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Tuning a strain-induced orbital selective Mott transition in epitaxial VO_2

Shantanu Mukherjee,[1] N. F. Quackenbush,[1] H. Paik,[2] C. Schlueter,[3] T.-L. Lee,[3] D. G. Schlom,[2,4] L. F. J. Piper,[1,5,*] and Wei-Cheng Lee[1,†]

[1]*Department of Physics, Applied Physics and Astronomy, Binghamton University, Binghamton, New York 13902, USA*

[2]*Department of Materials Science and Engineering, Cornell University, Ithaca, New York 14853-1501, USA*

[3]*Diamond Light Source Ltd., Harwell Science and Innovation Campus, Didcot, Oxfordshire OX11 0DE, United Kingdom*

[4]*Kavli Institute at Cornell for Nanoscale Science, Ithaca, New York 14853, USA*

[5]*Materials Science & Engineering, Binghamton University, Binghamton, New York 13902, USA*

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We present evidence of strain-induced modulation of electron correlation effects and increased orbital anisotropy in the rutile phase of epitaxial VO_2/TiO_2 films from hard x-ray photoelectron spectroscopy and soft V L-edge x-ray absorption spectroscopy, respectively. By using the U(1) slave spin formalism, we further argue that the observed anisotropic correlation effects can be understood by a model of orbital selective Mott transition at a filling that is noninteger but close to the half filling. Because the overlaps of wave functions between d orbitals are modified by the strain, orbital-dependent renormalizations of the bandwidths and the onsite energy occur. These renormalizations generally result in different occupation numbers in different orbitals. We find that if the system has a noninteger filling number near the half filling such as for VO_2, certain orbitals could reach an occupation number closer to half filling under the strain, resulting in a strong reduction in the quasiparticle weight Z_α of that orbital. Our work demonstrates that such an orbital selective Mott transition, defined as the case with $Z_\alpha = 0$ in some but not all orbitals, could be accessed by epitaxial-strain engineering of correlated electron systems.

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Introduction. Mott insulators are characterized by the ratio of U/W, where U refers to the correlation strength and W is the full bandwidth. A Mott state is usually predicted from theoretical models to exist in materials at half filling and when $U/W \sim 1$. However in multiorbital systems an incipient Mott picture has been proposed with the possibility of an "orbital selective Mott transition" (OSMT). The OSMT scenario was first proposed to understand the physical properties of $Ca_{2-x}Sr_xRuO_4$ by Anisimov [1], stimulating a lot of research efforts on this subject [2–6]. More recently, in the iron based superconductors, OSMT has been suggested to account for the insulating properties driven by the iron vacancy in $K_{1-x}Fe_{2-y}Se_2$ [7–14]. In general, the physics of OSMT has relevance to a variety of multiband materials that are close to a Mott transition, and a better understanding of this phase both theoretically and experimentally would be crucial for advancing our understanding of Mott physics.

Vanadium dioxide (VO_2) is one of the early prototypes for strongly correlated systems near half filling [15,16]. VO_2 exhibits a metal to insulator transition (MIT) with a concomitant formation of V-V dimers that is generally considered to be driven cooperatively by both Mott and Peierls physics [16–20]. For example, it has been pointed out that the massive orbital switching that occurs upon entering the insulating phase can only be achieved if the system is already close to a Mott insulating regime [16]. A significant theoretical effort has been made to understand this MIT using local density approximation (LDA), LDA + U, LDA + DMFT, etc. [16,19,21,22]. Specifically, a Peierls-assisted OSMT mechanism has been proposed to understand the MIT between metallic R and insulating $M1$ phases in bulk VO_2 [22]. Furthermore, recent progress in ultrathin epitaxial VO_2 growth using TiO_2 substrates has provided surmounting evidence that electron correlation effects may become enhanced by the large strains, thus pushing the system further into the Mott regime without introducing any dopants [23–26]. These results suggest that VO_2 is an ideal candidate for exploring the OSMT with epitaxial strain.

