Self-healing of GaAs nanowires: An atomistic study

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Summary Fractured GaAs nanowires (NWs) with a zinc-blende structure can spontaneously self-heal throughout Ga–As re-bonding at fracture sites. In this paper, a systematic molecular dynamics study has been made with focus on the influence of lateral dimensions of GaAs NWs, multiple fractures and atomistic diffusion on the self-healing process. The results show that, as the lateral dimension increases from 2.31 to 9.23 nm, GaAs NWs lose their 46.0% capacity of self-healing. After 24 repeated cycles of fracture, the restored tensile strength of a NW reduces by 64.4%. Atomistic diffusion enhances the healing efficiency by eliminating mismatch of atoms.

INTRODUCTION

Self-healing is a widely observed phenomenon in natural materials, particularly in biomaterials such as the healing of a small cut in skin and restoration of fractured bones. It has been one important emerging field in nanotechnology since self-healing behaviors have been observed in a wide range of nanostructured materials. In synthetic materials, there is no circulatory system to mimic biochemical components of self-healing, and thus, a more direct route to self-healing is re-bonding of atoms at fracture sites. However, it is difficult to happen in a macroscopic system because damaged surfaces are so rough that even mechanical contact is impossible. At nanoscale, surface roughness is limited by the characteristic dimension of a structure. With the distance between two fractured surfaces being substantially reduced, atoms on one surface can react with their counterparts on the opposite side. It can thus be expected that self-healing might be an intrinsic property of one dimensional nanostructured materials at least under near-vacuum conditions. This study is motivated by in-situ deformation experiments that demonstrated repeatable self-healing of fractured GaAs nanowires (NWs) inside a transmission electron microscope [1]. Based on molecular dynamics simulations of the self-healing process between fractured sections of GaAs NWs, our focus is on the influence of lateral dimensions, multiple healing cycles and atomistic diffusion.

RESULTS AND DISCUSSION

The self-healing behavior in a GaAs NW can be assessed in three steps: loading, self-healing and re-loading. Firstly, a uniaxial tensile load is applied on a GaAs NW until its fracture. Then, two fractured sections are attached along their axes. Finally, a uniaxial tensile load is re-applied and mechanical properties of the restored NW are evaluated.

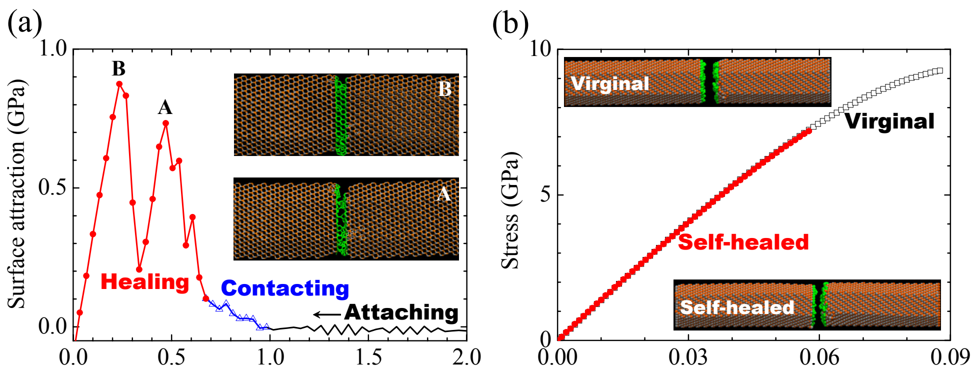

Figure 1: (a) The self-healing process of a fractured GaAs NW, where insets are patterns at two peaks (A and B) in the healing stage. (b) Stress versus strain curves of virginal and self-healed GaAs NWs.

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A typical self-healing process consists of three stages: attaching, contacting and healing, as shown in Fig. 1(a). (i) As the distance between two fractured surfaces is more than 1.0 nm, no interaction can be detected. (ii) As the distance reduces from 1.0 to 0.7 nm, a substantial surface attraction emerges. The attractive force per unit area is about 0.1 GPa, which enables a small amount of broken Ga–As bonds between two fractured surfaces to be rebuilt. (iii) With a further decrease of the distance, the surface attraction between two fractured surfaces reaches a maximum of 0.87 GPa, which is much stronger than that in the contacting stage. The two peaks of surface attraction in Fig. 1(a) correspond to two healing events: the partial healing in rough regions (peak A) and the full healing of fractured NWs (peak B). The tensile test on a self-healed GaAs NW shows that the tensile strength can reach 7.19 GPa. In comparison with its original strength of 9.27 GPa, 77.6% (the healing efficiency) tensile strength is restored, see Fig. 1(b). Here, it is of interest to note that the second brittle failure happens at the same location [2].

