Core-level x-ray photoemission and Raman spectroscopy studies on electronic structures in Mott-Hubbard type nickelate oxide NdNiO$_2$

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We perform core-level X-ray photoemission spectroscopy (XPS) and electronic Raman scattering studies of electronic structures and spin fluctuations in the bulk samples of the nickelate oxide NdNiO$_2$. According to Nd $3d$ and O $1s$ XPS spectra, we conclude that NdNiO$_2$ has a large transfer energy. From the analysis of the main line of the Ni 2p$_{3/2}$ XPS, we confirm the NiO$_2$ planes in NdNiO$_2$ are of Mott-Hubbard type in the Zaanen-Sawatzky-Allen scheme. The two-magnon peak in the Raman scattering provides direct evidence for the strong spin-fluctuation in NdNiO$_2$. The peak position determines the antiferromagnetic exchange $J = 25$ meV. Our experimental results agree well with our previous theoretical results.

Introduction – Nickel has the formal valences Ni$^{3+}$, Ni$^{2+}$ and Ni$^{+}$ with electronic configurations of of $3d^7$, $3d^8$ and $3d^9$, respectively, in the transition-metal oxides. The nickelate compounds exhibit lots of strongly correlated electronic properties, such as the metal-insulator transitions, unusual magnetic order, charge order and even superconductivity [1–17]. The recent discovery of the superconductivity in the thin film LaNiO$_2$ and NdNiO$_2$ [18], and motivates the experimental [17] and lots of theoretical works [19–35] to explore its electronic properties. The recent superconductivity in the nickelate oxides, due to the proximity to a Mott insulator [43, 44]. Raman spectroscopy probes spin fluctuations in the transition-metal compounds, even without a long-range magnetic order [45]. The exchange interaction $J$ for cuprates is very large, and $J$ was determined from the two-magnon peak to be of order 125 meV [45–56]. The absence of long-range magnetic order in LaNiO$_2$ and NdNiO$_2$ in Refs. [7] may be due to poor sample qualities, or due to the “self-doping” effects of the Nd $5d$ electron pockets [10, 17, 25]. We perform Raman measurements to explore spin fluctuations, and observe a broad two-magnon peak in NdNiO$_2$. The antiferromagnetic exchange is determined as $J = 25$ meV in NdNiO$_2$, close to our previous theoretical estimation [25].

Experimental setup. – We carried out the XPS investiga-
which evacuated to 2 \text{tegral time}. The samples were placed in a He-flow cryostat µ400 tation line of a He-Ne laser. The power of the laser is about 1\text{ng a HORIBA iHR550 spectrometer and the 632.8 nm exci-}

quasi-back-scattering geometry on our home-built system us-

was calibrated by 1\text{effect in our insulating samples. The binding energy in XPS}

tron flood gun was turned on to eliminate electric charging

the sol-gel with stoichiometric ratio of Ni and Nd [57]. Af-

Single crystal synthesis. – The NdNiO\textsubscript{3} polycrystals were

thesized by a combination precursor method with high

pressure technique. The precursor was prepared by sintering

the bottom profiles are the difference between the observed and cal-

culated results. Insets of each panel are crystal pictures and the poly-

hedral view of the corresponding crystal structures.

ions on Thermo Fisher ESCALAB 250Xi using monochro-

mated Al K\text{radiation at room temperature, and the elec-}

tron flood gun was turned on to eliminate electric charging

effect in our insulating samples. The binding energy in XPS

was calibrated by 1\text{s spectra of carbon. The Shirley back-

ground of the XPS spectra has been subtracted in this work.

The energy dispersive X-ray (EDX) and scanning electron mi-

croscopy (SEM) studies were performed on Phenom ProX

ground of the XRD patterns for NdNiO\textsubscript{2}, especially in the peak indexed by \langle hkl \rangle with nonzero value for l. The anisotropic broadening of the

Bragg peaks was also observed in both thin films and poly-

crystals [7, 8, 11, 12, 16, 58], and could be ascribed to the anisotropic crystal size or stacking disorder. NdNiO\textsubscript{2} has inten-
sitive peaks along \langle h00 \rangle direction in XRD pattern as shown in

Fig. 1 (b), probably due to the preferred a-axis of crystal

grains. The orientation preference was reported for the thin-

film LaNiO\textsubscript{2} where the preferred orientation changes from c-

axis to a-axis for the over-time reduction [12, 13].

