

# STM Study of (BEDT-TTF)<sub>2</sub>Cu(NCS)<sub>2</sub> Surface

M. Yoshimura<sup>1</sup>, N. Ara<sup>1</sup>, M. Kageshima<sup>1</sup>, R. Shioda<sup>1</sup>, A. Kawazu<sup>1</sup>,  
H. Shigekawa<sup>2</sup>, H. Mori<sup>3</sup> [1], M. Oshima<sup>3</sup> [2], H. Yamochi<sup>3</sup>, and G. Saito<sup>3</sup>

<sup>1</sup>Department of Applied Physics, University of Tokyo,  
Bunkyo-ku, Tokyo 113, Japan

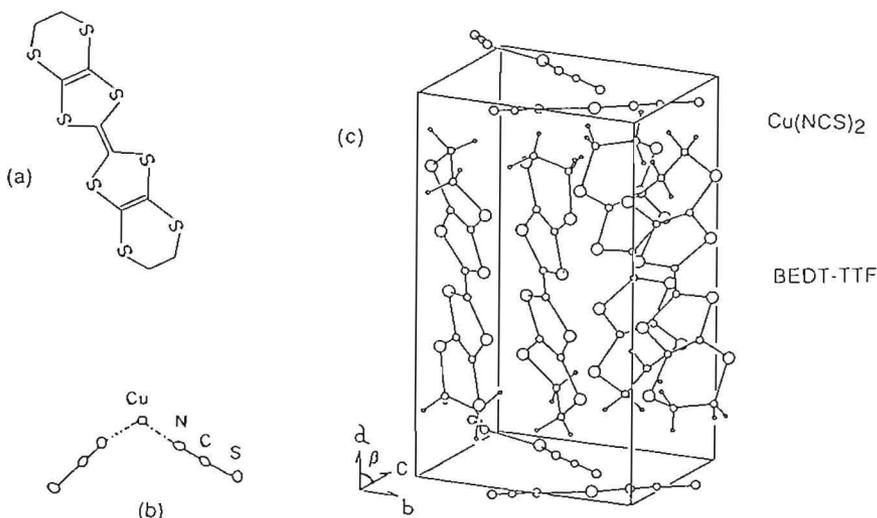
<sup>2</sup>Institute of Materials Science, University of Tsukuba,  
Tsukuba Science City 305, Japan

<sup>3</sup>Institute for Solid State Physics, University of Tokyo,  
Roppongi, Minato-ku, Tokyo 106, Japan

The surface structure of an organic superconductor (BEDT-TTF)<sub>2</sub>Cu(NCS)<sub>2</sub> was observed by means of a scanning tunneling microscope (STM) in air and at room temperature. Observed periodic structures were in good agreement with the two dimensional BEDT-TTF molecular structure projected onto its crystal b-c plane. Strong tunneling voltage dependence of STM image was also observed.

## 1. Introduction

(BEDT-TTF)<sub>2</sub>Cu(NCS)<sub>2</sub> crystal has a monoclinic structure which consists of alternating stacking of BEDT-TTF molecular layers and Cu(NCS)<sub>2</sub> molecular layers (Fig.1,  $a=16.248\text{\AA}$ ,  $b=8.440\text{\AA}$ ,  $c=13.124\text{\AA}$ ,  $\beta=110.30$  degree,  $V=1688.0\text{\AA}^3$ )[3]. Through the electron transfer from the BEDT-TTF layer to the Cu(NCS)<sub>2</sub> layer, the former has two dimensional



**Fig.1** (a) Molecular structure of BEDT-TTF. (b) Molecular structure of Cu(NCS)<sub>2</sub>. (c) Crystal structure of (BEDT-TTF)<sub>2</sub>Cu(NCS)<sub>2</sub> determined by X-ray diffraction, which has a monoclinic structure[3].

