Electronic Band Structures of $CuBa_2Ca_{n-1}Cu_nO_{2n+2}$ and $Cu(Tl)Ba_2Ca_{n-1}Cu_nO_{2n+1}F$ $(n = 3-5)$

N. Hamada[a], I. Hase[b] and H. Ihara[b]
[a]*Science University of Tokyo, Noda 278-8510*
[b]*Electrotechnical Laboratory, Tsukuba 305-8568*

Electronic band structures of

$CuBa_2Ca_2Cu_3O_8$ ($Cu1223O_8$)		$CuBa_2Ca_2Cu_3O_7F$ ($Cu1223O_7F$)
$CuBa_2Ca_3Cu_4O_{10}$ ($Cu1234O_{10}$)	and	$CuBa_2Ca_3Cu_4O_9F$ ($Cu1234O_9F$)
$CuBa_2Ca_4Cu_5O_{12}$ ($Cu1245O_{12}$)		$CuBa_2Ca_4Cu_5O_{11}F$ ($Cu1245O_{11}F$)

are calculated by using the full-potential linearized augmented plane wave (FLAPW) method in the local density approximation (LDA). The calculations show that large Fermi surfaces contains 1.05–1.61 holes in $Cu1223O_8$, 0.99–1.55 holes in $Cu1234O_{10}$, and 0.97–1.58 holes in $Cu1245O_{12}$. From the viewpoint of optimum doping, the hole numbers are deficient for Fermi surfaces derived from the inner CuO_2 planes, while they are excessive for Fermi surfaces derived from the outer CuO_2 planes. The oxygen dope to the Cu plane in the charge-reservoir layer changes the hole number in the outer CuO_2 planes and reduces the anisotropy of the conductivity, while it does not give a strong effect on the hole number in the inner CuO_2 planes.

To study the possibility of designing the Fermi surfaces, we substitute some of the apical oxygen atom with the F atom. If we substitute 50% of apical O with F in $Cu1223O_8$, we obtain $Cu1223O_7F$. Band strucutures of $Cu1223O_8$ and $Cu1223O_7F$ are shown in Figures 1 and 2. In $Cu1223O_7F$, the system is doped with electrons and the Fermi surfaces derived from the outer CuO_2 planes becomes electron-doped: Three Fermi surfaces contains 0.87, 0.98 and 1.15 holes. We conclude that the F doping can control the size of the Fermi surface and is useful to design an optimum set of the Fermi surfaces for superconductivity.

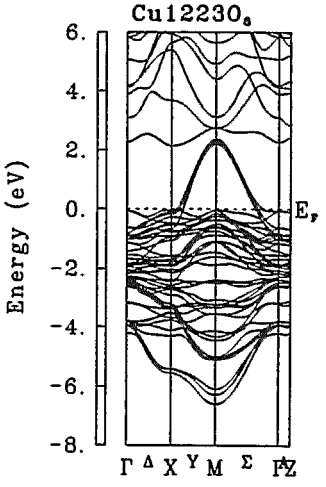

Figure 1: Band structure of $Cu1223O_8$.

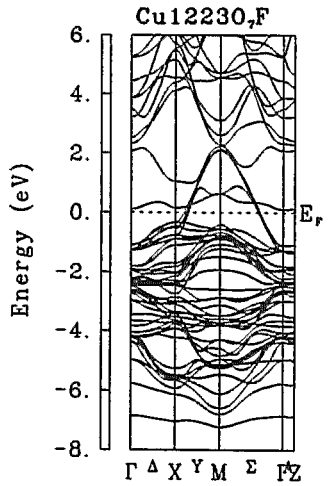

Figure 2: Band structure of $Cu1223O_7F$.