In this Rapid Communication we present a generalized theory of OSMT to describe how strain can result in quasiparticle weight variation and preferential orbital switching. We perform theoretical calculations to show that an OSMT can be tuned within the metallic phase of VO_2 (R phase) by applying a strain that enhances the electron correlations. We find that the application of a uniaxial strain tends to make the occupation number on each orbital unequal. As a result, even if the system is slightly away from half filling, the presence of a moderate anisotropic strain along particular directions could render an occupation number in certain orbitals closer to half filling, leading to an OSMT. Further, by performing hard x-ray photoelectron spectroscopy (HAXPES) and V L-edge x-ray absorption spectroscopy (XAS) on 10 nm epitaxial VO_2 films on TiO_2(001), (100), and (110), referred to as VO_2(001), VO_2(100), and VO_2(110) (see Supplemental Material [27]), we show that strain induced electronic effects indeed exist in the metallic phase of VO_2, in an agreement with our theoretical predictions.

Model and Formalism. We have employed the $U(1)$ slave spin formalism [10] on a two orbital model to investigate the effect of strain on the quasiparticle weight near the transition to the featureless Mott phase. The slave spin formalism [6,28] has been shown to reproduce the Mott transition at the mean-field level in good agreement with DMFT results, and the $U(1)$ version can even obtain the correct noninteracting

*lpiper@binghamton.edu
†wlee@binghamton.edu

limit at the mean-field level [9]. We start from a generic two orbital model containing a tight binding Hamiltonian and a multiorbital Hubbard interaction term representing onsite electron correlations (see Supplemental Material [27]). Below we briefly summarize the mechanism for studying OSMT in a $U(1)$ slave spin formalism [10] applied to our model Hamiltonian.

Representing the charge degree of freedom by a quantum spin 1/2, the electron creation operator $d^{\dagger}_{i\alpha\sigma}$ can be written as $d^{\dagger}_{i\alpha\sigma} = S^{+}_{i\alpha\sigma} f^{\dagger}_{i\alpha\sigma}$, where $d^{\dagger}_{i\alpha\sigma}$ creates an electron on the orbital α with spin σ at site i, $S^{+}_{i\alpha\sigma}$ is the spin raising operator for the slave spin describing a charge on the orbital α with physical spin σ on the site i, and $f^{\dagger}_{i\alpha\sigma}$ is the fermionic spinon associated with the physical spin. After solving the mean-field equations subject to the constraints to eliminate the unphysical Hilbert spaces due to the introduction of the slave spins, the quasiparticle weight on orbital α can be obtained by $Z_{\alpha\sigma} \propto |\langle S^{+}_{\alpha\sigma}\rangle|^2$ [10]. Finally, the correlated metallic phase (Mott insulating phase) corresponds to $Z_{\alpha\sigma} \neq 0$ ($Z_{\alpha\sigma} = 0$) for every orbital, and the OSMT is given by $Z_{\alpha\sigma} = 0$ for some orbitals. Note that the OSMT is not a complete insulating state since the quasiparticle weight in certain bands is still finite. We perform the calculations at zero temperature and limit our attention only to the featureless Mott insulating phases. As a result, we have $\langle n_{\alpha\sigma}\rangle = \frac{n_\alpha}{2}$ and $Z_{\alpha\sigma} = Z_\alpha$. In a two orbital model, the half filling corresponds to $n = n_1 + n_2 = 2$, and we focus on the case with $1 < n < 2$.

Results. Although the generic tight binding model can describe any two orbital system, we begin by choosing a $|1\rangle = d_{xz}$ and $|2\rangle = d_{yz}$ two orbital system for the purpose of demonstration (see Supplemental Material [27]). Now assume that the strain is applied to elongate the system along the $\hat{x}$ direction. This strain significantly reduces the wave function overlaps associated with the d_{xz} but has much less effect on the wave function overlaps associated with the d_{yz}. As a result, the bandwidth of d_{xz} orbital should reduce, and we may introduce an effective parameter d such that $t^{11,strain}_{\vec{k}} \equiv (1-d)t^{11}_{\vec{k}}$. Here t^{11} is the hopping matrix element associated with the d_{xz} orbital and $(1-d)$ reflects the bandwidth reduction in the d_{xz} orbital. As a test, we have studied the case with C_4 symmetry and $d = 0$, which is summarized in the Supplemental Material [27].