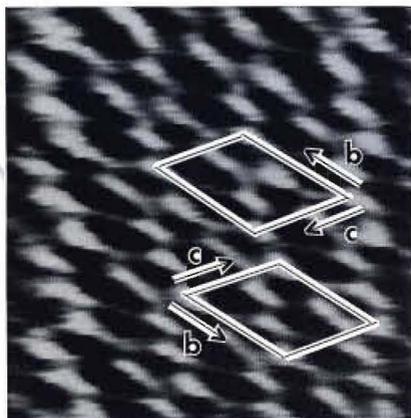
conductivity in its crystal b-c plane, while the latter becomes insulating. This crystal shows superconductivity at  $T_c=10.4\text{K}$  under ambient pressure. In order to reveal the microscopic mechanism of this high- $T_c$  organic superconductor, we must have knowledge of the atomically resolved electronic and geometric structure of the crystal.

## 2. Experimental Results and Discussion

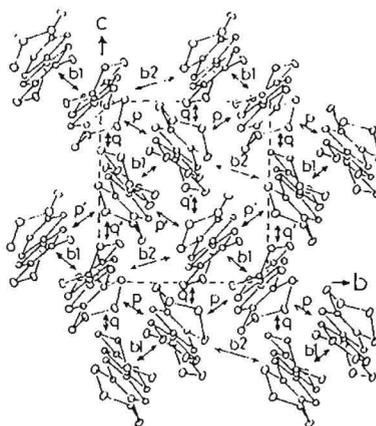
STM observations were performed over the crystal b-c plane in air and at room temperature. A platinum-iridium tip was used to probe the surface. Figure 2 shows a gray scale image obtained by the constant current mode (66mV tip to sample, 4.6nA, scan area is  $60 \times 60 \text{ \AA}^2$ ). The voltage dependence of tunneling current indicates that the surface has a metallic property (images were the same on both signs of the bias voltage), and the periodic structure in Fig.2 is expected to correspond to the surface electronic structure of BEDT-TTF layers[4].

The arrangement of BEDT-TTF molecules, projected onto the b-c plane, is shown in Fig.3[5]. When the crystal axis determined by X-ray diffraction is taken into consideration two choices for the unit cell are possible (drawn in Fig.2). In addition, STM images showed a strong tunneling voltage dependence (Fig.4), which corresponds to the change of local distribution of electronic states according to their energy. In order to give a comprehensive explanation of the observed images, we shall have to perform further experiments and detailed calculations on the local density of states of this crystal.

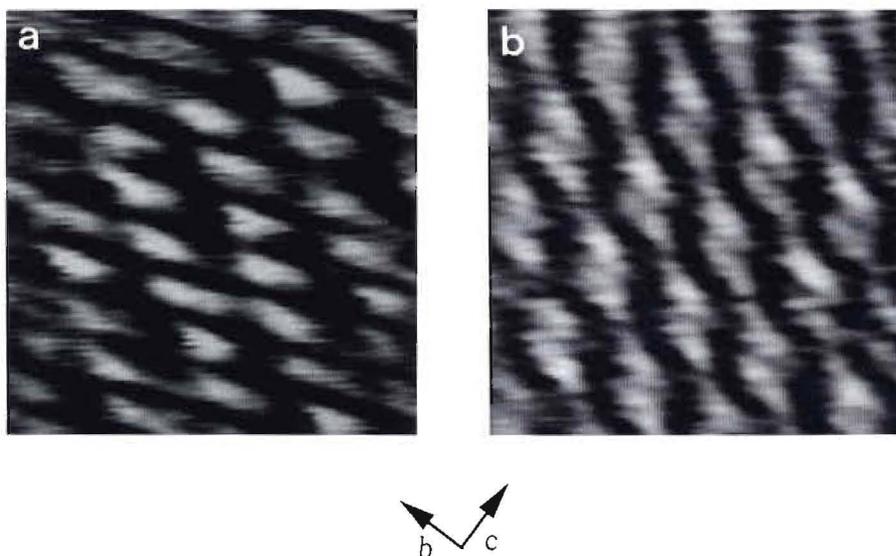
The mechanism of superconductivity for organic materials[6] will be revealed by a systematic STM study of those materials. For comparison an STM image of  $(\text{BEDT-TTF})_2\text{KHg}(\text{SCN})_4$  surface acquired over the a-c plane is shown in Fig.5 together with the crystal structure determined by X ray diffraction[7,8].



