

Strain Distribution Analysis during Tensile Deformation of Silicon Nanowire with 4D-STEM

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Deformation in materials is a multiscale problem, which is usually identified by three characteristic length scales: atomic scale, micrometer scale, and macroscale [1]. The atomistic deformation, including lattice distortion and dislocation interactions, results in various deformation mechanisms [2-7]. Although the deformation at the large scale is regarded as the average of the atomic scale properties [1], the connection between atomic scale and larger length scales is unclear. The statistical distribution of the lattice distortion at a specific tensile strain can correlate the atomic-level strain to micro/macro strain, if the strain in both dimensions can be measured simultaneously. In this work, we performed four-dimensional scanning transmission electron microscopy (4D-STEM) during in-situ TEM tensile test to bridge the global tensile strain with maps of the local lattice distortion on silicon (Si) nanowires.

The in-situ tensile test was carried out at room temperature using a MEMS based mechanical testing stage. The single crystalline Si nanowire was clamped on the sample stage (**Fig. 1a**), with its length of about 3 μm and its diameter of about 200 nm. The HRTEM image (**Fig. 1b**) and the diffraction pattern (**Fig. 1c**) indicate that the sample is in its [111] zone-axis. During the tensile test, the MEMS applied a uniaxial tensile force on the nanowire, resulting in lattice distortions and increasing strain in the nanowire. The tensile strain on the nanowire was measured by the method based on digital image correlation [7]. In situ 4D-STEM data was captured by a Thermo Scientific Titan aberration corrected STEM equipped with an EMPAD detector [8]. At each step in the tensile test, a 4D-STEM dataset was recorded which consists of more than 5,000 convergent-beam electron diffraction (CBED) patterns taken as the electron probe scanned on the sample. Local lattice can be measured by automated analysis of the diffraction patterns using AutoDisk [9], which detects the positions of diffraction disks in each diffraction pattern and calculates lattice constants via a lattice fitting process. To map the strain, lattice constants measured in each diffraction pattern are compared with a reference determined as the lattice constants of the sample before the tensile test. The variation of the lattice parameters indicates the local lattice distortions of the sample. A map of the lattice distortion can reveal the distribution of the local strain at the corresponding tensile condition.

Using the average lattice of the Si nanowire before deformation as the reference, the normal strain ϵ_{xx} along the tensile direction based on the coordinate system marked in **Fig. 1** can be determined. In **Fig. 2a**, the strain maps before the tensile test, during the tensile test and near the fracture are plotted corresponding to the tensile conditions colored with labels in the strain-stress curve (**Fig. 2b**). This study helps us to understand the distribution of the strain during the tensile test and provides us some insights on the contribution of local lattice distortions evolution on the deformation process. Details of the strain evolution during the tensile test and its correlation with the overall deformation will be discussed in the presentation. [10]

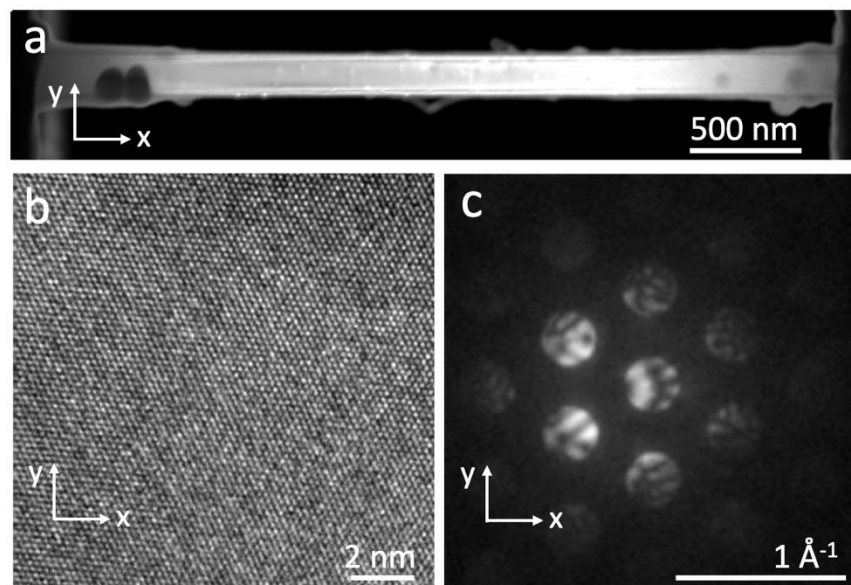


Figure 1. (a) HAADF STEM image of the Si nanowire before the tensile test. (b) HRTEM image of the Si nanowire. (c) CBED pattern of the nanowire.

