Electronic Supplementary Information (ESI) for RSC Advances

Mechanical properties of zigzag-shaped carbon nanotubes: roles of geometric parameters

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1. Strain−stress curves of the Z-CNTs and their straight CNT counterparts.

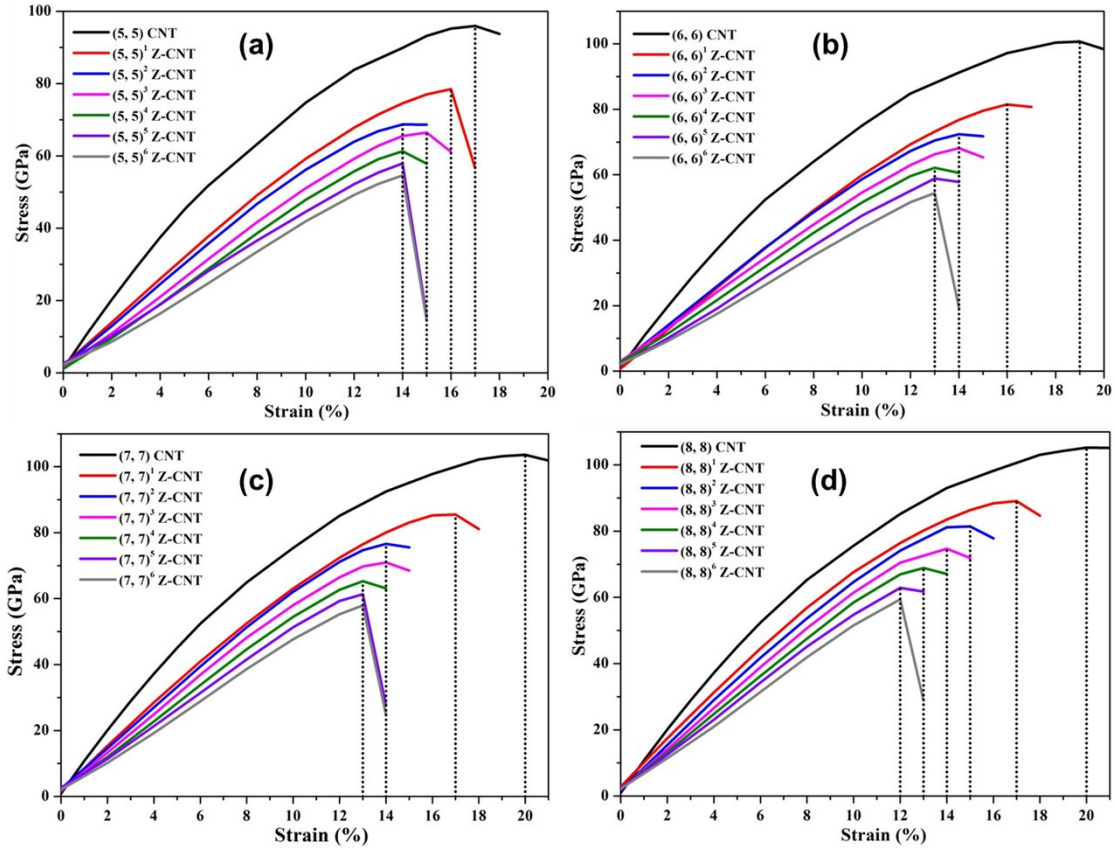

Fig. S1 1.Strain−stress curves of the (n, n)^{m} Z-CNTs with n = 5−8 and m = 1−6 and their straight CNT counterparts. The dot-dashed line indicates the fracture strain. (a), (b), (c), and (d) correspond to the (5, 5)^{m}, (6, 6)^{m}, (7, 7)^{m}, (8, 8)^{m} Z-CNTs, along with their CNT counterparts, respectively.

2. Fitting process for the relationship between the intrinsic strength τ / Young's modulus E and curvature $1/r$ for the $(n, n)^m$ Z-CNTs with n = 5−8 and m = 1−6.

Using the OriginPro 8.5 software, the calculated data of the τ and E and at different curvatures were plotted, as shown in Fig. S3. The adopting the built-in mathematical tools in the OriginPro 8.5 software, the calculated data were fitted using an exponential function through the "Nonlinear Curve Fit" module in the OriginPro 8.5. All of the fitting results were presented in Fig. S3. As a result, the relationship between the intrinsic strength / Young's modulus and curvature $1/r$ can be written into simple equations:

$\tau = A + Be^{-(C/r)}$, and

$E = A' + B'e^{-(C'/r)}$,

which are the Equations (5) and (7) in the manuscript.

3. Fitting results of the relationship between the intrinsic strength τ and curvature $1/r$ for the $(n, n)^m$ Z-CNTs with n = 5−8 and m = 1−6.