Now we turn on the strain by setting $d \neq 0$. There are two effects of d on the d_{xz} orbital. First, since the bandwidth W_1 is reduced, the ratio of the interaction to the bandwidth U/W_1 increases, leading to stronger correlation effect on the d_{xz} orbital. Second, if $n < 2$, the reduction of the bandwidth W_1 tends to attract more electrons to occupy the d_{xz} orbital. Therefore we can expect that under the strain, $n_1 = n/2 + x$ and $n_2 = n/2 - x$. This indicates that the d_{xz} orbital is pushed even closer to the half filling and consequently much more correlated. As a result, both effects favor driving d_{xz} more correlated, and an OSMT could be obtained if n is near the half filling.

The orbitally-dependent quasiparticle weight Z_α as a function of strain with fixed U at different n is presented in Fig. 1. For $n = 1$, the strain does not affect Z_α too much even at quite large d. As n is closer to 2, the difference between Z_1 and Z_2 becomes more prominent, consistent with our discussion above. It should be noted that this result is quite general for a multiorbital system, and an intriguing point is that one could engineer the OSMT by the strain effect even in a system with noninteger fillings. In the next section, we study the MIT in VO_2 under high strain using the same formalism developed above.

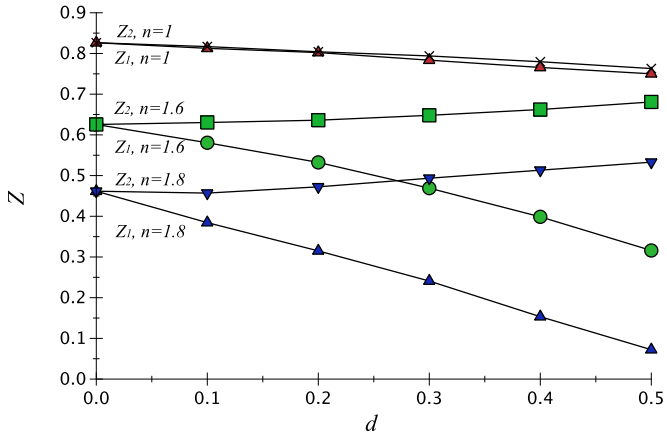

FIG. 1. The orbital-dependent quasiparticle weight in the case under the strain with $U = 4.5$ for different filling n. At the filling away from the half filling ($n = 1$), the quasiparticle weights remain almost the same even at large d. In contrast, at the filling near the half filling ($n = 1.8$), the quasiparticle weight in d_{xz} (Z_1) reduces significantly as d increases.

