Supplementary Information of "Band gap engineering and manipulating electronic and optical properties of ZnO nanowires by uniaxial strain"

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1. Reproducibility and the stability of the strain effect on the current

We investigated the reproducibility and the stability of the strain effect on the current in ZnO NWs, and the results are shown in Fig. S1 and Movie 1. In this test, we obtained the current response of a typical ZnO NW over an entire compress-release-stretch-release cycle under a fixed bias of 1V (Movie 1 shows the entire

deformation process). At the initial stage, no strain was applied and the current was maintained at 296±5nA. By controlling the movement of the W tip and by applying a compressive strain to the NW, the current is found to decrease with increasing the compressive strain. When we released the applied strain, the current returned to the initial state. Then, we stretched the ZnO NW and the current increases to 378±5nA when the tensile strain is ~ 1.75%. It has been found that the current was fully recovered again when the strain was fully relieved. These results indicate that deformation of the ZnO NW is highly reproducible and has good stability in the case of a stress-induced change in the electrical properties.

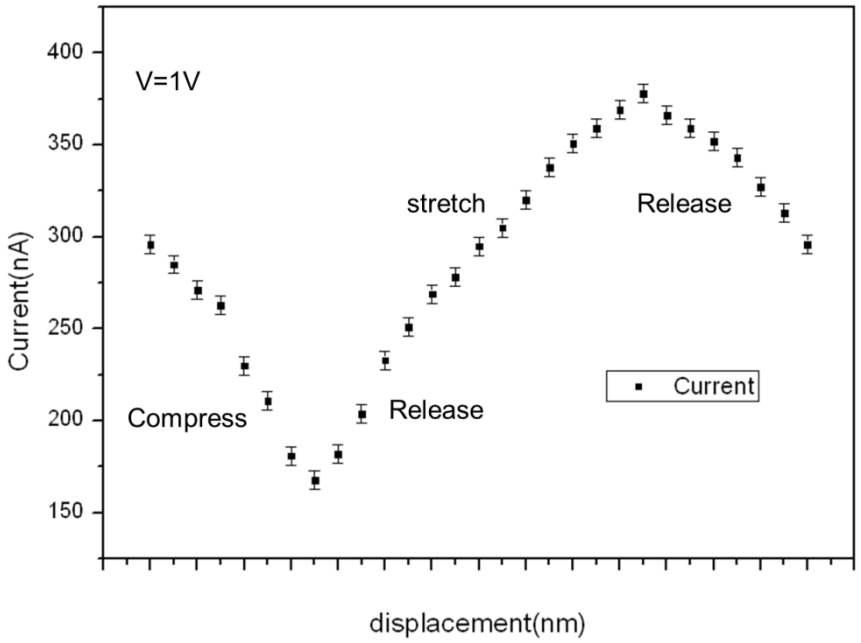

Figure S1. The relationship of the current response of a typical ZnO NW over an entire compress-release-stretch-release cycle under a fixed bias of 1v *Vs* the displacement of the tungsten tip.

2. Strain simulation using the finite element method

To avoid the common limitations when applying strain, such as buckling and strain localization, we employed two strategies: a) the small aspect ratio of length and diameter (in our case, the ratio is ~ 5), and b) a small strain (<2%) is employed which is far below their elastic limitation.[1] These strategies can ensure no buckling and plastic deformation during our experiment. To obtain the information on possible strain localization in segments of the nanowire, a strain simulation using the finite element method (FEM) is utilized, in which the density ρ= 5.606g/cm^3 and the Young modulus Y= 160Gpa [2] were used in the numerical modelling. The simulation results are shown in Fig. S2, with the length of the nanowire of 822nm and the thickness of 136 nm. The nanowire was subjected to large deformation, assuming that the wire was fixed at one end and pinned at the other end.

The free end of the cantilever was displaced by 15 nm towards or backwards with respect to the fixed end, as shown in Fig. S2(b) and (c). As can be seen, the strain along the nanowire axial direction is uniform except at the contact end where a small strain fluctuation is seen, consistent with the *in situ* TEM data.

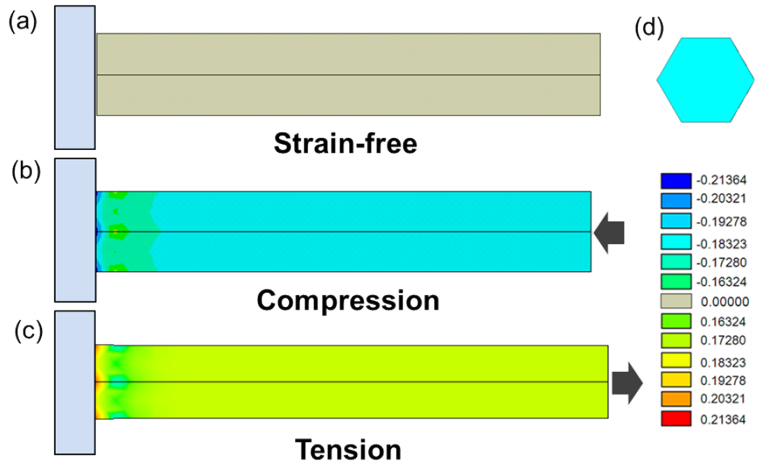

Figure S2. Strain simulation using the finite element method (FEM). (a)~(c) The model of ZnO NW with (a) unstained state, (b) tensile deformed, (c) compressively deformed; (d) Cross section of the ZnO NW model used in the FEM simulation.

