Supplementary Materials

Mapping of Strain-Piezopotential Relationship along Bent Zinc Oxide Microwires

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SI: Extract strain distribution from SEM image of a bent ZnO MW

A Matlab algorithm was written to extract strain distribution from SEM images. The algorithm scans the SEM image to find the points representing the edges of the wire. When the locations of the edges are identified, a smooth function is generated to describe the shape of the wire. The function can then be used to find the strain in the wire. Ideally the algorithm should be fed with AFM topography data. Since it is not always possible to obtain such data, a method was developed to extract topography information from 2D images.

Topography information can be extracted from 2D images by exploiting contrast between the wire and its background. Such contrast is evident in Figure S1 where the wire is much brighter than the background. Most digital images use the RGB color space, which defines red, green, and blue as the primary colors. Arbitrary colors are defined by the relative proportions of the primary colors they contain, on a scale from 0 to 255 for each. The apparent brightness of a color can be measured by its relative luminance. In the RGB color space, relative luminance is given by

$$Y = 0.2126\,R + 0.7152\,G + 0.0722\,B \tag{1}$$

where R, G, and B are the relative proportions of red, green, and blue as defined in the color space. In a digital image, pixels are arranged in an evenly spaced grid, and the color of each pixel is stored as a set of three integers from 0 to 255 representing its position in the RGB color space. The data extraction routine maps each pixel to a location in 3D space. The length scale of an image of a wire is used to map each pixel to a position in the x-y plane (with origin at the bottom left corner of the image) based on its location within the grid of the image. Then the color data from each pixel is used to compute its relative luminance. Once this is complete, the routine maps the relative luminance of each pixel to a height above the x-y plane. The contrast between the wire and background results in a large difference in luminance and correspondingly a large difference in height. This mapping mimics the structure of AFM topography data, and allows SEM or even optical images to be used in the strain algorithm.

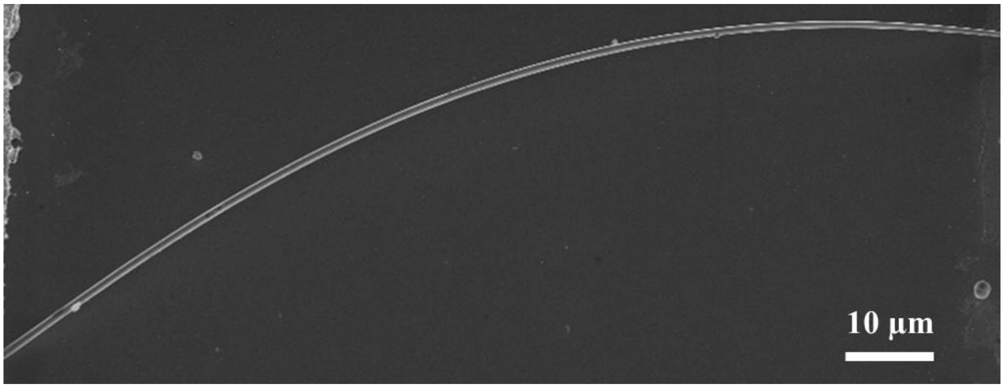

Figure S1: SEM image of a ZnO microwire showing the typical contrast with the background. Topography information can be extracted from such images by exploiting contrast between the wire and its background. The ZnO wire in this SEM image is bent and secured by two Au electrode walls.

The strain algorithm begins with data in the form of points in 3-dimensional space, representing a surface above the x-y plane. The coordinate system is defined to place the surface above the first quadrant, with the origin at the bottom-left corner of the image. Figure S2 shows an example of such a topography image, with height represented by color. Since the AFM takes data in a regular grid pattern with respect to that plane, each data point has a unique set of x-y coordinates. The algorithm scans the data points in a way analogous to the AFM. The data points can be considered a set of lines in the y-direction, and the algorithm considers these lines one at a time. Starting at the x-axis, it compares each point in succession. Since the wire generally appears much taller that the surface it rests on, it can be expected that the algorithm will encounter a large slope when it reaches the edge of the wire.