Application to epitaxially strained VO_2. Although the origin of the MIT in VO_2 is a complicated issue, the dominant bands near the Fermi surface are well known. The orbital compositions of the three dominant bands near the Fermi surface can be expressed as $|\sigma(d_\parallel)\rangle = |x^2 - y^2\rangle$, and $|\pi_\pm\rangle = \frac{1}{\sqrt{2}}(|xz\rangle \pm |yz\rangle)$. While the leading hopping parameter of the σ band mostly comes from the strong direct σ bonding between nearest V-V pairs, the leading hopping parameters of $\pi_\pm$ bands come from a combination of the direct π bonding between nearest V-V pairs and the second order hoppings via the V-O bonds between $3d$ and $2p$ orbitals [16,29]. Tanaka estimated [29] $|t^{\sigma\sigma}| \sim |t^{\pi_-\pi_-}| \gg |t^{\pi_+\pi_+}|$, which is in close agreement with LDA calculations [16]. Moreover, due to the crystal field effect coming from the oxygen atoms, $\pi_\pm$ bands are pushed to the higher energy, leading to a lower onsite energy in the σ band. As a result, this system can be reasonably approximated as a two-band system with comparable bandwidths in the metallic R phase. A strain on VO_2 due to the (110) or (100)-oriented TiO_2 substrate leads to two important effects that support the OSMT scenario. Firstly, because the c-axis lattice constant of the bulk TiO_2 is longer than that of bulk VO_2 by 3.62% [30], the c axis is stretched in both VO_2(110) and VO_2(100). Here the $\hat{x}$, $\hat{y}$, and $\hat{z}$ axes are defined to be parallel to the rutile (001), (110), and (−110) directions, respectively [19,31]. It is found in LDA calculations that a longer c axis primarily leads to a reduction of the σ orbital hoppings $t^{\sigma\sigma}$ and suppression of the corresponding bandwidth W_σ [31]. Consequently a larger U/W_σ would enhance the electronic correlations in the σ band. Secondly, due to the elongation of the c axis, the average V-O bond length would shorten due to the effect of a volume conserving strain $2\epsilon_{cc} - \epsilon_{aa} - \epsilon_{bb}$,

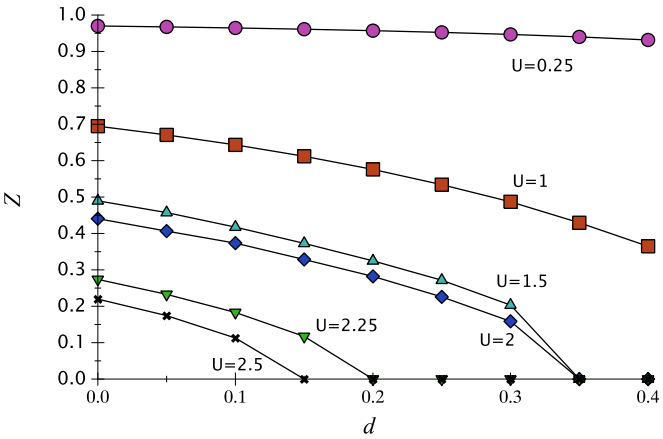

FIG. 2. The quasiparticle weight in the σ band of VO_2 under the strain as a function of U at $n = 1.5$. The hopping parameters for VO_2 are $t^{\sigma\sigma}_{i,i+\hat{x}} = t^{\sigma\sigma}_{i,i+\hat{y}} = -0.25$, $t^{\pi-\pi-}_{i,i+\hat{x}} = t^{\pi-\pi-}_{i,i+\hat{y}} = 0.22$. The onsite energy due to the crystal field splitting without the strain is $\Delta_\sigma = -0.1$ and $\Delta_\pi = 0.05$. These values are taken from Ref. [29], and the unit of energy is eV. The interband hoppings are small and neglected in Ref. [29], and we set a representative value $t^{\sigma\pi-}_{i,i+\hat{x}+\hat{y}} = t^{\pi-\sigma}_{i,i+\hat{x}+\hat{y}} = 0.01$. At large U, an OSMT could occur at small to moderate d.