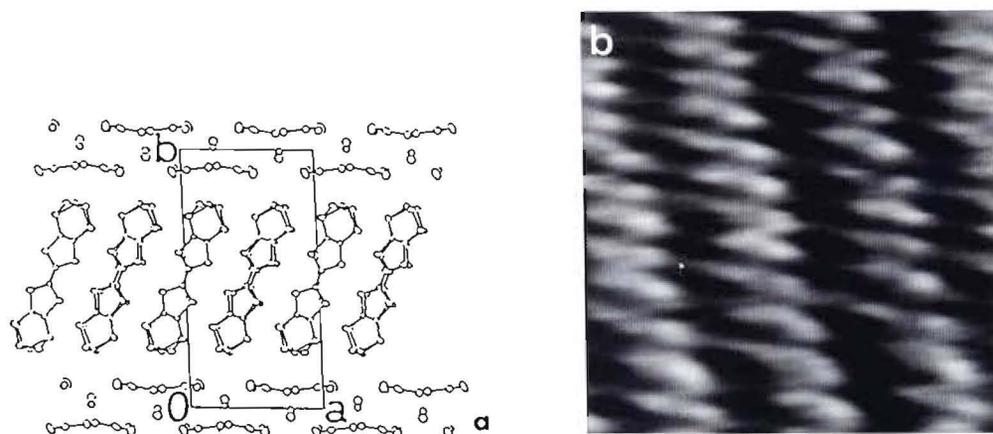
**Fig.2** Gray scale image of  $(\text{BEDT-TTF})_2\text{Cu}(\text{NCS})_2$  surface obtained by the constant current mode (66mV tip to sample, 4.6nA). Scan area is  $60 \times 60 \text{ \AA}^2$ . Two possible unit cells are drawn.



**Fig.3** BEDT-TTF molecular structure projected onto the crystal b-c plane[5]. The unit cell is drawn.



**Fig.4** Tunneling voltage dependence of STM images (a) 180mV,  $30 \times 40\text{-}\text{\AA}^2$ . (b) 300mV,  $50 \times 50\text{-}\text{\AA}^2$ .



**Fig.5** (a) Crystal structure of  $(\text{BEDT-TTF})_2\text{KHg}(\text{SCN})_4$  determined by X-ray diffraction[7]. (b) Surface image obtained by STM (90mV, 1.01nA,  $75 \times 75\text{-}\text{\AA}^2$ ).

### 3. Conclusion

In summary, we obtained STM images of  $(\text{BEDT-TTF})_2\text{Cu}(\text{NCS})_2$  surface structure. The observed images indicate that the surface is metallic and the periodic structure observed was in good agreement with the BEDT-TTF molecular structure projected onto the crystal b-c plane. STM images showed a strong tunneling voltage dependence.

It is a pleasure to acknowledge many helpful discussions with Prof. T.Mori, Institute for Molecular Science.

## References

- [1] Present address: International Superconductivity Technology Center, Atsuta, Nagoya 456
- [2] On leave of absence from Japan Carlit Co., Ltd., Shibukawa Gunma 377
- [3] H.Urayama, H. Yamochi, G. Saito, S. Sato, A. Kawamoto, J. Tanaka, T. Mori, Y. Maruyama, and H. Inokuchi, *Chem.Lett.*,1988(1988)463.
- [4] M. Yoshimura, N. Ara, M. Kageshima, R. Shioda, A. Kawazu, H. Shigekawa, and S. Hyodo, *J.Vac.Sci.Technol.A*, to be published
- [5] K. Oshima, T. Mori, H. Inokuchi, H. Urayama, H. Yamochi, and G. Saito *Phys.Rev.B*,38(1988)938
- [6] K. Yamaji, *Synthetic Metals*, 27(1988)A115
- [7] M. Oshima, H. Mori, G. Saito, and K. Oshima, *Chem.Lett.*,1989(1989)1159
- [8] M. Yoshimura, N. Ara, M. Kageshima, R. Shioda, A. Kawazu, H. Shigekawa, M.Oshima, H. Yamochi, and G. Saito, *Jpn.J.Appl.Phys.*, to be submitted