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Electron correlations, oxygen vacancies, or both ? Revisiting a foundational paradigm of strongly-correlated electron systems

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1 Introduction

$SrTiO_3$ and $SrVO_3$ are model examples of, respectively, a band insulator and a correlated electron metal. However, our previous work unveiled that a 2D electron gas (2DEG) can be created at the surface of $SrTiO_3$ [1]. Moreover the spectrum of such 2DEG looks identical to that of $SrVO_3$, namely composed of dispersing quasi-particles near the Fermi level (E_F) and an incoherent peak around -1.5 eV, assigned to the lower Hubbard band in the case of $SrVO_3$ [2], but known to arise merely from oxygen vacancies in the case of $SrTiO_3$ [1]. The purpose of this work is to determine what part of the measured spectrum of $SrVO_3$ is due to correlations, and what part is imputable to oxygen vacancies created by the preparation methods and/or by the UV light used for photoemission measurements. The issue at stake is to understand to what extent the *drosophila* of correlated-electron materials can be described in the framework of modern theories of interacting electrons in solids.

2 Experiment

The bulk-like, crystalline $SrVO_3(001)$ thin films were grown by pulsed laser deposition (PLD) in a chamber directly connected to the ARPES setup at beamline 2A of KEK-PF. The PLD growth was performed in a pressure below 10^{-7} Torr, to obtain clean surfaces, using a $Sr_2V_2O_7$ target, which has excess oxygen with respect to $SrVO_3$, thus minimizing the formation of vacancies during the growth. For the ARPES measurements we used linearly polarized photons in the energy range 30–110 eV and a hemispherical electron analyzer with horizontal slits. The angular and energy resolutions were 0.25° and 15 meV. The mean diameter of the incident photon beam was smaller than 100 μm. The UV light brilliance was about 5×10^7 photons/(s μm^2). Such low brilliance, about 100 times smaller than the one found in standard 3[d] generation synchrotrons, was crucial for our measurements, to avoid the rapid generation of oxygen vacancies under UV dose. The samples were measured at $T = 20$ K.

3 Results and Discussion

The experiments successfully provided the information we were looking for. As shown in Fig. 1(a), when the preparation procedure carefully avoids the introduction of vacancies, and the UV dose is kept sufficiently small, a weak but clearly dispersive Hubbard peak is observed. On the other hand, as seen in Fig. 1(b), once the UV dose is large again, hence creating a significant amount of oxygen vacancies, the incoherent peak becomes very intense and non-dispersive. Such dramatic enhancement of the incoherent peak at -1.5 eV demonstrates that states arising from oxygen vacancies can completely mask any intrinsic Hubbard band. All these observations prove that the measured line-shape of the Mott-Hubbard band and the ratio of intensities between the quasi-particle and the Mott-Hubbard peaks, which are crucial to quantify the strength of electron correlations, can be dramatically affected by the conditions used in the photoemission experiments, and must be seriously considered to validate theories and first-principles calculation schemes of the physics of strongly-interacting electron materials [3].

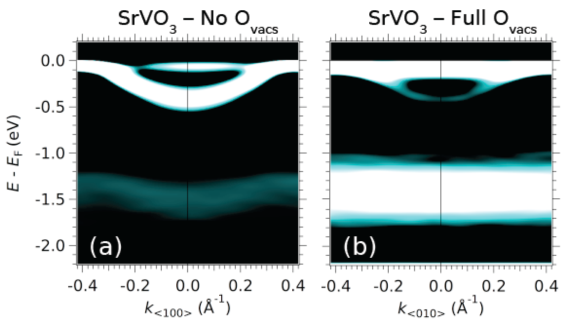

Fig. 1: (a) ARPES energy-momentum map at the Γ point in an $SrVO_3$ sample prepared and measured at BL-2A of KEK-PF under conditions that minimize the introduction of oxygen vacancies. (b) Same as (a) after irradiation with a large UV dose during complementary measurements at synchrotron SOLEIL (France). Adapted from Ref. [3]

References

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Research Achievements

1. Our results were published in Phys. Rev. B Rapid Communications [3]. The paper was an "Editors' Suggestion" for the issue of Dec. 2016.

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