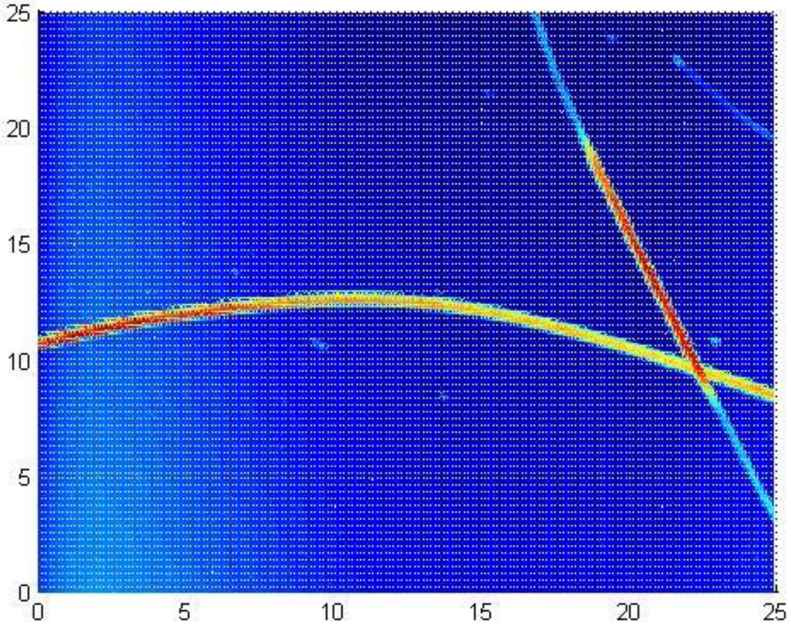

Figure S2: A typical topography image, with wires clearly visible against the blue substrate surface. Dimensions are in μm.

To define the edge of the wire, a slope is determined to trigger the algorithm. The presence of noise in the data is a source of uncertainty, as it must be determined that the slope is the actually the wire, and not an artifact on the substrate surface. To minimize that problem, a statistical analysis is used to define the critical slope. The algorithm scans each line in its entirety, starting at the x-axis (the minimum y-value), and records the value of each positive slope it encounters. The critical slope is then defined as some number of standard deviations greater than the average. The precise number of standard deviations is not fixed to allow adjustment for different data sets. This procedure is repeated for each line, as it is not assumed that the slope on the edge of the wire will be constant along its length. The algorithm also takes the maximum height of the structure into account. When performing the data collection pass on each line, it calculates the average z-position for all the points. A critical height is then determined in the same way as the critical slope. This step allows out most large artifacts to be automatically ruled out, as well as most objects smaller than the wire. After collecting data, the algorithm performs a second pass, again examining slopes. When it encounters a slope greater than the critical slope, it then finds the maximum height of structure containing that slope and compares it to the critical height. If the maximum height is greater than the critical height, the slope is accepted as the edge of the wire. Once one edge has been found, the entire procedure is repeated, this time starting at the top of the image (the maximum y-value), to find the other edge.

Once both edges are defined, the center of the wire along each line is determined to be half way between the edges on that line. The line defined by these center points is assumed to represent the neutral surface of the wire. A polynomial function is fit to the center points:

$$f(x) = \sum_{i=1}^{N} a_i x^{N-1} \tag{2}$$

where N-1 is the degree of the polynomial. The degree is determined by the overall shape of the wire. It must be high enough to accommodate all bends in the wire, as for example, a second degree polynomial can only model a single bend. The degree must also be low enough to eliminate any local changes in concavity not found in the wire.

