Fabrication of nanocontacts for molecular devices using nanoimprint lithography

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(Received 14 June 2001; accepted for publication 21 January 2002)

We present a simple process to fabricate gold nanocontacts with a gap as small as sub-10 nm. This method uses a two-step process of nanoimprint lithography (NIL) and electromigration. First, 20 nm wide gold nanowires were fabricated by NIL on a silicon dioxide substrate. Then by passing an electric current through a nanowire, the nanowire is split into two wires with a gap as small as sub-10 nm by electromigration. This fabrication method offers a fast and effective process for producing large numbers of nanocontacts for use in molecular self-assembly, and thus greatly enhances the probability of successful capture of single molecules. *© 2002 American Vacuum Society.* [DOI: 10.1116/1.1463068]

I. INTRODUCTION

As conventional transistors are scaled into the sub-30 nm region, the exploration of single molecules as electronic devices becomes of great interest. Single molecule devices offer many unique properties unattainable with traditional silicon based devices. These properties include the ultimate in feature size scaling whereby sub-1 nm quantum dot devices could possibly be fabricated.[1] In addition, the molecules can be functionalized with various end groups for self-assembly onto prefabricated contacts[2] and can be chemically customized for a particular application.

One key challenge in making single molecule devices is to fabricate contacts to a single molecule. Typically, two contact wires with a sub-10 nm gap are made first, and then single molecules are self-assembled between the contacts. Current attempts to fabricate the contacts have included: break junctions,[2] vertical sandwich structures,[3] electron-beam lithography (EBL) and shadow evaporation,[4] electron-beam deposition,[5] electrochemical growth,[6] and electromigration.[7] Although successful, these processes are ill suited for large-scale integrations, as each gap must be fabricated individually in a time consuming fashion.

Here we present a way of fabricating nanocontacts by using electromigration and nanoimprint lithography (NIL), a parallel lithography technique with proven sub-10 nm resolution over large areas.[8] Using NIL, 20 nm gold nanowires were fabricated on a silicon dioxide substrate. The nanowires were then split with electromigration to form contacts with gaps as small as sub-10 nm. This process for fabricating nanocontacts with electromigration is an improvement over previous attempts, as the 20 nm nanowires being split were fabricated with a parallel process, and are significantly narrower.[7]

II. FABRICATION OF NANOCONTACTS

The fabrication sequence for the nanocontacts is shown in Fig. 1. A 20 nm Au wire was made with NIL on a silicon dioxide substrate. The wire was then split by electromigration induced by passing a current through the wire. This method produces nanocontacts separated by gaps as small as sub-10 nm.

The NIL process uses a silicon dioxide mold with 20 nm wide nanowires of 70 nm height as shown in Fig. 2. The mold was patterned with EBL for the nanowires, and with photolithography for the larger features. Once the mold is fabricated, the nanowires can be replicated in parallel using NIL as described in detail in Ref. 8, and briefly described here. The mold was pressed into a 90 nm film of 15 kg/mol average molecular weight polymethylmethacrylate polymer on a silicon dioxide substrate with a pressure of 650 psi while heated to 175 °C, which is above the glass transition temperature of the polymer. The polymer flows, conforming to the features of the imprint mold. Once cooled, the mold was separated from the polymer, leaving the polymer surface patterned. An anisotropic oxygen plasma reactive ion etch was used to remove the residual polymer. Next, 15 nm of gold was deposited using electron-beam evaporation, followed by liftoff in acetone heated to 60 °C. Au pads to the nanowires were then added to allow for measurements to be conducted with a probe station. The result is a chip with 60 gold nanowires of uniform width and thickness.

