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## Reduction of Electrical Damage due to Au/Pentacene Contact Formation by Introducing Ar Gas during Au Evaporation

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### 1. Introduction

Obtaining an ideal metal/organic ‘top’ contact has been an important subject not only for the study of molecular scale electronics but also for that of organic macroscopic devices. Characteristics of metal/organic contacts vary depending on the deposition conditions of metals, since the metal atoms easily migrate deep into the organic layer and form composites or defects. A Au top contact is widely adopted for drain and source electrodes in pentacene-based organic field-effect transistors (OTFTs), and has been believed to form nearly ohmic contact with relatively low contact resistance only by a conventional vacuum deposition technique. However, atomic force microscope potentiometry (AFMP) measurement has shown the existence of significant potential drops near the electrodes where Au was deposited on pentacene films, which suggests that the conventional Au deposition deteriorates the physical property of pentacene films [1].

In this study, we have demonstrated the reduction of the electrical damage in a simple Au/Pentacene/Al diode structure by filling the Au evaporation chamber with Ar to an appropriate pressure. Collisions of the Au atoms with the back-filled Ar atoms reduce the kinetic energy of the Au atoms reaching pentacene films, resulting in soft-landing deposition. These ‘cold’ Au atoms are expected to suppress the reactivity with organic materials [2, 3].

### 2. Experimental

Glass substrates cleaned by ultrasonic agitation in acetone were used for the diode samples. An Al film (70nm-thick) was deposited on the substrate by RF-sputtering. A pentacene polycrystalline film (150nm-thick) was then deposited by evaporation under a vacuum of  $10^{-5}$  Pa. The deposition rate of the pentacene layer is maintained to be 0.1nm/s. Finally, a Au electrode (70nm-thick) was evaporated in vacuum or an Ar ambient (0.1, 0.2 and 0.4 Pa). The active area of the diodes was 0.04 cm<sup>2</sup>. The  $I$ - $V$  characteristics of the diodes were measured at 295K and 90K under a vacuum of  $10^{-5}$  Pa and a dark condition.

### 3. Results and discussion

Prior to the experiments, the Ar pressure for the Au deposition was optimized for our evaporation chamber using a 3D rarefied gas dynamic simulation software (*RGS3D* package, *Pegasus Software, Inc.*). The energy distribution started low shift when the pressure reached 0.1 Pa and became low enough to suppress pentacene decomposition when 0.4 Pa.

Figure 1 shows the  $I$ - $V$  characteristics of the fabricated devices against the Ar pressure. The current is obviously composed of two components, those in low and high voltage region. The low-voltage component strongly depends

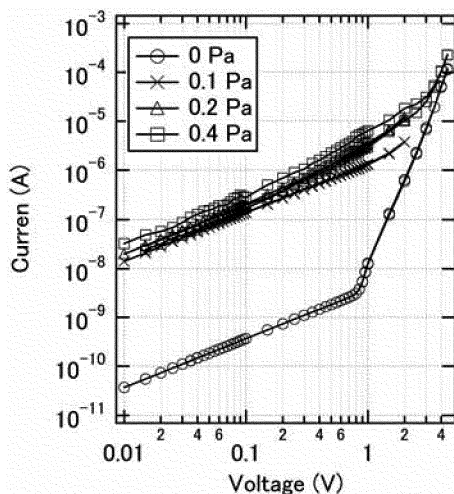


Fig.1  $I$ - $V$  characteristics of Au/pentacene/Al diodes against the Ar pressure during Au evaporation. Au electrodes were positively biased against Al.

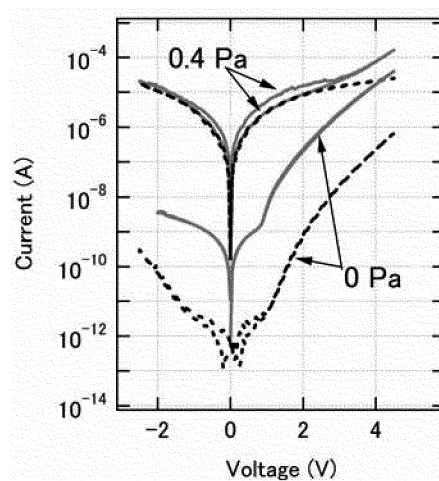


Fig.2  $I$ - $V$  characteristics of Au/pentacene/Al diodes of which Au electrodes were deposited under 0 and 0.4 Pa Ar. Solid lines represent those measured at 295K and dashed lines at 90K.