Figure S3 shows the coordinate system used for strain analysis. The neutral surface is given by line DE. The algorithm assumes that only bending stresses are present. Under those conditions, the strain in the x-direction is given by

$$\varepsilon_x = -\frac{y}{\rho} \tag{3}$$

where ρ is the radius of curvature. The strains in the y and z directions are related to Poisson's Ratio as follows:

$$\varepsilon_y = \varepsilon_z = \nu\varepsilon_x \tag{4}$$

The radius of curvature is given by the reciprocal of curvature.

$$\rho = \frac{1}{\kappa} \tag{5}$$

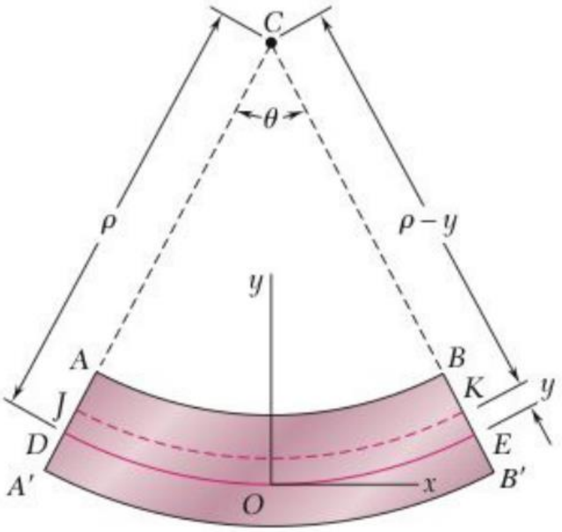

Figure S3: The coordinate system used for strain analysis. [1]

As strain does not depend on arc length, it is reasonable to assume that the relation is preserved even when arc length approaches zero. Thus the local curvature of a function can be used to find the local strain. For a function $y = f(x)$ in the x-y plane, the signed curvature is given by

$$\kappa(x) = \frac{\frac{d^2 f}{dx^2}}{\left[1 + \left(\frac{df}{dx}\right)^2\right]^{3/2}} \tag{6}$$

Substituting equations 5 and 6 into equation 3 gives

$$\varepsilon_x = -y\left[\frac{\frac{d^2 f}{dx^2}}{\left[1+\left(\frac{df}{dx}\right)^2\right]^{3/2}}\right] \tag{7}$$

Equation 7 is applied to the polynomial from equation 2 to yield a strain field for the wire.

The preceding equation for strain can be checked against the case of Euler beam theory, which also assumes pure bending. It also assumes small deformations. In that theory the strain is

$$\varepsilon_x = -y\frac{d^2 f}{dx^2} \tag{8}$$

Under the assumption of small deformations, the slope of f(x) must be much smaller than unity. Thus

$$\left[1+\left(\frac{df}{dx}\right)^2\right]^{3/2} \approx 1 \tag{9}$$

and equation 7 reduces to equation 8.