We performed the Rietveld profile refinement for NdNiO\textsubscript{3} and

NdNiO\textsubscript{2} using the Fullprof suite of programs [59]. The

NdNiO\textsubscript{3} has the space group of \textit{Pbnm} with lattice parameters

\(a=5.38500\ \text{Å}, b=5.38400\ \text{Å}, \text{and } c=7.61314\ \text{Å} \) (\(R_{wp}=8.83\%\text{ and } R_B=13.25\%\)), consistent with the previous re-

port [60]. The refinement results for NdNiO\textsubscript{2} is \(a=b=3.93110\ \text{Å} \) and \(c=3.30200\ \text{Å} \) ( with \(R_{wp}=11.6\%\text{ and } R_B=7.35\%\)), which is in agreement with previous results

which used NaH as reduction agent [8]. It is worth noting that the metal nickel phase usually appears in NdNiO\textsubscript{2} after

duction, as reported in refs [7, 8, 11, 58]. Although the

metal nickel phase is almost invisible in our PXRD result, we

observed the metal nickel impurities embedded in surface-

polished NdNiO\textsubscript{2} crystal by SEM, as shown in inset of Fig. 5.

Electronic structures from XPS. – The core-level x-ray spec-

troscopy is a powerful tool to study electronic properties of

transition-metal oxides [62, 63]. It helps to determine the

FIG. 2. Nd 3\text{d} core-level XPS spectra of NiO, NdNiO\textsubscript{3} and NdNiO\textsubscript{2}.
on-site Coulomb interaction and the charge-transfer energy, and classify materials as charge-transfer or Mott-Hubbard insulators in the Zaanen-Sawatzky-Allen scheme [1, 64–67].

Figure 2 is the Nd $3d$ core-level XPS spectra for Nd$_2$O$_3$, NdNiO$_3$ and NdNiO$_2$. The similar overall pattern indicates the trivalent Nd$^{3+}$ with the $4f^3$ ground state in the three compounds. There is a blue shift of the binding energy around $\Delta E_b \simeq 1.1$ eV for NdNiO$_2$, comparing to NdNiO$_3$ as shown in the inset. Thus the formal chemical valence is Ni$^{3+}$ and Ni$^{1+}$ in NdNiO$_3$ and NdNiO$_2$, respectively. In the Nd$^{3+}$ $3d$ XPS, the spectral structure is mainly determined by the effect of the covalency hybridization, and the two peaks of the $3d$ XPS correspond to the bonding and antibonding states between the $3d^94f^3$ and $3d^94f^44d^1$ configurations ($4d^1$ is the hole in the ligand) in the final states [62]. The ground state of Nd$_2$O$_3$ is in the almost pure $4f^3$ configuration, and hence the main peak at around 981-983 eV in the Nd $3d_{5/2}$ XPS spectra is the unscreened $3d^94f^3$ final state. The screened $3d^94f^44d^1$ final state has a lower binding energy around 977 eV.

Figure 3 compares the O $1s$ XPS spectra in NiO, NdNiO$_3$ and NdNiO$_2$. The O $1s$ XPS has often used in the experiments for the transition-metal oxides, however, the nature of the 531 eV O $1s$ spectral peak in NiO is unclear [68, 69], and has been proposed to be due to defective sites within the oxide crystal [70, 71], adsorbed oxygen [72], or hydroxide species [73], and also attributed to an intrinsic feature [68, 74]. We can’t exclude the contaminant origin for the 530.9 eV feature, however, we have measure the O $1s$ XPS spectra on both different samples and different XPS instruments and obtain the consistent similar results, which is hardly attributed to an extrinsic feature. In O $1s$ XPS spectra, NiO and NdNiO$_2$ have the best-screened states at around 529 eV. In NdNiO$_3$, an extra peak appears at the lowest binding energy 528.3 eV, indicating the concentration of the oxygen holes in the ground state, due to a negative charge transfer energy [75–78].