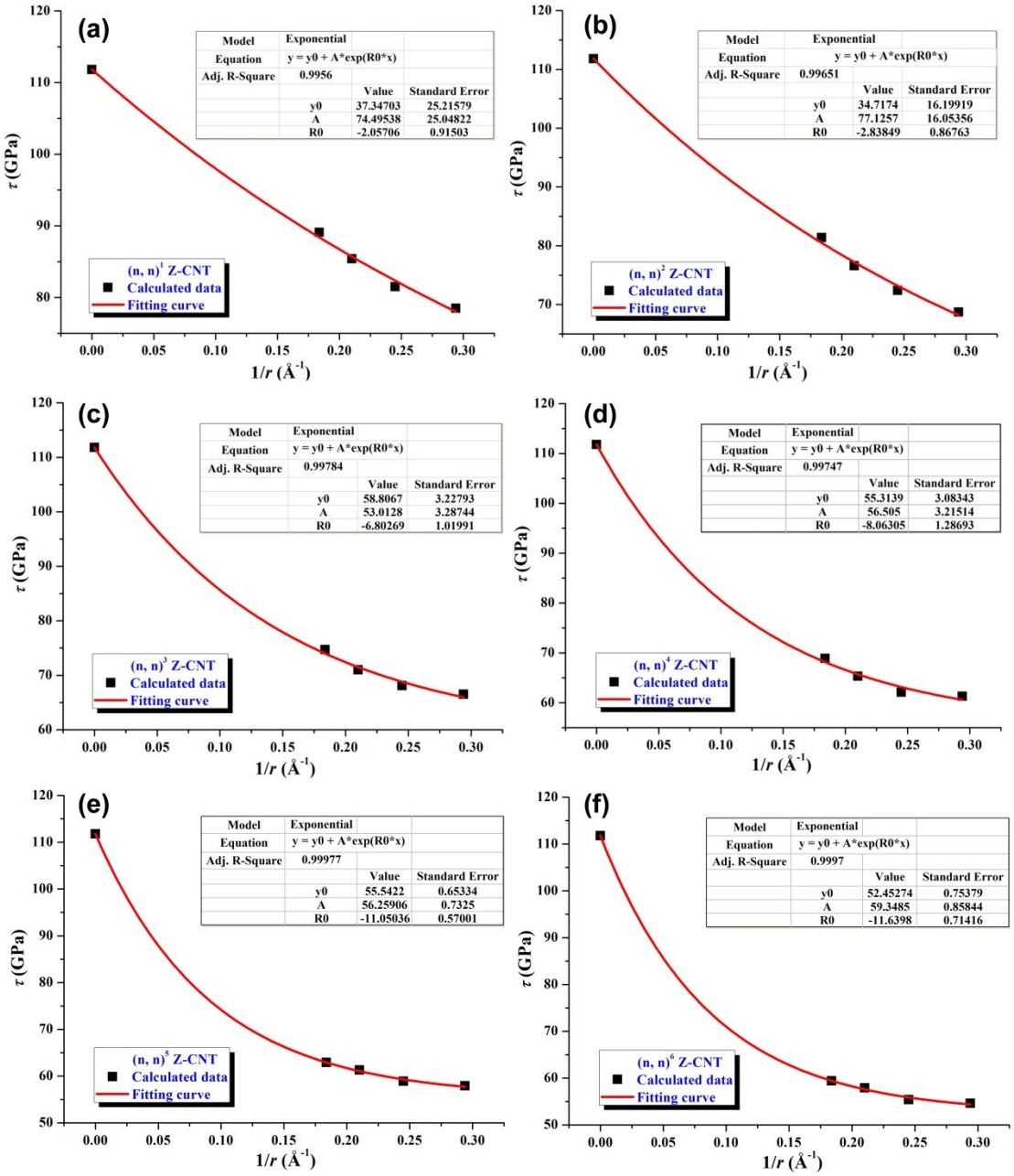

Fig. S2 Exponential fitting of the relationship between the intrinsic strength τ and curvature $1/r$ for the $(n, n)^m$ Z-CNTs with n = 5−8 and m = 1−6. (a), (b), (c), (d), (e), and (f) correspond to the fitting of $(n, n)^1$, $(n, n)^2$, $(n, n)^3$, $(n, n)^4$, $(n, n)^5$, and $(n, n)^6$ Z-CNTs, respectively. The calculated data are plotted in square and the fitting curves are highlighted in red. The inserted table in each figure give the values and standard errors of fitting parameters y0, A, and R0, which correspond to the parameters A, B and C in the manuscript respectively. Adj. R-Square is adjusted R^2, which is used to describe goodness of a fitting curve. The closer the value of Adj. R-Square goes to 1, the better the fitting curve will be.