The nanowire gaps were then fabricated with electromigration, where large electron current densities induce drift among the gold atoms due to momentum transfer from the electrons. This phenomenon has been extensively studied due to its importance in wire failures in integrated circuits.[9] Electromigration requires vacancies for the metal atoms to propagate. For larger wires, networks of grain boundaries can provide pathways for atoms to move. However, for nanowires, the grain size is much larger than the wire width, resulting in ‘‘bamboo’’ grains which run perpendicular to the direction of current flow. Electromigration in nanowires thus relies on lattice vacancies within the metal, or along the surfaces and therefore requires much higher current densities than wires of larger size.[9,10]

A circuit, shown in Fig. 3, was designed to break the

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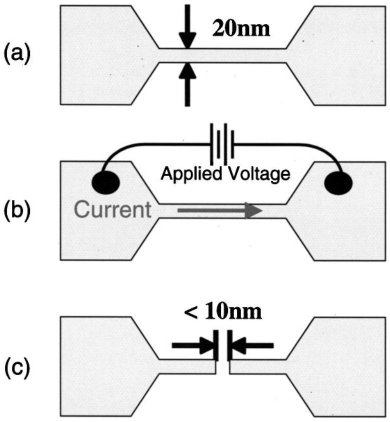

FIG. 1. Summary of the nanocontact fabrication process: (a) 20 nm Au wires are made with nanoimprint lithography; (b) an electric current is passed through the wires; and (c) high current densities break the wire with electromigration, forming gaps as small as sub-10 nm.

nanowires by carefully controlling the current through the nanowire and protecting the nanowire from large applied voltages with a shunt path. First, the potentiometer resistance and the variable dc voltage source was set to zero, ensuring that all static charge in the circuit has been dissipated. The voltage source was increased until 1 mA passed through the potentiometer. Then the 1 kΩ potentiometer resistance was increased until it equaled that of the nanowire, typically around 100 Ω, and 0.5 mA flows through both branches. The current was then slowly increased by 0.1 mA increments every 5 min by increasing the voltage source until electromigration broke the nanowire. This event was detected by observing when the current through the nanowire falls sharply to zero. Breakage due to electromigration typically occurred between 1 and 2 mA, a current density of about 10^8 A/cm^2. The shunt branch through the potentiometer protected the nanowire from a large applied voltage across the nanocontacts after the gap formation.

In this work, each wire was individually broken by electromigration. However, multiple wires could be broken by wiring the nanowires in parallel and repeating the experiment. This is possible as the gap formation is a self-halting process: once the gap is formed the current can no longer flow, and thus electromigration within the wire ceases. This is significant as the nanowires will not break in unison, but randomly, so a voltage must be applied on all nanowires in parallel until all are broken. Attempting multiple gap formation in such a manner with electrochemical growth would fail, as growth must stop when the wire with the smallest gap comes close to connecting the nanocontacts, regardless of the gap size of the other wires.

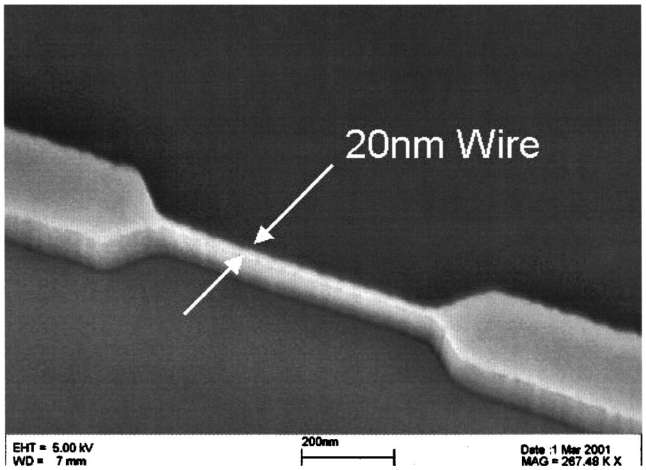

FIG. 2. NIL silicon dioxide mold of a nanowire of width 20 nm and height 70 nm.

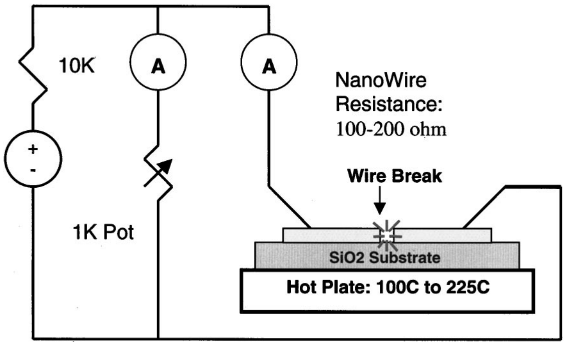

FIG. 3. When a sufficient current density passes through the nanowire, electromigration will break the nanowire, producing nanocontacts. Since the nanowire can break uncontrollably due to static charge or large changes in applied voltage, a potentiometer shunt is used to steer the current into the nanowire.

