Microstructure-Dependent Mechanical Behaviors of SiC Nanowires

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Summary The tensile behaviors of [111]-oriented SiC nanowires (NWs) with various microstructures are investigated by using molecular dynamics simulations. The results elucidate the influence of microstructures on brittleness and plasticity of SiC NWs. Plastic deformation is mainly induced by the anti-parallel sliding of 3C grains along an intergranular amorphous film parallel to the $(11\bar{1})$ plane and inclined at an angle of 19.47° with respect to the NW axis. Also revealed is that the wide dispersion of mechanical properties of SiC NWs observed in experiments is attributed to their diverse microstructures.

INTRODUCTION

At the macroscopic scale, ceramics are brittle at room temperature, but novel experimental findings emerge when the characteristic dimension of a structure is reduced to the nanoscale. For example, large plastic deformation of SiC nanowires (NWs) has recently been observed [1]. Oppositely, most theoretical analysis reveals only the elastic behavior and brittle failure. There is still lack of a good understanding on large plastic deformation of SiC NWs at room temperature. On the other hand, the values of Young's modulus of [111]-orientated SiC NWs vary widely in the range from 20 to 750 GPa, without a consensus value even for a specific, fixed wire dimension. The similar phenomenon also exists in their strengths. In addition to differences in experimental protocols and testing error, so far there is no satisfactory explanation on the wide dispersion of mechanical properties. It is generally believed that mechanical properties of a material critically depend on its internal structures at different length scales. The microstructures of SiC NWs synthesized in laboratories usually consist of [111]-oriented 3C-structured segments, stacking defects and twins. Moreover, an intergranular amorphous film (IAF) with a thickness of ~0.6 to 0.9 nm between grains was formed as a result of aluminum added as a sintering aid. For [111]-oriented 3C-structured segments, the reported side morphologies include: an ultra-thin amorphous shell, (112) or (110) facets and Wulff twinning blocks with (111) facets. Si and C vacancies were also recognized as intrinsic point defects in SiC nanostructures. As shown in Fig. 1, the influence of a specific microstructure on mechanical properties can hardly be evaluated by experiments since an individual SiC NW may contain one or more these microstructures. Such a gap can be at least partially addressed with numerical simulations.

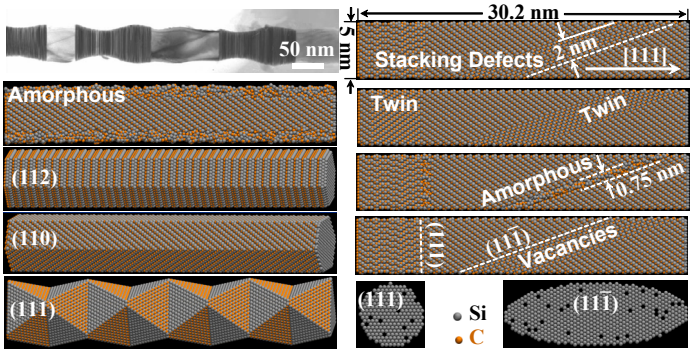

Figure 1: Various microstructures of SiC nanowires, where the transmission electron microscope image is adapted from Ref. [1]

RESULTS AND DISCUSSION

Tensile tests show that all microstructures result in brittle fracture after the tensile strength is reached except for IAF−19.47º (defined as IAFs at an angle of 19.47º to the NW axis). In IAF−19.47º, plastic deformation occurs after the tensile strength of 10.1 GPa is reached and the maximum elongation is up to 20.9%, which is 4.6 times of the corresponding value of 4.5% in the case of IAF−90º (Fig. 2a). The plastic deformation is through the anti-parallel sliding of two 3C−grains along the $(11\bar{1})$ plane, as shown in Fig. 2(b). The tensile response shows saw-tooth jumps that result from stretching, breaking and re-forming of Si–C bonds in IAF; see Figs. 2(c) to (e). Specifically, as strain

