Cold welding assisted self-healing of fractured ultrathin Au nanowires

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Abstract

In nano-electronic field, cold welding is a simple novel method to join ultrathin noble metal nanowires (NWs) without introducing extra energy and defects. In previous works, it always occurred between ultrathin noble metal NWs, tensile fracture parts of a single NW, or a NW formation from nanoparticles. However, some external force is still needed to drive the materials as close to each other as possible before the process. Here, we proposed a new method to achieve cold welding without introducing artificial loadings. The bending fractured ultrathin gold (Au) NW can be self-healed assisted by cold welding during the removal of the tungsten (W) tip by in situ transmission electron microscope (TEM). A new interface with lattice mismatch formed in the welding zone after multiple periodic cycles, leaving an angle between the two rebonded fracture parts. Furthermore, the cold welding assisted self-healing of the bending fractured ultrathin Au NW and atom evolutions were also confirmed by molecular dynamics (MD) simulations. The successful implementation of cold welding makes the self-healing come true when the ultrathin Au NW fractures under the unexpected vibrations.

Introduction

Ultrathin (diameter < 10 nm) gold nanowires (Au NWs) open up an era of synthesizing one dimensional (1 D) ultrathin metallic nanostructures [1–4]. Then, ultrathin Au NWs were considered as one of the most promising candidates for future nano-electronics and interconnect applications as the critical feature size of integrated circuits approaching sub-10 nm [5–11]. How to assemble the ultrathin Au NWs is a challenge [12, 15]. Thus, cold welding was proposed as a nanotechnology to weld ultrathin metallic NWs in nano-electronics applications, avoiding local heating, precise control of heating mechanism and introduction of damage compared with traditional electric welding [12, 15]. The final NW after cold welding still had a fairly perfect crystal structure [16]. The Au NWs can be assembled through the cold welding of nanoparticles (NPs) or nanorods (NRs) [16–20]. The method was also suitable for silver (Ag), copper (Cu), and Ag-Au NWs [21, 22].

The cold welding was also considered as a repairing nanotechnology in nanoelectronics field, such as repairing the pre-damaged Au nanomesh flexible transparent electrodes [23] and transparent Ag nano-network electrodes [24, 25].

Currently, the researches focus on the behaviors of cold welding of ultrathin noble metal NWs, re-welding of the single stretching fractured NW, and the NW formation from welding of NP/NRs. However, there are few concerns on the behaviors of the bending fractured nanostructures [26] which are regular to happen in practical
applications. In this work, we proposed a new method to achieve the cold welding assisted self-healing of bending fractured ultrathin Au NWs without introducing subjective forces. The research results would be benefit to the repair of interconnects composed of ultrathin noble metal nanostructures when it fractures in the undesired bending or vibrations.

**Experimental section**

Figure 1(a) shows the TEM image of an ultrathin Au NW, with diameter around 10 nm. The HRTEM image in figure 1(b) reveals that the Au NW has a good crystal structure.

In order to investigate the behaviors of the ultrathin Au NW under the compression (bending) and release processes, the following preparation procedures were adopted. Firstly, the Au NW was stuck on an Au electrode by AB conductive glue. Secondly, the Au electrode was fixed on one end of the Nanofactory holder, and a tungsten (W) tip was fixed on the other end, whose movement (forward and backward) is controlled by the piezoelectric ceramics. Finally, the holder was inserted into TEM (JEM 2100) to be observed.

The schematics shown in figure. S1 (available online at stacks.iop.org/NANOX/1/020014/mmedia) reveal the movement routes of the W tip. Its movement directions are marked with red arrows. The whole processes include approach (figure S1(a)), contact (figure S1(b)), compression (figure S1(c)), maximum compression (figure S1(d)), release, (figure S1(e)), contact (figure S1(f)), and separation (figure S1(g)). The force states of the Au NW are marked with green arrows. The Au NW experienced bending and release processes that is controlled by the forward and backward of the W tip, respectively.

Finally, molecular dynamics (MD) simulation with embedded–atom model (EAM) potential was performed on FCC Au (111) NWs without defects [27–30]. The diameter and length of the NW are 2.0 nm and 21.1 nm, respectively. The NW was subjected to the uniaxial compression at a strain rate of $1.0 \times 10^9 \text{ s}^{-1}$ in the [001] crystallographic direction.

**Results and discussion**

Figure 2 shows the deformation behaviors of an ultrathin Au NW with smooth surface (marked with red dotted line in the inset in figure 2(a)) under the bending and release processes. Firstly, the W tip is controlled to approach the free end of the Au NW (figure 2(a), the red arrow reveals the move direction of the W tip, and the same below) until they are in contact with each other (figure 2(b)). Secondly, the Au NW starts to be compressed and bends as the tip continues to move forward (figure 2(c)). The first compression cycle ends when the tip stops (figure 2(d)). Thirdly, the tip is controlled to move back along the red arrow in figure 2(e), accompanied with the pressure removal on the Au NW gradually. When the pressure just disappears, the Au NW restores to its original state before bending (inset in figure 2(e)). So far, one complete compression and release cycle has been ended. More details of the process can be seen from Movie S1.