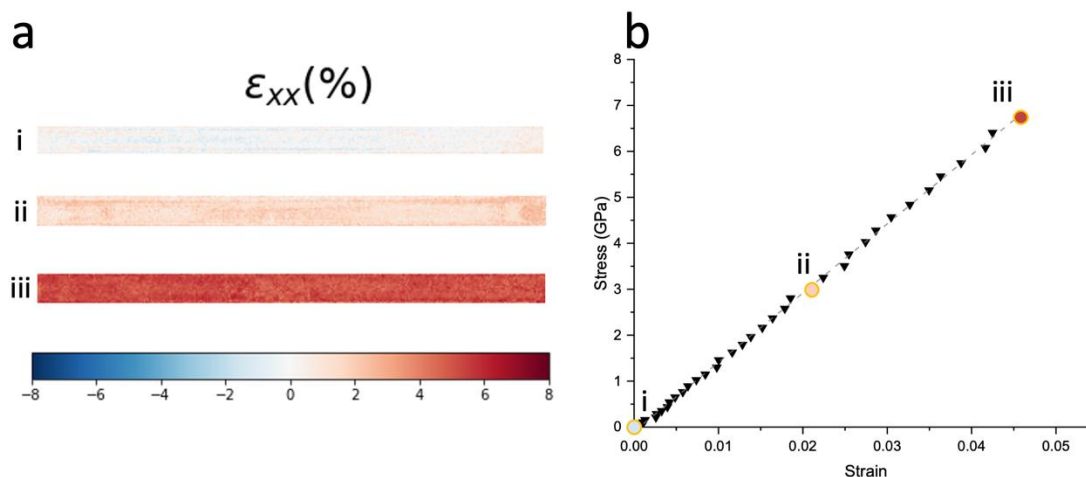


Figure 2. (a) Strain maps of the Si nanowire corresponding to the state (i) before the tensile test, (ii) at the middle of the tensile test, and (iii) approaching to the failure, colored in the strain-stress curve (b).

References:

- [1] Tang, A., Liu, H., Liu, G., Zhong, Y., Wang, L., Lu, Q., ... & Shen, Y. (2020). Lognormal distribution of local strain: a universal law of plastic deformation in material. *Physical Review Letters*, 124(15), 155501.
- [2] Field, J. E. (1971). Brittle fracture: its study and application. *Contemporary Physics*, 12(1), 1-31.
- [3] Kang, K., & Cai, W. (2007). Brittle and ductile fracture of semiconductor nanowires—molecular dynamics simulations. *Philosophical Magazine*, 87(14-15), 2169-2189.
- [4] Zhu, Y., Xu, F., Qin, Q., Fung, W. Y., & Lu, W. (2009). Mechanical properties of vapor–liquid–solid synthesized silicon nanowires. *Nano letters*, 9(11), 3934-3939.

- [5] Zhang, H., Fung, K. Y., Zhuang, Y., Cao, K., Song, J., Hu, A., & Lu, Y. (2019). Fracture of a silicon nanowire at ultra-large elastic strain. *Acta Mechanica*, 230(4), 1441-1449.
- [6] Cheng, G., Chang, T. H., Qin, Q., Huang, H., & Zhu, Y. (2014). Mechanical properties of silicon carbide nanowires: effect of size-dependent defect density. *Nano letters*, 14(2), 754-758.
- [7] Cheng, G., Zhang, Y., Chang, T. H., Liu, Q., Chen, L., Lu, W. D., ... & Zhu, Y. (2019). In situ nano-thermomechanical experiment reveals brittle to ductile transition in silicon nanowires. *Nano Letters*, 19(8), 5327-5334.
- [8] Tate, M. W., Purohit, P., Chamberlain, D., Nguyen, K. X., Hovden, R., Chang, C. S., ... & Gruner, S. M. (2016). High dynamic range pixel array detector for scanning transmission electron microscopy. *Microscopy and Microanalysis*, 22(1), 237-249.
- [9] Wang, S., Eldred, T., Smith, J., & Gao, W. (2022). AutoDisk: Automated Diffraction Processing and Strain Mapping in 4D-STEM. *Ultramicroscopy*, 236, 113513.
- [10] The electron microscopy was carried out at the Analytical Instrumentation Facility (AIF) at North Carolina State University, which is supported by the State of North Carolina and the National Science Foundation (award number ECCS-2025064). The AIF is a member of the North Carolina Research Triangle Nanotechnology Network (RTNN), a site in the National Nanotechnology Coordinated Infrastructure (NNCI).