text{out}}_z E^{\text{in}}_y) \int d\varepsilon \frac{\beta(\varepsilon)}{\omega - \varepsilon + \varepsilon_{1s} + i\Gamma}; \]

\[ f^{(011)}(\omega) = A(E^{\text{out}}_z E^{\text{in}}_x + E^{\text{out}}_x E^{\text{in}}_x) \int d\varepsilon \frac{\gamma(\varepsilon)}{\omega - \varepsilon + \varepsilon_{1s} + i\Gamma}. \]

Only one of the off-diagonal elements remains in each expression of the scattering amplitudes, with the diagonal elements \( a, b, \) and \( c \) completely vanishing. Therefore, we can select out one of them by choosing the reflection index. The photon energy dependence is factored out from the polarization of photon in Eqs. (3.5), (3.7), and (3.8). The RXS intensities \( I^{(100)}, I^{(001)}, \) and \( I^{(011)} \) are given by \( |f^{(100)}|^2, |f^{(001)}|^2, \) and \( |f^{(011)}|^2, \) respectively.

**B. Calculated results**

We calculate the RXS spectra on the crystal structure determined at room temperature in Ref. 1 using the above formulas. We show in the following the results calculated in the ferromagnetic ground state of YTiO₃, although the RXS experimental data are given above the Curie temperature \( T_c \). We checked that the RXS spectra are insensitive to the magnetic states by calculating the spectra also in a nonmagnetic state. This is consistent with the 4p DOS above 15 eV in Fig. 3 which shows no exchange splitting.
FIG. 4. RXS spectra as a function of photon energy. The left panels are the calculated spectra for the (100), (001), and (011) reflections on YTiO$_3$. The origin of energy corresponds to the photon energy of exciting an electron from the 1s state to the Fermi level. Right panels are the experimental spectra in the low temperature phase of YVO$_3$ (ref. 6).

Figure 4 shows the calculated spectra as a function of photon energy for the (100), (001) and (011) reflections. Note that the anisotropy of the Coulomb interaction between the 4$p$ and 3$d$ states is eliminated in the calculation by using the muffin-tin approximation. The experimental spectra in the low temperature phase of YVO$_3$ are also shown for the sake of comparison since their shapes are quite similar to the unpublished experimental data for the RXS spectra of YTiO$_3$. As already mentioned, the resemblance of the RXS spectra is quite understandable in the light of the mechanism of the distorted crystal structure, since both the JTD and the tilt of the VO$_6$ octahedra in the low temperature phase of YVO$_3$ are quite similar to those in YTiO$_3$. In the (100) and (001) reflections, the intensities vanish for the $\sigma \rightarrow \sigma'$ channel. For the $\sigma \rightarrow \pi'$ channel, we have three peaks denoted by A, B, and C, whose intensities are comparable to each other in the (100) reflection, while we have two peaks denoted as D and E in the (001) reflection. In the experimental data of YTiO$_3$, three peaks appear at 4.974 keV, 4.986 keV, and 5.0 keV, corresponding to peaks A, B, C, for the (100) reflection, while two peaks appear at 4.974 keV and 4.984 keV with the former intensity about twice as the latter, corresponding to peaks D and E. In the (011) reflection, both the $\sigma \rightarrow \sigma'$ and the $\sigma \rightarrow \pi'$ channels contribute to the intensities; we have a dominant peak denoted as F and a small peak denoted as G. The energy of peak F is found slightly higher ($\sim 2$ eV) than that of the peaks A and D. In the experimental data of YTiO$_3$, two peaks appear at 4.976 keV (2 eV higher than the positions of peaks A and D) and 4.986 keV with the former intensity dominating the latter.

FIG. 5. Azimuthal angle dependence of the RXS intensities for the (100), (001) and (011) reflections.

Figure 5 shows the azimuthal angle dependence of the RXS spectra. As clear from Eqs. (3.6), (3.7), and (3.8), the peaks belonging to the same scattering vectors show the same dependence. In the (100) and (001) reflections, the intensities are proportional to $\cos^2 \psi$ for the $\sigma \rightarrow \pi'$ channel, with the condition $E^{\text{in}} \parallel b$ at $\psi = 0$. In the the (011) reflection, the intensities are proportional to $\sin^2 2\psi$ for the $\sigma \rightarrow \pi'$ channel, with the condition $E^{\text{in}} \parallel a$ at $\psi = 0$, while the dependence is rather complicated for the $\sigma \rightarrow \pi'$ channel. The calculated results are in agreement with those of YVO$_3$ (and also YTiO$_3$).