As depicted in the inset of Fig. 2, NdNiO$_2$ has a higher binding energy than NdNiO$_3$ in the Nd $3d$ XPS by around $\Delta E_b \simeq 1.1$ eV. The Nd$^{3+}$ binding energy blue shift $\Delta E_b$ indicates the increasing of the Fermi energy in NdNiO$_2$. Since Nd$^{3+}$ has a weaker hybridization than Ni$^{+}$ with the oxygen, the Fermi energy increasing is mainly due to the increasing chemical potential of Ni$^{3+}$ in NdNiO$_2$, assuming the unchanged chemical potential of oxygen. Hence NdNiO$_2$ has a larger charge-transfer energy $\Delta$. Taking account for the covalency of the transition-metal ions and ligands, the effective charge transfer energy is $\Delta' = \Delta - (W + w)/2$ [79], where $W$ and $w$ are the bandwidths for the transition-metal $3d$-band and oxygen $2p$-band, respectively. NdNiO$_2$ has the nearly two-dimensional transition-metal $3d$-band and oxygen $2p$-band which are narrower than the three-dimensional ones in NdNiO$_3$; then it has a larger effective charge transfer energy $\Delta'$. From the comparison between NdNiO$_2$ and NdNiO$_3$, the former has a larger charge-transfer energy than the latter, and is not a negative/small charge-transfer insulator. NdNiO$_2$ has the quite similar pattern of O $1s$ XPS to NiO, but the covalence peak is significantly suppressed as shown in Fig. 3. Since NiO is a three-dimensional charge-transfer insulator, NdNiO$_2$ could have a larger effective charge-transfer energy $\Delta'$ than NiO, and is likely to be a Mott-Hubbard type as suggested in Ref. [16, 17, 21, 25], which need further confirmation in the Ni $2p$ XPS as demonstrated below.

Next, we examine the Ni $2p$ XPS spectra to confirm whether NdNiO$_2$ is a charge-transfer or Mott-Hubbard type. Figure 4 displays Ni $2p$ XPS spectra of NiO, NdNiO$_3$ and NdNiO$_2$. The Ni $2p$ spectrum is composed of $2p_{3/2}$ and $2p_{1/2}$ components due to the large spin-orbit coupling in the Ni $2p$ core level. The main line region of the $2p_{3/2}$ spectra around 852-859 eV corresponds to the screened final states, and can

![FIG. 3. O $1s$ core-level XPS spectra of NiO (a), NdNiO$_3$ (b) and NdNiO$_2$ (c) powder samples.](image-url)

![FIG. 4. Ni $2p_{3/2}$ and $2p_{1/2}$ core-level XPS spectra of NiO (a), NdNiO$_3$ (b) and NdNiO$_2$ (c) powder samples.](image-url)
be fitted by two peaks. The removal of the $2p$ core electron leads to the creation of a strong local potential on the nickel site, and an electron is transferred from the environment to the Ni site. The different types, i.e., small/negative charge-transfer, charge-transfer and Mott-Hubbard types according to the ZSA scheme, of the transition-metal compounds have different non-local screening effects in the main line of the $2p$ transition-metal XPS spectra [40, 41].

The perovskite NdNiO$_3$ has a negative effective charge-transfer energy, giving rise to “self-doped” holes on the ligands [79]. It mainly has a local Ni $3d^8$ configuration, a predominant $O 2p$ character across the Fermi level and a consequent ground state of mainly Ni $3d^9L$ in the metallic state at the room temperature. The two peaks in the main lines correspond to the $2p^33d^0L^1$ and $2p^33d^0L^2$ final states [77]. NdNiO$_2$ has a larger transfer energy $\Delta$ than NdNiO$_3$ as demonstrated above according to Fig. 2 and Fig. 3, and hence displays a different shape of the main line of Ni $2p_{3/2}$ XPS. Again, we confirm NdNiO$_2$ is not a negative charge-transfer insulator.

In the charge-transfer insulator NiO, the main line have the double-peak structure. The higher binding energy peak corresponds to the $2p^33d^0L^1$ final state, where an electron is transferred from the neighboring oxygen atoms (local screening) leaving a hole in the oxygen ligand orbital $L$. The peak at the lowest energy corresponds to the final state where an electron is transferred from oxygen in the neighboring NiO$_6$ octahedron, thereby creating a Zhang-Rice singlet in the faraway octahedron (non-local screening) [37, 40, 41].

The non-local screening peak is a signature for the presence of the Zhang-Rice singlet in the charge-transfer insulators, as observed in the cuprate oxides and NiO [38–41]. Compared with NiO, the non-local screening peak in NdNiO$_2$ is significantly suppressed. Hence the NiO$_2$ layer in NdNiO$_2$ is not a large-$\Delta$ charge-transfer type, but a Mott-Hubbard one. The initial ground state and the final screened state are mainly $3d^0$ and $3d^{10}L^2$, respectively.

Two-magnon mode in Raman spectroscopy. – Figure 5 is the Raman spectra of NdNiO$_3$ and NdNiO$_2$ at 300 K and 120 K measured on the sub-millimeter sized single crystals. The Raman susceptibility $\chi''(\omega)$ deduced from the Raman intensity $I(\omega)$ according to the fluctuation-dissipation theorem, $I(\omega) = (1 + n_B(\omega))\chi''(\omega)$ where $n_B(\omega)$ is the boson factor.