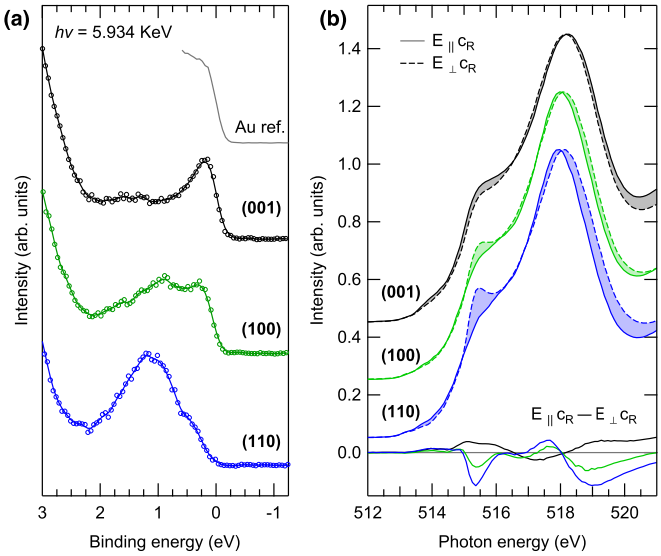

FIG. 3. (a) HAXPES of the metallic phases of the three VO_2 strain orientations close to the Fermi level. (b) The corresponding polarization dependent V L-edge XAS for the films along with the orbital dichroism for each case plotted underneath on a common intensity scale.

which enhances the d-p hybridizations, increases the onsite energy of the π orbital, and leads to a larger energy difference between the σ and π orbitals. For simplicity, we model the change in the onsite energy as an effective lowering of σ orbital onsite energy. The effects of the strain can then be taken into account by

$$t^{\sigma\sigma,\text{strain}}_{\vec{k}} \equiv (1-d)t^{\sigma\sigma}_{\vec{k}}$$
$$\Delta^{\text{strain}}_{\sigma} = -(1+Cd)\Delta_\sigma, \quad (1)$$

where C is a positive constant. It can be seen easily that both effects from the strain strongly favor more occupation numbers in the σ band, thus pushing it closer to half filling.

Moreover, because of the large hybridization between $3d$ orbitals of V and $2p$ orbitals of O, the total occupation number in $3d$ orbitals is in fact in the range of $n = 1.2$–2 instead of 1 as one might expect from a direct counting of the valence charges. Consequently, the OSMT due to the strain effect discussed in the last section is very likely to occur with a moderate d. We adopt the values of $t^{\sigma\sigma}$, $t^{\pi-\pi-}$, and the onsite energies derived in Ref. [29] and Eq. (1) to model the strain effect. The quasiparticle weight in the σ band Z_σ at $n = 1.5$ as a function of U and d is plotted in Fig. 2. For small U, Z_σ remains close to 1 and does not depend on d. As U increases, Z_σ develops a significant dependence on d, and an orbital selective Mott transition occurs at a critical $d = d_c$ if U is large enough. Clearly, d_c decreases as U increases, indicating that the OSMT is indeed driven by the strong Coulomb repulsive interaction. Furthermore, we notice that the behavior would be fundamentally different when the c axis is compressed rather than elongated, as is the case for VO_2(001). This will shorten σ bond distance along the c direction and would reduce the energy difference between σ and π orbitals, thus keeping their occupations away from half filling in the R phase. As a result, the OSMT would be expected to occur in VO_2(100) and VO_2(110), but not in VO_2(001).

We emphasize that the increase of the occupation number in the σ band is a direct consequence of the balance between kinetic and interaction energies. Because the bandwidth and the effective onsite energy of the σ band are both lowered by the strain, it is energetically favorable to put more electrons in the σ than in the π_- bands to compromise the interaction energy. While this trend in the occupation numbers can be captured by LDA-based approaches, the significant change in the quasiparticle weight as well as the OSMT found here is attributed to the advantage of the $U(1)$ slave spin formalism. We predict that the occupation number in the σ band could be substantially increased under the strain even in R phase without the dimerization of V-V pairs, and the metallic phase in this region would be a strongly correlated metallic state with vanishing quasiparticle weight in the σ band Z_σ.

To investigate the predicted effect of strain on VO_2 thin films, we have performed HAXPES and polarization dependent XAS of the V L-edge on VO_2(001), VO_2(100), and VO_2(110) in the metallic R phase close to the MIT (see Supplemental Material [27]). Figure 3(a) shows the HAXPES of the topmost valence states, while Fig. 3(b) shows the corresponding V L XAS spectra collected from each VO_2 film. All presented spectra were collected at $\sim 20\,^\circ$C above their respective T_{MIT}, i.e., in the metallic phase. The XAS at the V L edge were collected with the polarization vector either parallel to the [001] ($E_\parallel c_R$) or [110] ($E_\perp c_R$) crystallographic axis. Included at the bottom of Fig. 3(b) are the difference spectra ($E_\parallel c_R$-$E_\perp c_R$) representing the linear orbital dichroism.