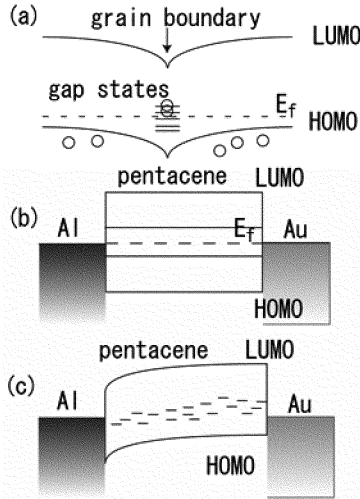


Fig.3 Schematic band diagrams at grain boundaries: (a) diagram across a boundary with gap states, (b) diagram along a boundary with a metallic gap-state band, and (c) that with discrete gap states.

on the Ar pressure and increases by thousand fold when 0.4 Pa Ar is filled, which agrees well with the gas simulation results. The unity slope in this region indicates that this component is an ohmic current. On the contrary, high-voltage component converges to the same curve independently of Ar pressure. Figure 2 shows  $I$ - $V$  characteristics measured at 295K and 90K. The low-voltage component of 0.4 Pa sample is almost independent of temperature although that of 0 Pa depend on temperature. High-voltage components depend on measurement temperature for both samples.

The high-voltage component was concluded to be originated from thermionic emission of holes from the Au electrode by fitting those curves with a theoretical  $I$ - $V$ - $T$  equation [4]:

$$J \propto T^2 \exp\left(a\sqrt{V}/T - q\phi_B/kT\right), \quad (1)$$

where  $J$  is the current density,  $T$  the measurement temperature,  $V$  the applied voltage, and  $\phi_B$  the barrier height.

For the low-voltage components, the carrier mobility was estimated using acceptor concentration,  $1 \times 10^{15} \text{ cm}^{-3}$ , which was measured by  $C$ - $V$  measurement. The estimated value was in the order of  $10^{-6}$  and too small even if the anisotropy of the mobility is considered. The result suggests that this component is a current flowing through a local structure, such as gap states at grain boundaries {Fig.3 (a)}. When Au is evaporated in Ar ambient, no electrical damage is induced and gap states at grain boundaries form a metal-like band {Fig.3(b)}. The low-voltage ohmic current flows through the metal-like band and is therefore independent of temperature. When a damage is caused by the conventional Au deposition, the metal-like band is broken and the low voltage components thus behave as a hopping conduction {Fig.3 (c)}.

To know the Au migration depth, depth profiles were

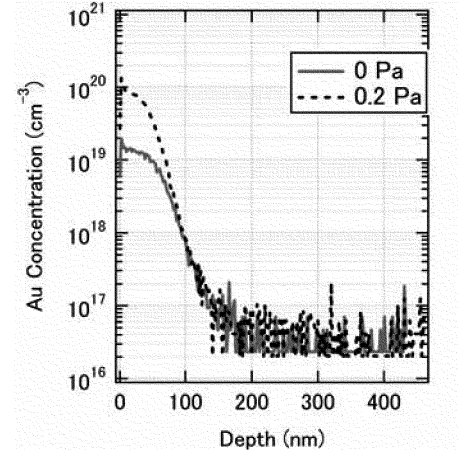


Fig.4 Au depth profiles for Au/pentacene/Al diodes of which Au electrodes were deposited under 0 and 0.2 Pa Ar. Zero in the depth scale corresponds to the Au/pentacene interface.

measured with secondary ion mass spectrometry (SIMS). Figure 4 shows SIMS depth profiles of Ar 0.2 Pa and without Ar. The Au films were removed by adhesive tapes before the measurements to prevent the knock-on effect. The Au density near the surface in the 0.2 Pa sample is higher than that without Ar. This is supposed to be due to the Au nano-clusters formed in Ar ambient which tend to remain on the pentacene surface. Taking notice of the decay slopes in deeper region, there is no difference between both samples. Au is included down to the depth of around 200nm. This migration range is surprisingly large. However, the influence of Au deposition was confirmed to continue even in much thicker films both for vertical and lateral conduction. The damage is therefore assumed to be caused by a phase transition of pentacene crystal structure, of which detail is currently under study.

### 3. Conclusion

To reduce an electrical damage in pentacene due to Au top-electrode formation, an evaporation technique of Au in Ar ambient was employed and the influence on electrical properties was studied. By this simple technique, the characteristics of vertical-type devices and short-channel transistors are expected to be improved.

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### References

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