FIG. 6. The 4$p$ density matrix $\rho_{\text{Ti}1}^{(1)}(\varepsilon)$ at the Ti 1 site, as a function of energy $\varepsilon$. (a) in the $xyz$ coordinate system, and (b) in the $\xi\eta\zeta$ coordinate system. The thick lines represent the off-diagonal elements, and the thin lines represent the diagonal elements. The origin of energy is at the Fermi level.

To see more closely how the 4$p$ states are modified, we examine the 4$p$ density matrix $\rho_{\text{Ti}1}^{(1)}(\varepsilon)$ at the Ti 1 site, which is shown in Fig. 6. The left panel shows the representation in the $xyz$ system. Although the diagonal...
elements are larger than the off-diagonal elements, the former quantity does not contribute to the RXS intensity. The right panel shows the representation in the local \( \xi \eta \zeta \) coordinate system. The off-diagonal elements remain comparable to those in the \( xyz \) system, indicating that the \( \xi \eta \zeta \) axes are still deviating from the principal axes of the density matrix. Since the off-diagonal elements are fluctuating with changing energy, the principal axes may also be fluctuating. One may think that the principal axes of the density matrix are related to the direction of the 3d orbital polarization. However, this is not the case in the present calculation, since the 3d orbital polarization has little effect on the 4p states within the muffin-tin approximation. We interpret this as the sensitiveness of the 4p states to the tilt of the TiO\(_6\) octahedra which makes the local \( \xi \eta \zeta \) coordinate axes no longer principal axes.

**IV. CONCLUDING REMARKS**

We have studied the effect of the crystal structure to the RXS spectra of YTiO\(_3\), using the band structure calculation within the LDA. The calculated spectra are mainly compared with the experimental data of YVO\(_3\), since the unpublished data of YTiO\(_3\) are similar to those of YVO\(_3\). This similarity is consistent with the mechanism of the distorted crystal structure. The obtained spectra as a function of photon energy are in agreement with the experiments of YVO\(_3\) (and also YTiO\(_3\)). Since the muffin-tin approximation averages the Coulomb interaction between the 4p states and the 3d states, the anisotropy of the Coulomb interaction is eliminated in the calculation of the RXS spectra. We have clearly shown that along with the JTD the tilts of the transition-metal oxide octahedra need to be taken into account. The agreement between the calculation and the experiment suggests that the RXS intensity originates mainly from the distorted crystal structure, casting doubt on a prevailing assertion that the RXS is a direct observation of the orbital order. We hope that the present work could accelerate further study on the relation between the RXS and the orbital order.

In spite of the above findings, there are several points to be made clear. First, since the crystal structure includes both the JTD and the tilt of the TiO\(_6\) octahedra, it is not clear which effect is important. Closely related to this question, the crystal structure of YVO\(_3\) changes into a state of a very small JTD for \( T > 100 \) K (the tilt is not changed so much). According to this change, the intensities of peaks a and c were found to become very small, while those of other peaks were found to remain similar. This suggests that the effect of the JTD on the RXS spectra is different from that of the tilt of the octahedra. For clarifying this point and for a direct comparison with the experiment, the calculation of the RXS spectra in the two cases of the atomic coordinates for YVO\(_3\) is now under progress. Second, the intensities in the (100) reflection are 1/5 ~ 1/10 smaller than those in the other reflections in the experiment of YVO\(_3\) (and YTiO\(_3\)). Note that the samples are different for different reflections in the experiment. This may make the comparison of the data between different reflections less accurate. In any event, this behavior is not reproduced by the present calculation. It might improve the situation to go beyond the muffin-tin approximation in which the potential is crudely treated as a constant in the interstitial region. Third, in addition to the RXS spectra mentioned above, another small peak has been observed about 10 eV below the main \( K \) edge peak. Since its azimuthal angle dependence is nearly the same as in other peaks, this pre-edge peak must come from the dipolar process. The presence of such pre-edge peaks has been predicted for LaMnO\(_3\). This study suggests that the pre-edge peak arises from the \( p \) symmetric states (centered at a Ti site) hybridizing to neighboring 3d states in the intermediate states. Since the orbital polarization is obtained very small in the present calculation, we are unable to handle the pre-\( K \) edge structure. The LDA+\( U \) method may be suitable to treat this problem.

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