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μ-ARPES study of Kagome superconductor $Cs(V_{1-x}Nb_x)_3Sb_5$

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1 Introduction

Recently, a family of kagome metals AV_3Sb_5 (AVS; A = K, Rb, Cs) with a V kagome network has emerged as a new platform to study the physics associated with the saddle point (SP) singularity due to its proximity to E_F, as revealed by density-functional-theory calculations [1–10] and angle-resolved photoemission spectroscopy (ARPES) [11–18]. AVS commonly exhibits superconductivity (T_c = 0.9–2.5 K) and a charge density wave (CDW; T_{CDW} = 78–103 K). The mechanism has been intensively discussed in terms of the characteristic band structure with the SP at the M point of the BZ [2-4,5–18]. For instance, the scattering connecting different SPs would promote unconventional superconducting pairing, whereas the same scattering also contributes to the energy gain to stabilize the chiral CDW with an in-plane 2 × 2 periodicity.

A promising strategy to study the interplay among superconductivity, a CDW, and electronic states is to modulate the band structure by varying key physical parameters that characterize the electronic phase diagram, such as pressure and carrier concentration. Such attempts have been made in AVS. For example, transport measurements under high pressure have clarified the anticorrelation between T_c and T_{CDW} as well as an unconventional double superconducting dome [19–22], whereas the relevant band structure is under debate. Chemical substitution in crystal is a useful method to tune chemical pressure and carrier concentrations, but such studies are still limited in AVS.

Here, we report an μ-ARPES study of Nb-substituted CVS, $Cs(V_{1-x}Nb_x)_3Sb_5$ (x=0, 0.03, and 0.07), in which the substitution of V ions with isovalent Nb ions leads to T_c enhancement and simultaneously T_{CDW} reduction [23].

2 Experiment

High-quality single crystals of $Cs(V_{1-x}Nb_x)_3Sb_5$ were synthesized with the self-flux method. VUV-ARPES measurements with micro-focused synchrotron light were performed with a DA30 electron analyzer at BL28A [24], as well as SES2002 spectrometers at Tohoku University. The energy resolution was set to be at 35 meV at Photon factory and 7 meV at Tohoku University. The angular resolution was set to be 0.2-0.3˚. Crystals were cleaved *in-situ* in an ultrahigh vacuum of ~ 1×10^{-10} Torr.

3 Results and Discussion

Figures 1(a) and 1(b) display a comparison of the ARPES intensity between x = 0.07 and x = 0 measured along the ΓKM cut at T = 120 K. In both measurements, the electron-like α band at Γ, the linearly dispersive γ/ε bands crossing E_F, and the δ band forming a SP at M are commonly resolved. This indicates that the overall band structure is unchanged after the Nb substitution. To clarify quantitative differences in the band position, we have determined the experimental band dispersion (red and black crosses), and directly compared them in Fig. 1(c). At first glance, both band structures for x = 0.07 and 0 well overlap each other. However, a closer look reveals a finite difference in the energy position of the α band, which shifts downward ~20 meV at x = 0.07 relative to that at x = 0. The shift is also seen by a comparison of momentum distribution curves (MDCs) at E_F in Fig. 1(d) where the peaks for x = 0.07 are located outside of the peaks for x =

0 (note that the peak width is slightly wider in $x = 0.07$ due to the increase of impurity scattering by Nb substitution). Moreover, as shown by the energy distribution curves (EDCs) at Γ in Fig. 1(e), the bottom of the α band moves toward higher EB by ~20 meV with Nb substitution, One can also see from Fig. 1(c) that the ε-band bottom and the η-band top at M are shifted downward (by ~20 meV) upon Nb substitution. These results suggest that the Nb substitution affects both the Sb- and V-derived bands. In contrast to the downward shift of the α, ε, and η bands, the γ and δ bands near EF look relatively stationary.

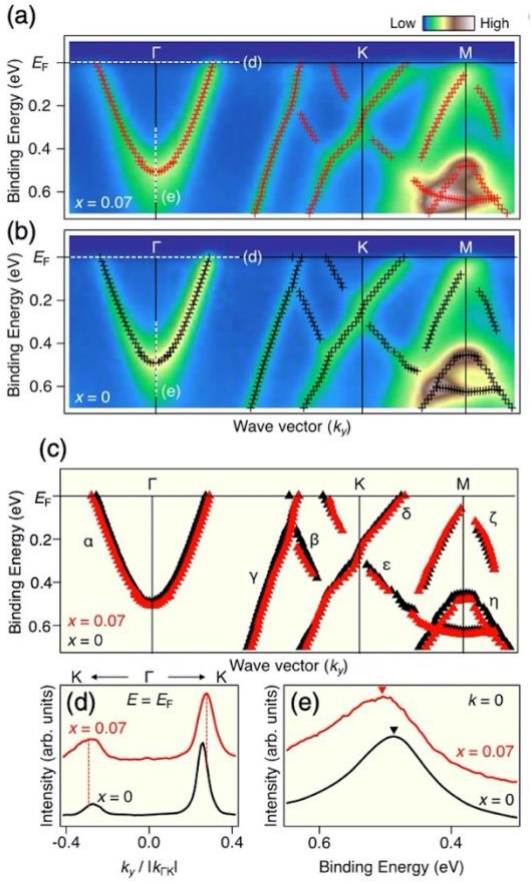

Fig. 1 (a) ARPES-intensity plot along the ΓKM cut for $x = 0.07$ measured at $T = 120$ K with hν = 106 eV. Crosses show experimental band dispersion extracted from the peak position in EDCs and MDCs. (b) Same as (a) but for $x = 0$. (c) Comparison of band dispersions between $x = 0.07$ and $x = 0$ [same as red and black crosses in (a) and (b)]. (d),(e) Comparison of MDCs at E_F and EDCs at $k_y = 0$ [the cuts are indicated by white dashed lines in (a)], respectively, between $x = 0.07$ (red) and $x = 0$ (black). The horizontal axis in (d), $k_y/|k_{ΓK}|$, is defined as the k_y value in units of the ΓK length where the Γ and K points correspond to 0 and 1, respectively. Red dashed lines in (d) are a guide for the eye to trace the peak position of $x = 0.07$. Triangles in (e) indicate the peak position.

In addition to the experiment at synchrotron, we also performed high-resolution experiment to observe the CDW gap at Tohoku University. We found that the Nb substitution shifts the Sb-derived electron band at the Γ point downward and simultaneously moves the V-derived band around the M point upward to lift up the saddle point (SP) away from the Fermi level, leading to the reduction of the CDW-gap magnitude and T_{CDW}. This indicates a primary role of the SP density of states to stabilize the CDW. The present result also suggests that the enhancement of superconductivity by Nb substitution is caused by the cooperation between the expansion of the Sb-derived electron pocket and the recovery of the V-derived density of states at the Fermi level [23].

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