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Spiral Band Structure Hidden in the Bulk Chiral Crystal $NbSi_2$

Cheng Zhang[a], Koji Miyamoto[a], Tatsuya Shishidou[b], Ryoga Amano[c], Taisei Sayo[c], Chiho Shimada[c], Yusuke Kousaka[c], Michael Weinert[b], Yoshihiko Togawa[c], and Taichi Okuda[a]

[a]*Hiroshima synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan.*
[b] *Department of Physics, University of Wisconsin-Milwaukee, Wisconsin 53201, USA.*
[c] *Deparment of Physics and Electronics, Osaka Metropolitan University, Osaka 599-8531, Japan.*

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Recently, so-called chirality induced spin selectivity effect (CISS) has been observed in the chiral crystal $NbSi_2$ through electrical conductivity measurement [1], CISS effect refers to a phenomenon that a spin-polarized current is generated when a current is passed through a material with a chiral structure [2,3].

To investigate the electronic structure of $NbSi_2$, we performed synchrotron-radiation angle resolved photoemission spectroscopy for both right-($P6_222$) and left-handed ($P6_422$) samples. Since the $NbSi_2$ crystal is difficult to cleave, the clean surface was obtained by mechanical polishing, Ar ion sputtering and annealing. We found not only the clear energy bands, but also spiral-shaped constant energy contours (CEC) at specific binding energies (E_B). The fact that the helicity of this pattern is reversed in the crystal having opposite chirality indicates that the observed intriguing pattern has its origin in the structural chirality. Our density functional theory (DFT) calculations confirmed this point. This result demonstrates that a photoemission experiment can be a new way to distinguish the chirality of crystals.

Figure 1 (a) and (b) show energy band structure of the right-handed $NbSi_2$ observed by ARPES along the high-symmetry lines $\bar{M}$-$\bar{\Gamma}$-$\bar{M}$ and $\bar{K}$-$\bar{\Gamma}$-$\bar{K}$. Figure 1 (c) and (d) show the bulk and surface calculated energy band structure, respectively. Bulk bands and surface states of ARPES data can be distinguished. Figure 2 (a) and (b) are CEC patterns for the right- and left-handed $NbSi_2$, respectively. Figure 2 (c) and (d) are the bulk calculated results without the showing spiral patterns. By comparing the surface calculated results, as shown in Figure 2 (e) and (f), we can confirm that the spiral structure is a surface effect.

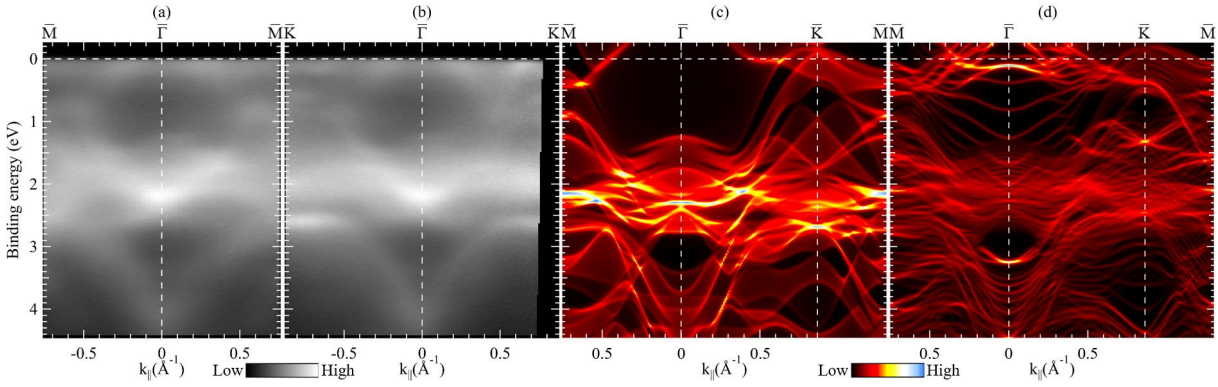

Figure 1. (a), (b) ARPES band structures of right-handed $NbSi_2$ crystal ($P6_222$) along lines $\bar{M}$-$\bar{\Gamma}$-$\bar{M}$ and $\bar{K}$-$\bar{\Gamma}$-$\bar{K}$. (c), (d) Bulk and surface calculated energy band structures by DFT along the high-symmetry lines.

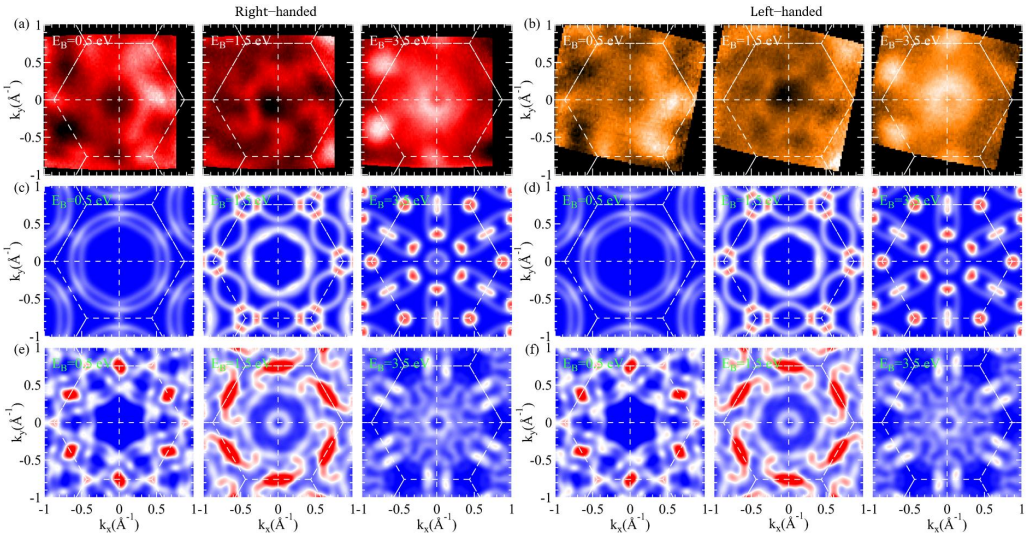

Figure 2. (a), (b) ARPES CEC patterns for the right-handed ($P6_222$) and left-handed $NbSi_2$ ($P6_422$) at some typical E_B, respectively, which are constant energy cut at E_B through a $E(k_x, k_y)$ data set obtained at a photon energy of 50 eV. (c), (d) Bulk calculated results for some corresponding E_B. (e), (f) Surface calculated results.

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