3. The method for calculating resistivity

The system in our experiment can be regarded as a metal-semiconductor-metal (M-S-M) circuit,[3] so that the *I-V* curves should be nearly linear under the high bias,[4] as shown in Fig. S3; their slopes can then be directly related to the resistances $R=dV/dI$. Since the length l and the thickness t of the NW can be directly measured from TEM images for different strains, the area of the cross section can be obtained using the relationship $s=0.789t^2$, the resistivity ρ can then be calculated using the formula of $R=\rho l/s$. The data are shown in Table S1 and Figure 4 (Main text).

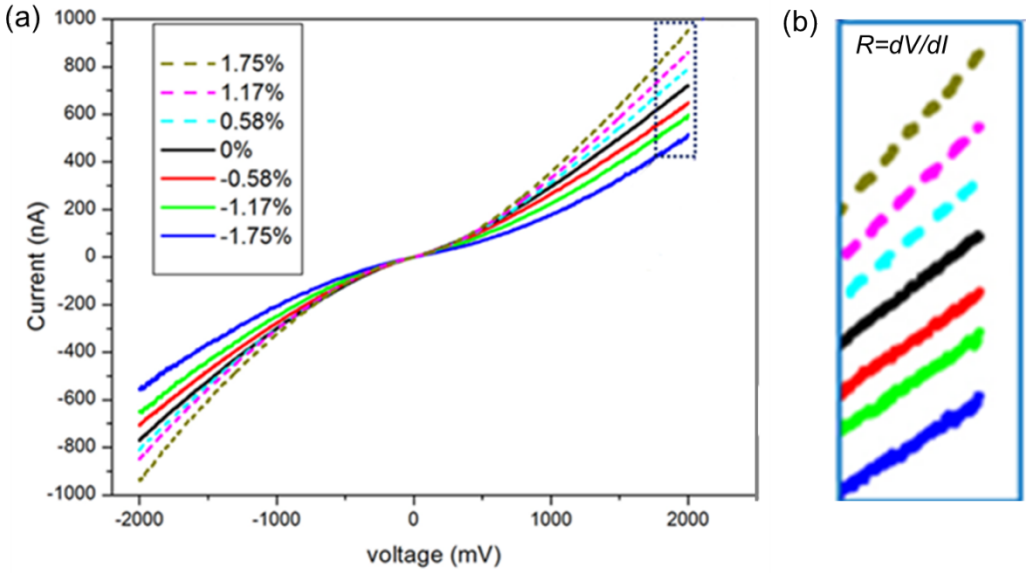

Figure S3. The *I-V* curves under the higher bias. (a) Corresponding *I-V* characteristics of Figure 2; (b) The enlarge region of the dashed frame region.

Table S1 The data for resistance, resistivity of a ZnO NW under different strains.

Strain (%)	-1.75	-1.17	-0.58	0	0.58	1.17	1.75
Resistance($\times 10^6 \Omega$)	2.90	2.50	2.33	2.20	1.90	1.70	1.53
Resistivity($\Omega \cdot$cm)	5.66	4.88	4.54	4.29	3.70	3.32	2.98

4. The change of electron concentration and electron mobility with applied strain

In our M-S-M system,[3] the changes of electrical properties can be retrieved from the experimental *I-V* curve. Based on the M-S-M model, under the lower bias, the current is expressed as[4,5]

$$\ln I = \ln(SJ) = \ln(S) + V(q/k_B t - 1/E_0) + \ln(J_s), \quad (1)$$

where S is the contact area associated with this barrier; J is the current density through the Schottky barrier; q is the elemental charge; k_B is Boltzmann constant; T is temperature in Kelvin; E_0 is a parameter that depends on the carrier density; J_s is a slowly varying function of the applied bias.

The ln *I-V* curves under lower bias are basically fitted to straight lines; their slope k is used to extract the electron concentration n. The relationship between the slope k and n can be deduced by the following equation[6]

$$k = q / q_B T - 1 / E_0, \quad (2)$$

where $E_0 = E_{00}\coth(E_{00}/k_B T)$ and $E_{00} = (\hbar q/2)(n/m^*\varepsilon)^{1/2}$, m^* is an effective electron mass of the ZnO nanowire; n is the electron concentration, and ε is the dielectric constant.

For ZnO materials, $\varepsilon = 7.8\varepsilon_0$, ε_0 is dielectric constant of vacuum and $m^* = 0.28m_0$.[7] Thus, the electron concentration n can be determined. The results are shown in Fig. 5(a); from which, we can see that the electron concentration varies slightly with the strain. Then, the electron mobility μ can be obtained from the resistivity ρ (Main Text, Figure 4 and Supplementary Information, Table 1) of the NW according to the formula $\rho = 1/ne\mu$. The results are shown in Fig. 5(b).

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