Electronic states of potassium intercalated picene thin film on Au substrate

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A picene molecule is constituted by a zigzag chain structure of five benzene rings sharing some of their edges as shown in Fig. 1. A solid picene has a layer structure stack to *c* axis, where each layer consists of a herringbone structure with the picene molecules inclining a little from the *ab* plane as shown in Fig. 2[1]. Thus the structure is two dimensional. Also this material is an organic-semiconductor which has an optical band-gap of 3.3 eV[2]. Then this material has been interested for an application such as a solar battery and an organic-thin-film transistor, et al., because of band-gap near sun light and high electron mobility. On the other hand, physical property as superconductor with *T*c=7 and 18 K when doped with potassium in the solid of molecule picene has been discovered[3]. However, the pristine solid picene does not appear the property of the superconductivity. Therefore it is interested that origin of superconductivity appearance is clear from a viewpoint of electron spectroscopy. So the discovery of the superconducting molecule picene motivates us to search for new molecular superconductors such as the potassium intercalated picene thin film. Thus it is considered that electronic states of the potassium intercalated picene play an important role in superconductivity.

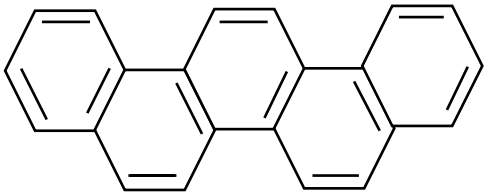

Fig. 1. A structure of a picene molecule.

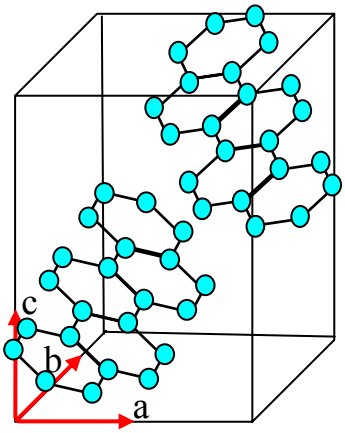

Fig. 2. A three-dimensional structure of a solid picene.

In this report the electronic states for specimens of the potassium intercalated picene is studied by X-ray emission spectroscopy (XES). The XES spectra have characteristics to give information of partial density of states in the valence band density of states (VB-DOS) because different wave functions for each element in a material under study can be separated due to the dipole selection rule of electron transitions. Therefore, we can obtain a specific signal for an element which can be used as a finger print, otherwise it is difficult.

A substrate of gold evaporated on a stainless steel was prepared. Picene thin film with thickness of 100 nm was deposited on this substrate by Joule heating of alumina coated tungsten-basket within picene powder in vacuum. After potassium was intercalated into this picene thin film by evaporation at room temperature, XES measurement was performed in

situ. The XES spectra were obtained in an XES apparatus which is installed to a beamline BL-19B at synchrotron radiation facility of Photon Factory (PF) in High Energy Accelerator Research Organization (KEK).

Figure 3 show XES spectra of C Kα, where the energy of incident photon is 350 eV. Blue dots are an XES spectrum obtained from pure picene thin film. Red dots are an XES spectrum obtained from potassium intercalated picene thin film. Right part of figure is partially expanded from the left part of figure. The shape of both XES spectra (blue and red dots) is similar ones as C Kα of graphite without shown in figure. One can be seen that the spectrum shape of the allowed part is different by the potassium intercalation. Since the XES spectrum of C Kα has the information of partial density of states in VB-DOS because of a narrow core level, the increase in the intensity near 285 eV reflects on the increase of density of states near Fermi level. Because, after an electron at C 1s is excited by a photon of 350 eV and then a hole is formed, an only electron at 2p within 2s2p electrons in the valence band of solid picene is able to transfer into the hole of 1s for relaxation process to obey the dipole selection rule. The energy difference between the hole of C 1s and Fermi level is about 285 eV. That is, the intensity at allowed part means the increase in electron density with p states near Fermi level. Considering that the superconductivity appearance is closely related to electrons near Fermi level, 2p states in C atoms may be played the important role.

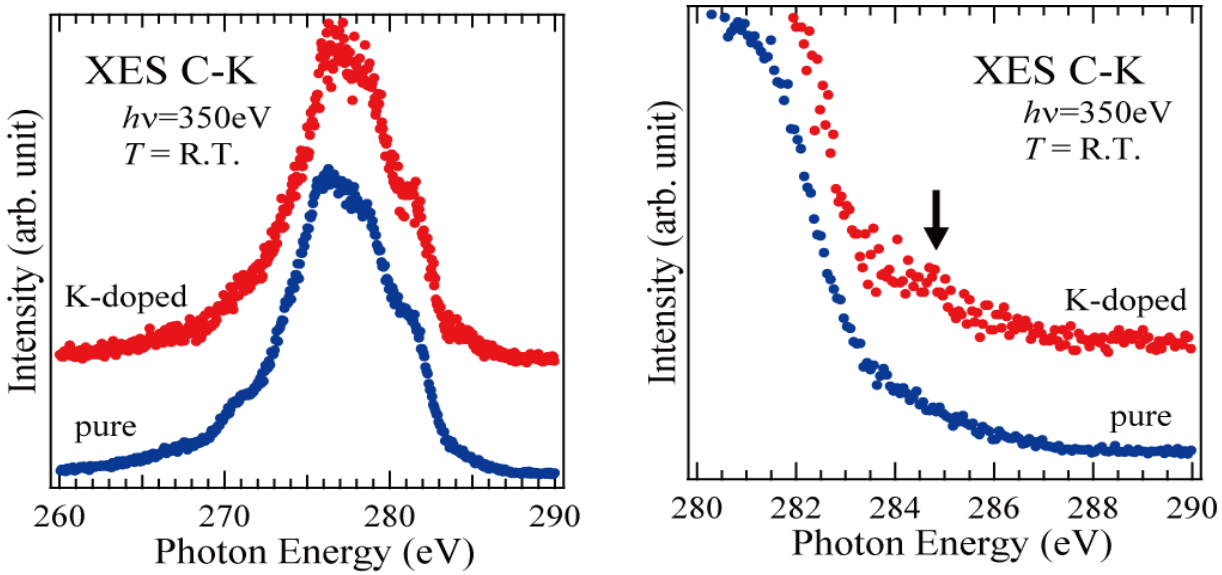

Fig.3. XES spectra of C Kα, where the energy of incident photon is 350 eV; Blue dots are pure picene thin film. Red dots are potassium intercalated picene thin film.

The samples of potassium intercalated picene thin film were made by the method of evaporation in situ. The XES measurements were performed at PF. The increase in intensity at the shoulder of high photon energy side in C Kα spectrum has been observed with the potassium intercalated samples. This is related to 2p states in C atoms near Fermi level.

References

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