Then, the above manipulations are repeated for multiple times. A damage (marked with blue arrow in figure 2(f), and the red dotted line in the inset) appears on the surface of the Au NW in the bending process at the site with stress concentration. The stress concentration becomes more obviously as the continuous compression, and a crack initiates in the bending Au NW (the gap in figure 2(g) and inset). Figure S2 show the atom arrangement evolution schematic of the Au NW around the crack in the compression and release processes. The Au NW has a perfect lattice match before the crack initiation (figure S2(a)), while the atom rows start to rotate in the crack initiation (figure S2(b)). As the compression goes on, the crack propagates (obvious

**Figure 1.** TEM images of an ultrathin Au NW at (a) low magnification, and (b) high magnification.
diameter reduction in figure 2(h) and inset) along the radial direction, and finally penetrates the whole cross section of the Au NW and makes it fracture into two parts (a gap formed in the cross section marked with red dotted ellipse in figure 2(i) and inset). The part of the Au NW contacted with the tip rotates due to the crack propagation. In the rotation process of the atom rows (figure S2(c)), the rotation angle gradually increases even to 90 degree, and its atom arrangements change dramatically as shown in figure S2(d). Interestingly, the two fractured parts are not separated from each other completely due to the pressure brought by the tip and the Van der Waals forces at the surfaces (figure 2(i) and inset). Then, the tip withdraws, companied with the pressure decreasing gradually. Simultaneously, the part of the Au NW contacted with the W tip rotates back to its original direction (figure 2(j) and inset), as the reverse rotation of the atom rows as shown in figures S2(d) to S2(e). Strikingly, the crack is healed [26, 31–33] gradually in the reverse rotation process (figures 2(j), (k) and insets), leading the two fractured parts of the Au NW re-bonded with each other. This behavior can be defined as cold welding assisted self-healing because of no extra energy consumption. The cold welding is attributed to the recombinantion of the crystal lattices that follows the principle of the ‘oriented-attachment’ mechanism [12].

When the pressure disappears completely, the atom rows restores to the state in figure S2(f) with a few lattice mismatches which leads the Au NW returned to the free state with damage defect (figure 2(l) and the red dotted line in the inset). Although the damage cannot be eliminated completely compared to the original state (figure 2(a)), the crack and fracture can be healed finally through the removal of the pressure. More details of the process can be seen from Movie S1.

In order to reveal the atom evolutions in the Au NW during the bending and release processes, the molecular dynamics (MD) simulation [27–30] is adopted as shown in figure 3. The Au NW possesses perfect atom arrangements before bending (free in figure 3(a) and just contacted with the W tip in figure 3(b)). When the compression starts, the Au NW first experiences slight bending deviation from the pressure axis (figure 3(c), reference the red dotted vertical line), without atom rotation. As the compression goes on, the atom rows rotate and local lattice mismatch or distortion (expressed of damage or even fracture in macroscopic observation) appears as shown in figure 3(d) (the area enclosed by the dotted ellipse, and the same as follows). The situation aggravates gradually as the compression displacement increasing to the maximum (figure 3(e)). Then, the atom rows rotate back and the local lattice distortion declines due to the release of the pressure (figure 3(f)), and some local lattice distortion disappears as the continuous release (figure 3(g)), and finally the local lattice distortion disappears completely or just leaves some lattice mismatch as the complete removal of the pressure (figure 3(h)).
The MD simulations also confirm the feasibility of cold welding to heal the bending damage or fracture in atomic level. More details can be seen from the Movie S2 (compression process) and Movie S3 (release process).

More importantly, the above deformation behaviors can be repeated perfectly that reveals the perfect cold welding repeatability of Au NWs. Figure S2 shows another two cycle compression and release processes. The cold welding repeatability can ensure the Au NW self-healed without external intervention once it fracture under some periodic compression or bending condition.

Furthermore, more periodic cycles are repeated with larger compression displacement to check the affordability of the ultrathin Au NW under extreme bending. After multiple cycle bending (figures 4(a), (d)) and fracture (figures 4(b), (e)), the cold welding (figures 4(c), (f)) can still be realized very well. However, it cannot return to the damage state like figures 2(l) and S2(f), displaying a certain angle about 30° between the rebonded two parts (figure 4(c)). Thus, a new interface is formed at the junction of the two parts. Under the repeated extrusion, an obvious welding zone unlike the original mother NW is formed gradually (figures 4(c)–(f)), with the disordered grain lattice. Figure S2(g) show the atom arrangements of the Au NW after release of multiple-cycle extreme bending. The crack healing can still be realized and the two fractured parts re-weld with each other when the pressure is removed completely. However, a new interface or a welding zone with significant lattice mismatch or distortion is formed at the junction of the two fractured parts during the cold welding process. The atom arrangements in the welding zone have a larger lattice mismatch (the purple color atoms). More details can be seen from Movie S4.

MD simulations are also adopted to verify the atom evolutions of the ultrathin Au NW under the multiple bending and release processes. After multiple bending and release, the free Au NW has a slight tilt but still possesses perfect atom arrangements (figure 5(a)). The atom rows rotate and local lattice distortion (the area enclosed by the dotted ellipse) appears and aggravates gradually under the continuous compression to the maximum displacement deformation (figures 5(b)–(e)). Then the atom rows rotate back and the local lattice distortion declines due to the release of the pressure (figures 5(f)–(g)), and a new interface is formed in the welding zone with disordered atom arrangements with lattice mismatch even after multiple completely release.
leaving an angle between the two rebonded fracture parts (Figure 5(h)). More details can be seen from Movie S5 (compression process) and Movie S6 (release process).

**Conclusions**

In summary, the bending fractured ultrathin Au NW can be self-healed repeatable assisted by cold welding during the release of the compression. However, a new interface in the welding zone with disordered atom arrangements and lattice mismatch was formed gradually, leaving an angle between the two rebonded fracture parts.
parts. In addition, the atom evolutions of ultrathin Au NW in the bending and cold welding processes were revealed by MD simulations. The cold welding provides a simple and fast self-healing strategy to repair the bending cracks and fracture in the ultrathin noble metal NW interconnects in practical applications without introducing artificial loadings, which can avoid the functional failure of nano-electronic devices. The self-healing function of the ultrathin noble metal NWs will be an important promoter of choosing them as the structural units of nanoelectronic devices.

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Notes

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