SII: A typical 3DKPM image

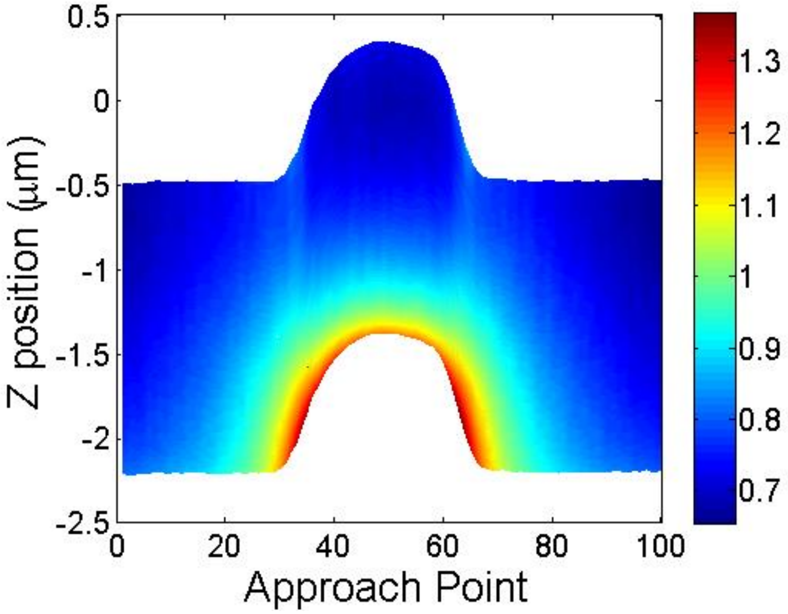

Figure S4: A typical 3DKPM image. The center blank area covered by red color is the cross section of a wire sitting on a flat substrate. A spatial electric potential map was constructed on the *x*-*z* plane after each 3DKPM scan. For each point on x axis, the conductive AFM tip was lifted over the sample surface and then moved downward until it contacts the sample surface. Spatial electric potential above this point is measured and recorded. Then the AFM tip moves laterally to the next approach point and repeats this cycle until a slice of electric potential map on the *x*-*z* plane is obtained. The magnitude of electric potential is represented by color. The unit of the color bar on right is volt.

SIII: 3DKPM results on a straight ZnO MW

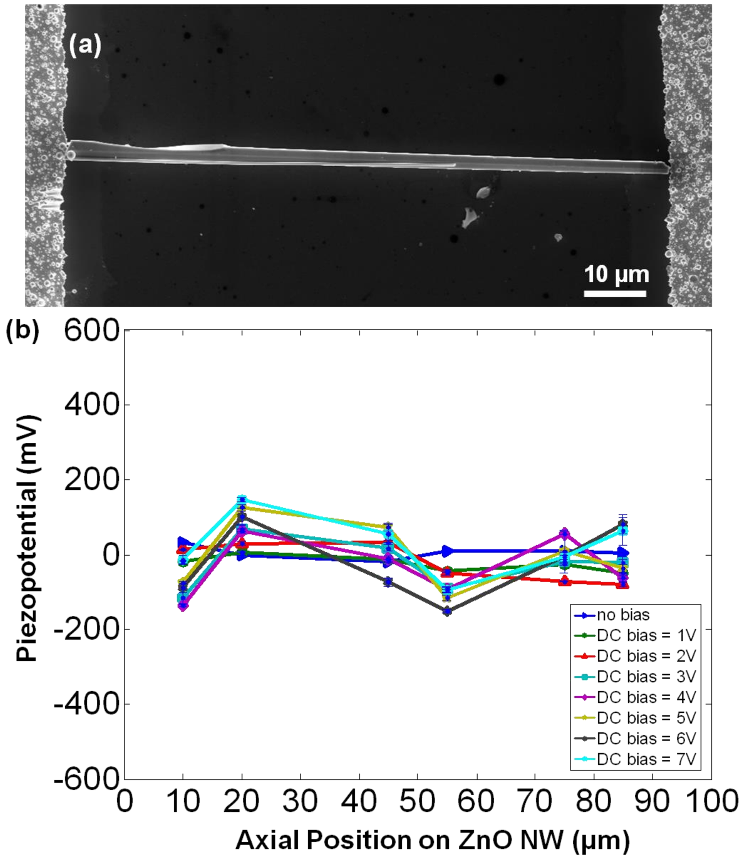

Figure S5: 3DKPM results on a straight ZnO MW. (a) SEM image of the straight ZnO MW without any strain sitting on the trench floor between the two Au electrodes. (b) Under different V_b, no obvious potential differences were detected when V_b was varied from 0V to 7V. This experiment suggests that the contribution of V_b to potential difference measured by 3DKPM is negligible and the detected values from deflected MW can reflect the piezopotential evolution from the bent ZnO MW.

Reference:

[1] F.P. Beer, E.R. Johnston, J.T. DeWolf, D.F. Mazurek, *Mechanics of Materials* 5th Ed., Mcgraw-Hill, NY, 2009.