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Chemical Soldering: New Method for Single Molecular Interconnects

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1. Introduction

In single-molecule electronics, each organic molecule performs the basic functions of electronics such as rectification, amplification, and storage. Though many efforts have been made to realize single-molecule electronics, it is still impossible to fabricate a practical single-molecule integrated circuit. One of the problems is the lack of viable methods for wiring each functional molecule. Since it is very difficult to reduce the width of metal wires to that of single molecules, we have to develop a viable method to connect each molecule with a single conductive polymer chain instead of a metal wire.

We found before that a stimulation with the probe tip of a scanning tunneling microscope (STM) could initiate a chain polymerization of diacetylene molecule (R–C≡C–C≡C–R'), where unsaturated diacetylene molecules add on to a growing polymer chain one after another like domino effect. As a result, we could fabricate a conjugated polydiacetylene (PDA; $(=RC–C\equiv C–CR'=)_n$) chain at designated positions (Fig. 1) [1–3]. Based on these previous studies, here we report a novel method for connecting single polymer chains to single organic molecules [4].

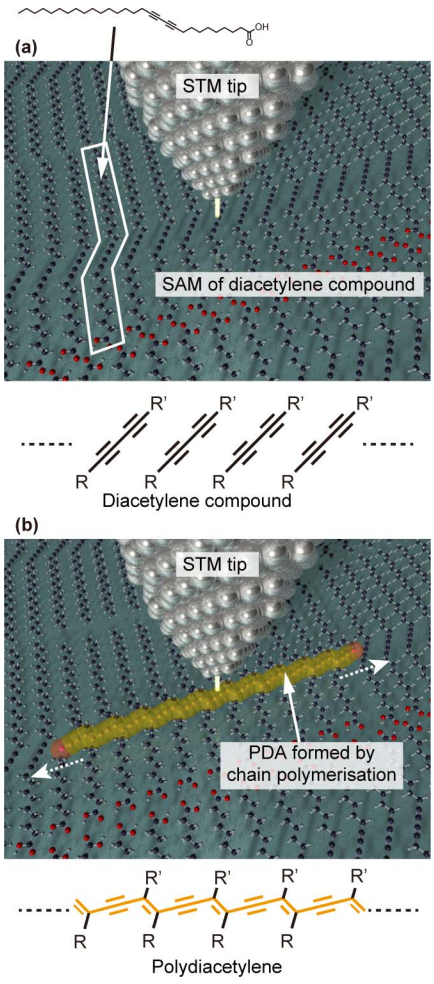

Fig. 1 (a) Chain polymerization of diacetylene compound is initiated by using an STM tip. (b) A single linear polydiacetylene chain can be created at any designated positions.

2. Experimental

We used 10,12-nonacosadiynoic acid ($CH_3(CH_2)_{15}$–C≡C–C≡C–$(CH_2)_8COOH$) as diacetylene compound in the present work. A thin film of 10,12-nonacosadiynoic acid on the surface of purified water was transferred to a freshly cleaved surface of graphite by nearly horizontal dipping. The molecules form a self-assembled monolayer (SAM) on the substrate. Then the sample was placed in a vacuum chamber and phthalocyanine was deposited.

STM experiments were performed in air at room temperature using a Bruker NanoScope STM system using Pt–Ir tips in the constant current mode.

3. Results and discussion

Figure 2 shows a scheme of this method, which we named "chemical soldering". First, relevant functional molecules are placed on a SAM of diacetylene compound. A probe tip of STM is then positioned on the molecular row of the diacetylene compound to which the functional mole-

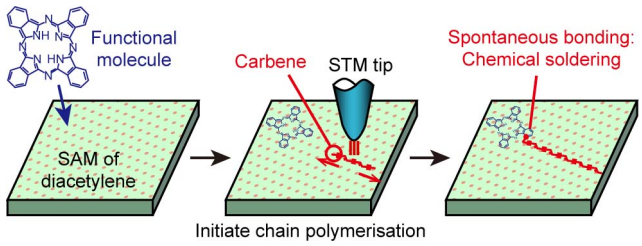

Fig. 2 Scheme of chemical soldering.

cule is adsorbed, and a conjugated PDA chain is fabricated by initiating chain polymerization by stimulation with the tip. During the propagation of chain polymerization, the propagating ends of PDA have reactive chemical species such as carbenes. Furthermore, the lifted-up structure of PDA [5] enables the reactive end to approach the adsorbed functional molecule. Hence, it is expected that the end of PDA spontaneously reacts with an encountered molecular element and forms chemical bonding.

