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Atomistic mechanical testing of nanostructures - seeing the invisible and bridging theory and experiments

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Abstract

Recently there has been a major thrust to develop novel nanomaterials exhibiting unique properties. These nanostructures are envisioned as building blocks for the next generation of electronic and energy harvesting systems. In this context, identification of their size-dependent properties is essential, but due to challenges in nanoscale experimentation, unambiguous characterization of mechanical and electromechanical behavior has been elusive. However, in the past few years, in-situ experimentation has emerged as a powerful technique to overcome these challenges. Furthermore, the coupling of such experimental findings to atomistic simulations has shown to have the potential to reveal mechanistic insights, essential for the deep understanding of nanoscale behavior. Here, we present a summary of a few significant results obtained by our group using this approach. Specifically, we discuss size effects that influence the mechanical and electromechanical properties of metallic and semiconducting nanowires.

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1. Introduction

Nanostructures, such as carbon-based nanomaterials (carbon nanotubes-CNTs, graphene and carbon nanofibers-CNFs) and nanowires (metallic and semiconducting), are envisioned as critical components in the next generation of advanced materials, electronic devices and autonomous sensor networks. CNTs and graphene, with their outstanding mechanical and electrical properties are now being studied as the building blocks of high-performance composite materials, and next-generation electronic and nano-electromechanical systems (NEMS). Crystalline nanowires, with enhanced moduli and fracture strengths below 100 nm, and active properties, such as piezoelectricity and piezoresistivity, are potential com-

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ponents of future post-CMOS electronics, energy harvesting architectures, and ultra-high density interconnects.

Although the potential of all these nanostructures is well recognized, challenges in nanoscale experimentation, and in scalability of computational modeling, has made difficult the obtention of unambiguous mechanical and electromechanical properties. For example, in the case of electromechanical properties, despite increased attention on the very high piezoresistivity in silicon nanowires [1], and energy harvesting using piezoelectric nanowires [2], some questions remain unanswered [3–5]. Even though high piezoresistance has been reported by several groups [1, 6, 7], recent findings point to experimental artifacts that may explain earlier measurements [3, 4]. In the case of energy harvesting, the correlation between conductivity, carrier concentration, and piezoelectric output has been the subject of controversy [5, 8, 9], although such systems have demonstrated the ability to produce usable electrical energy [10].

To address these challenges, our group has developed over the past several years a combined experimental-computational approach to characterize mechanical and electromechanical properties of nanostructures. For experimental measurements, we have developed a MEMS-based nanoscale material testing system (n-MTS) for in-situ SEM/TEM mechanical characterization of nanostructures [11–14], including CNTs [15] and nanowires [16, 17], in pure tension or compression. The n-MTS consists of a thermal actuator and a capacitive load sensor where the specimen to be tested is fixed between by EBID (electron beam induced deposition) of platinum. The device possesses nano-Newton load and nanometer displacement resolutions. To mount nanostructures on the n-MTS, we have perfected a nanomanipulation technique, within an SEM, using a 3-axis nanomanipulator with nanometer step resolution [13]. To complement the experimental effort, atomistic calculations using large scale molecular dynamics (MD) and density functional theory (DFT) methods have been used to model mechanical and electromechanical properties of nanostructures. Here, we present a summary of some of our results using this approach. For more details, the reader is referred to recent review articles that extensively discuss the techniques and findings [18–20].

2. Plasticity in penta-twinned silver nanowires [21]

Although there have been many molecular dynamics simulations on the plastic deformation of metal nanowires, most of the predictions have not been tested experimentally due to the difficulty of conducting in-situ TEM tensile measurements, which can directly identify plastic deformation mechanisms. In [21], we present the results of a combined study of in-situ TEM tensile testing and molecular dynamics (MD) simulations conducted on penta-twinned Ag NWs. We show that the coherent twin boundaries present in penta-twined Ag NWs result in a unique size-dependent strain hardening mechanism that can achieve both high strength and ductility.

Tensile tests were conducted in-situ with a JEOL 2100F field emission TEM operated at 200 keV using MEMS devices in which both stress and strain are measured during the deformation while the NW atomic structure is directly observed [13, 22]. The results show that the yield strain has a weak dependence on the NW diameter, as one would expect from the nucleation theory [23], which suggests that the onset of deformation is initiated by dislocation nucleation. However, the deformation behavior of the NWs after the initial yielding is significantly affected by the NW diameter. Thinner NWs show a more pronounced strain hardening effect. The thickest tested NW (118 nm diameter), however, quickly develops necking with no strain hardening, which is similar to the behavior of single crystalline NWs [24, 25].

TEM images have revealed that dislocations are nucleated and propagated in discrete localized regions along the NWs. Interestingly, the number of local plastic zones that develop during tensile testing is found to increase with decreasing NW diameter. In the thickest tested nanowire, only two plastic zones