With the lateral dimension of a GaAs NW being from 2.31 to 9.23 nm, the roughness of its fractured surface increases, see insets in Fig. 2. As a result, the healing efficiency reduces by 45.2% from 83.9% to 46.0% (Fig. 2). Based on tests of repeated fracture and cure of a GaAs NW with a lateral dimension of 5.54 nm, the restored tensile strength reduces dramatically by 64.4% from 7.19 to 2.56 GPa as the healing cycle reaches 24. During first 24 healing cycles, there is an attenuation trend. Further, the restored tensile strength is stable around 2.50 GPa, which accounts for 27.0% of the virginal strength (9.27 GPa), see Fig. 3. A bigger lateral dimension and multiple fractures increase the roughness of fractured surfaces, which cause con factors on self-healing such as a substantial reduction of surface attraction, mismatch of atoms during a healing process and local defects left in a self-healed GaAs NW. To improve the healing efficiency, enhancing atomistic diffusion is a better strategy to eliminate the mismatch of atoms between self-healed sites. To this regard, the self-healed NW after 32 healing cycles is annealed at 1400 K for 1 ns. The tensile test on the heat-treated sample shows that the healing efficiency dramatically increases from 27.0% to 85.5%.

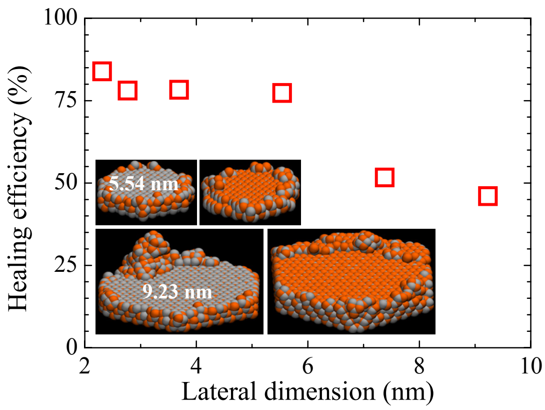

Figure 2: Healing efficiency versus lateral dimension.

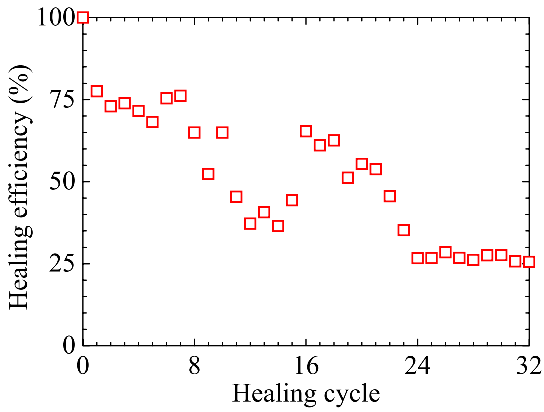

Figure 3: Healing efficiency varies with healing cycles.

CONCLUSIONS

In summary, molecular dynamics simulations have been carried out to investigate self-healing mechanisms of fractured GaAs NWs. The results show that smooth fractured surfaces are a precondition for self-healing of fractured GaAs NWs. In a healing process, the strong surface attraction, due to electrostatic interaction in the near-field region, contributes the Ga–As re-bonding. However, a bigger lateral dimension and repeated fractures increase the roughness of fractured surfaces, which are against self-healing of GaAs NWs. Atomistic diffusion can improve healing efficiency by eliminating mismatch of atoms. This study provides a deep understanding on the self-healing behavior of GaAs NWs and other nanostructured materials, which can help the design of novel nanostructured materials with the ability of self-healing.

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References

[1] Wang Y.B. et al.: Self-Healing of Fractured GaAs Nanowires. *Nano Lett.* **11:**1546, 2011.
[2] Wang J. et al.: Self-Healing of Fractured One Dimensional Brittle Nanostructures. *Appl. Phys. Lett.* 2012 submitted.