Figure 3 shows a demonstration of the chemical soldering, using phthalocyanine molecule as the functional molecule. After a small quantity of phthalocyanine was deposited on the molecular layer of diacetylene compound, we found that stable nano-cluster (pentamer) of phthalocyanine molecules, which were consisted of five phthalocyanine molecules, were adsorbed on the molecular layer (Fig. 3a). Then a pulsed bias voltage was applied between the substrate and the STM tip on the molecular row of the diacetylene compound to which the phthalocyanine molecule is adsorbed. As a result, a chain polymerization was initiated by the pulsed voltage, and the obtained PDA chain, observed as a very bright line in the image, was connected to the phthalocyanine molecule as shown in Fig. 3b. Similarly, the second PDA chain was connected to the same molecule as shown in Fig. 3c, by applying the second pulsed bias voltage on the opposite side of the same molecular row.

We also investigated the stability of possible configurations of the polymer and phthalocyanine by using density-functional first-principles calculations, and found that binding between the phthalocyanine and the polymer (Fig. 3d) gives the lowest energy among calculated structures. The distribution of calculated molecular orbitals is also consistent with the contrast of STM images.

4. Conclusions

This result enables us to connect single conductive polymer chains to single functional molecules, which is a key step in advancing the development of single-molecule electronic circuitry.

Acknowledgements

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References

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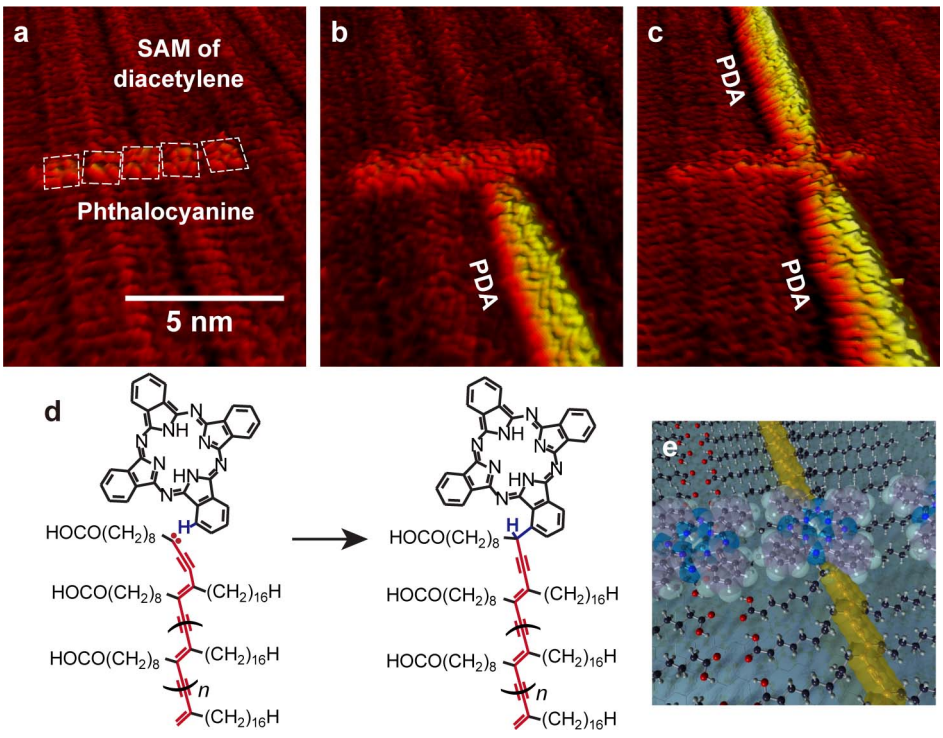

Fig. 3 (a-c) STM images showing the connection of two PDA chains to a single phthalocyanine molecule. (d) Proposed chemical reaction. The reactive end of PDA is inserted into a C–H bond of phthalocyanine. (e) Schematic structure model.