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increases from 8.5% to 9.6%, stretching of Si–C bonds in IAF dominates deformation (from C to D in Fig. 2(a)). As they reach the tensile limit, the stretched bonds break and lead to an abrupt stress drop until a new bond forms (from D to E). Thus, the anti-parallel sliding of two 3C–grains results in repeated saw-tooth jumps. It is worth noting that the local unloading curve at point D is consistent with the corresponding loading curve at point C. That is, the saw-tooth stage of C to D originates from the elastic stretching of Si–C bonds in IAF. Furthermore, the slope of upswing portion of each saw-tooth (from C to D) is similar to that of elastic regime of the stress-strain curve, indicating that mechanical properties of SiC NWs are determined by the stretching limit of Si–C bonds in IAF. Repetition of saw-tooth jumping behaviors produces large plastic deformation until brittle failure of the 3C–grain; see Fig. 2(f). For temperatures below 500 K, IAF–19.47º and IAF–90º are stable. Beyond 500 K, crystallization occurs in IAF–90º, which eventually changes to stacking defects. The critical temperature at initiation of crystallization in IAF–19.47º is 700 K. Beyond this temperature, brittle fracture dominates the mechanical behavior of SiC NWs. Many metallic NWs also exhibit large plastic deformation. However, in contrast to the plasticity of SiC NWs caused primarily by anti-parallel sliding of 3C–grains along IAFs, the deformation of metallic NWs is usually related to dislocation activities.

For brittle behaviors of SiC NWs with a lateral dimension of ~5 nm, microstructures have significant influence on mechanical properties such as Young's modulus and strength, see Fig. 3. The (110) faceted NW generates the highest Young's modulus, tensile strength and elongation of 318.6 GPa, 33.4 GPa and 12.1%. The amorphous shell brings the lowest Young's modulus and tensile strength of 158.4 and 12.4 GPa, while the Wulff blocks cause the smallest elongation of 7.9%. As a result, the discrepancy of Young's modulus can be as high as a factor of 2. Moreover, the dispersions of tensile strength and elongation are 2.7 and 1.5 times, respectively. The wide dispersion of mechanical properties is attributed to microstructural anisotropy. In a single crystal, physical and mechanical properties often vary with orientations. The increase of non-[111] orientated composition in SiC NWs causes reduction of Young's modulus and tensile strength [2,3].

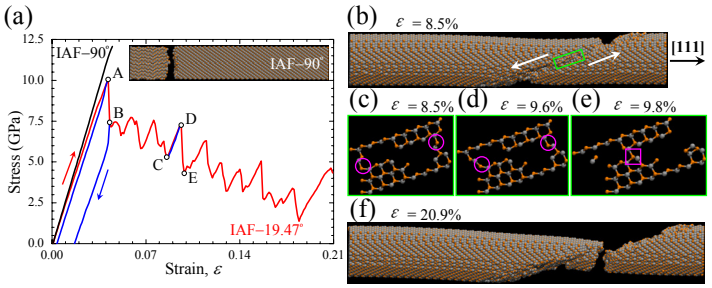

Figure 2: The self-healing process of a fractured GaAs NW. (a) The three-stages include attaching, contacting and healing. Insets are patterns at two peaks (A and B) in the healing stage. (b) Stress versus strain curves of virginal and self-healed GaAs NWs.

CONCLUSIONS

Molecular dynamics simulations have been carried out to investigate uniaxial tensile behaviors of SiC NWs with various microstructures. The main conclusions can be summarized as follows: (i) Large plastic deformation occurs as a result of anti-parallel sliding of 3C–grains along IAF–19.47º, and all other microstructures generate essentially brittle behaviors. The IAF–19.47º is thermally stable below 700 K. (ii) Wide dispersion of mechanical properties is attributed to microstructural anisotropy. The present study provides a better understanding of experimentally observed large plastic deformation and wide dispersion of mechanical properties in SiC NWs and similar nanostructured materials, as well as a potential guidance on microstructural design of ceramics with tailored properties.

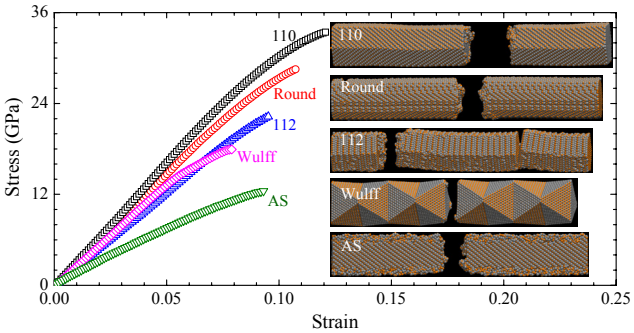

Figure 3: Stress-strain curves of SiC NWs with (110) facets, round cross section, (112) facets, Wulff twinning blocks, and amorphous shell (AS). Insets show fractured patterns.

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