III. RESULTS AND DISCUSSION

The initial attempts of gap fabrication with electromigration resulted in a large variation in gap size, from 5 to 500 nm, and often severe damage to the wire. This was due to the large current densities required to break the wire, resulting in a corresponding large force on the atoms. The lifetime of thin film conductors due to electromigration failure is a function of current density and temperature.[9,10] To reduce the current densities required, the sample is heated during the electromigration process. Our initial experiments suggest that temperatures from 100 to 225 °C are effective in reducing and controlling the gap size, as shown in Fig. 4. Figure 5 shows a scanning electron microscope picture of a nanowire before and after the electromigration process conducted at 175 °C. Although difficult to resolve, the gap size is approximately 8 nm.

Initial studies of nanocontacts for single molecular self-assembly have suggested the yields for successful capture are very low. Ideally, a very small and narrow gap should be fabricated to reduce the number of molecules captured between the contacts, with the ultimate goal of a single molecule captures. Fabrication methods such as electrochemical growth of wires have been shown to have nanometer control over the gap size,[6] however control over the wire width and potential for high throughput fabrication are lacking. A vertical structure is highly effective in capturing molecules,[3] however, adding a gate terminal and reducing the number of molecules captured from thousands to a few is problematic.

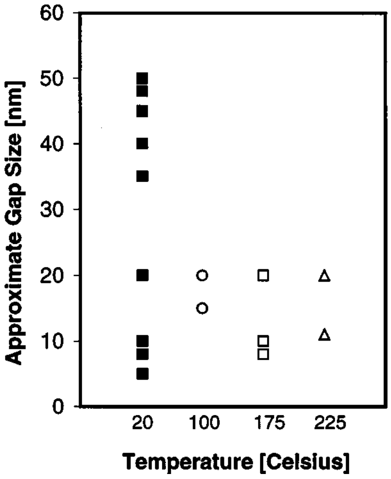

FIG. 4. Distribution of nanocontact gap size for 20 nm wires. Control over the gap size is improved by heating the wire during the electromigration process.

We have developed an effective tool for the study of single molecules. Admittedly, electromigration will not be able to control the gap size to the same accuracy as electrochemical growth; however, with its ease of processing, hundreds of contacts could be quickly fabricated with this process. This should substantially increase the likelihood of a successful capture. Since electromigration is inherently a destructive process, controlling the exact shape of the contacts is not possible, although precise control over the gap shape is lacking in all previous attempts as well.[2,4–7] However, since the gap is not grown, the width of gap maintains the original narrow wire dimension of 20 nm. Finally, a gate electrode is easily implemented by using the silicon substrate as backside gate.

IV. CONCLUSIONS

We have shown that nanoimprint lithography in combination with electromigration is an effective process for producing nanocontacts. Although electromigration is inherently a difficult process to control, by carefully allowing a current to flow and heating the wire, initial experiments suggest that the variation in gap size can be reduced. This simple process is potentially well suited for the fabrication of hundreds of contacts, thus greatly enhancing the chances of a successful capture of molecules within the gap. Future work will involve increasing the control over the gap size, and attempting to capture molecules between the nanocontacts.

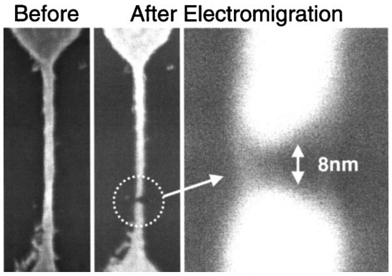

FIG. 5. 20 nm gold nanowire before and after the electromigration process conducted at 175 °C. The gap between contacts is approximately 8 nm.

ACKNOWLEDGMENT

This project was partially supported by DARPA.

Presented at the 45th International Conference on Electron, Ion, and Photon Beam Technology and Nanofabrication, Washington, DC, 29 May–1 June 2001.

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