The Raman spectra for NdNiO$_3$ agrees well with the previous measurements on the thin-film single crystal [80], implying the high-quality for our bulk NdNiO$_3$ samples. There are more phonon peaks at low temperatures due to the structure distortion during the metal-insulator transition around 200 K in NdNiO$_3$. The dramatically increasing of the phonon intensity is due to the metal-insulator transition in NdNiO$_3$.

The surface contaminant due to the formation of fluorite NdNiO$_2$H$_x$ reported in the previous thin-film NdNiO$_2$ [81, 82] is nearly invisible in our Nd 3d XPS. To remove the possible contaminant, we polish the NdNiO$_2$ single crystal as shown in the inset of Fig. 5. During the synthesis process, some pure nickel metal are embedded in NdNiO$_2$ crystal due to the perotectic phenomenon and forms the dark gray spots (marked by red circles) in the polished surface of NdNiO$_2$. The large light gray area in the SEM image is NdNiO$_2$ as identified by EDX. We perform the Raman scattering measurements on NdNiO$_2$ in the light gray area.

The ideal stoichiometric NdNiO$_2$ has the space group $P4/mmm$ and all the ions can be taken as the inversion center of the lattice. Therefore, there is no Raman active phonon mode in the Raman scattering. There is no sharp phonon modes in the spectra. A broad peak appears at 122 cm$^{-1}$, independent of the temperature and its origin is unclear. We suspect it comes from the defect due to the off-stoichiometry of NdNiO$_2$.

We attribute the mode at around 550 cm$^{-1}$ in the Raman susceptibility spectra of NdNiO$_2$ in Fig. 5 to the two-magnon peak in the two-dimensional Heisenberg antiferromagnet. The broadening of the two-magnon response with doping and temperature has been studied theoretically in the cuprate oxides [46–56]. The two-magnon identifies the strong spin fluctuations in the cuprate even when the long range antiferromagnetic order disappears at high temperatures or upon doping [45]. In a 2D Heisenberg antiferromagnet, the light in the Raman process flips two nearby spins on the nearest neighboring bond, leaving behind a locally disturbed antiferromagnet with 6 broken exchange bonds in the final state. Therefore the two-magnon has the energy scale at roughly $2.7J$ [45]. We equal $2.7J$ to 550 cm$^{-1}$, and obtain the antiferromagnetic exchange strength $J = 25$ meV.
The Mott-Hubbard scenario is also stressed in Ref. [21]. The 2NiO planes primarily locate on Ni sites. The presence of hybrid density functional and the exact diagonalization of NiO Hamiltonian for nickelate oxides Nd_{1−x}Sr_xNiO_2 reveals an insulating behavior without the presence of the superconductivity [58].

\[ H = J \sum_{i<j} S_i \cdot S_j + \text{exchange strength} \]
\[ J = 29 \text{ meV} \]

In summary, we perform core-level X-ray photoemission spectroscopy (XPS) and Raman spectroscopy studies of electronic structures and spin fluctuations in the bulk NdNiO_2. We find that the NdNiO_2 planes are Mott-Hubbard type in the ZSA scheme, consistent with Hepting’s electronic structure studies on the thin-film NdNiO_2 [17]. Two-magnon peak in the Raman scattering provides direct evidence for the strong spin-fluctuation in NdNiO_2. The peak position determines the antiferromagnetic exchange J = 25 meV. The present experimental investigation agrees well with our previous theoretical description of the electronic structures of NdNiO_2.

In the last, we make a remark on the three-dimensional electron pockets of Nd^{3+} 5d character in NdNiO_2 as demonstrated in Ref. [10, 17]. The presence of 5d electron pocket changes the hole count in the NiO_2 planes, resulting in spin-S = 0 Ni^{2+} states in the NiO_2 planes even without chemical doping [25]. A weakly-interacting three-dimensional 5d metallic state hybrids with the Ni^{2+} local moments in the NiO_2 layers, explaining the resonant inelastic x-ray scattering spectra in LaNiO_2 and NdNiO_2 [17]. In our Ni 2p_3/2 XPS spectra, the main line for NdNiO_2 has some weight around 853 eV (Fig. 4). We can’t rule out the minority nickel metal origin for this weight. However, XRD has the similar penetration depth as XPS and detect a tiny nickel peak in our samples. So the 853 eV weight in Fig. 4 for NdNiO_2 is likely to be intrinsic and related to the S = 0 Ni^{2+} states in the NiO_2 planes.

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