Both the valence band HAXPES and weak orbital dichroism of the VO_2(001) closely resemble that of bulk VO_2 [16,20,32]. In contrast, both the VO_2(100) and (110) films show dramatic deviations from the bulk. The sharp Fermi edge at E_F, indicating a Fermi liquid behavior, is weakened in the VO_2(100) case and further so for the (110) case resulting in a more smeared

out intensity distribution near the Fermi energy. This behavior is equivalent to the vanishing Z_σ in our model and is typically seen in Mott insulating materials such as in parent cuprate superconductors [15,33]. Along with these changes at E_F are concurrent increases in orbital anisotropy observed in the V L-edge spectra of the VO_2(100) and VO_2(110) films, indicating preferential filling of certain bands. This demonstrates that the strain, specifically when the c axis is elongated, can indeed effect both the electron correlations and the orbital occupancy.

The orbital dichroism observed here in the VO_2(100) and VO_2(110) films tends toward that observed for the insulating phase of unstrained VO_2, despite remaining in the metallic phase. Haverkort *et al.* [16] observed in unstrained bulk VO_2 a dramatic switching of the orbital occupancy going from the high temperature rutile to low temperature M1 phase, in which the σ (often referred to as $d_\parallel$) orbital becomes preferentially filled. Our results indicate a similar modification of the orbital occupancy purely induced by strain within the distorted rutile structure. Remarkably, the increased preferential filling of the σ orbital in this case does not require the formation of V-V dimers, supporting our OSMT picture.

Consistent with our OSMT prediction for VO_2, the weak orbital dichroism and the sharp Fermi edge for VO_2(001), when the c axis is contracted, resemble that of the bulk. Furthermore, we observe that while both VO_2(110) and VO_2(100) have the same stretched c axis, VO_2(110) exhibits larger orbital dichroism, as well as a weaker Fermi edge, indicating that VO_2(110) is more correlated than VO_2(100). This difference can be attributed to the contraction along the out-of-plane direction of the film due to the compensation of the biaxial strain, which is ignored in our theory. The contraction in VO_2(110) is along the rutile (110) direction, thus directly effecting the V-O bond lengths. This serves to increase the onsite energy of the π orbital due to the enhanced d-p hybridization, which leads to a larger energy difference between the σ and π orbitals. However, in VO_2(100) the contraction decreases the distance between V atoms along the rutile a axis [the ($\hat{y}$-$\hat{z}$) direction in the unit cell] [19,31], having a less direct effect on the V-O bond lengths. As a result, the strain effects distinguishing σ and π orbitals are expected to be stronger in VO_2(110). More rigorous theoretical efforts are required to obtain a quantitative description in this aspect.

Conclusion. To summarize, we have studied the effect of strain on multiorbital systems. Because the spatial profile of the orbital wave function is anisotropic, the strain-induced bandwidth reduction and the onsite energy due to the crystal field effect become orbital dependent. Based on the $U(1)$ slave spin formalism on a generic two orbital Hubbard model, we have demonstrated that if the system has a total filling which is noninteger, but close to the half filling, an orbital selective Mott transition could be engineered by the application of strain if the system has strong Coulomb repulsive interactions. By applying this theory to study the highly strained VO_2 in combination with experimental results from spectroscopic studies, we have proposed that an orbital selective Mott state exists in the high temperature phase of coherently strained VO_2 with an elongated c axis. This state could appear before the M_2 phase emerges, which explains why the region of M_2 phase found in experiments is much narrower than the prediction of Landau-Ginzburg theory [25]. Our results indicate that Mott physics is crucial to understand the properties of VO_2.

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