4. Fitting results of the relationship between the Young's modulus *E* and curvature 1/*r* for the (n, n)^{m} Z-CNTs with n = 5−8 and m = 1−6.

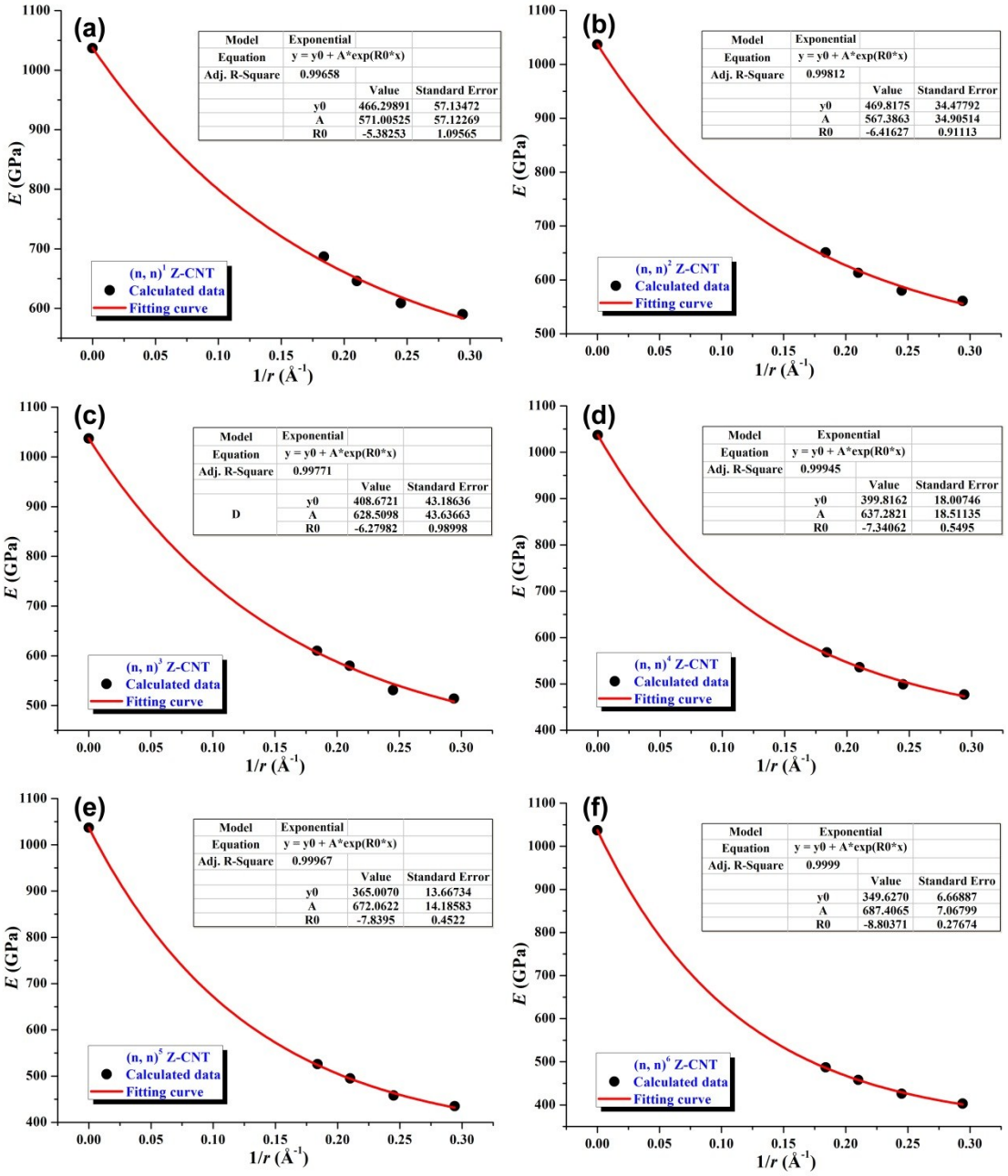

Fig. S3 Exponential fitting of the relationship between the Young's modulus ***E*** and curvature **1/*r*** for the (n, n)^{m} Z-CNTs with n = 5−8 and m = 1−6. (a), (b), (c), (d), (e), and (f) correspond to the fitting of (n, n)^{1}, (n, n)^{2}, (n, n)^{3}, (n, n)^{4}, (n, n)^{5}, and (n, n)^{6} Z-CNTs, respectively. The calculated data are plotted in square and the fitting curves are highlighted in red. The inserted table in each figure give the values and standard errors of fitting parameters y0, A, and R0, which correspond to the parameters A′, B′ and C′ in the manuscript respectively. Adj. R-Square is adjusted R^2, which is used to describe goodness of a fitting curve. The closer the value of Adj. R-Square goes to 1, the better the fitting curve will be.