Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information

Effect of geometry and loading on electromechanical response of 1D ZnO nanostructures

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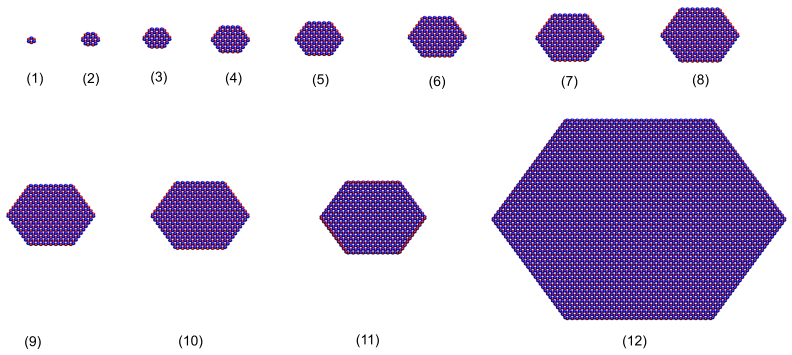
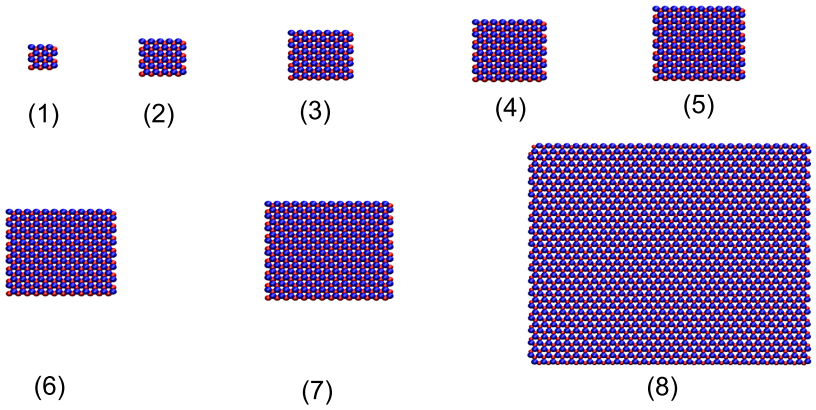
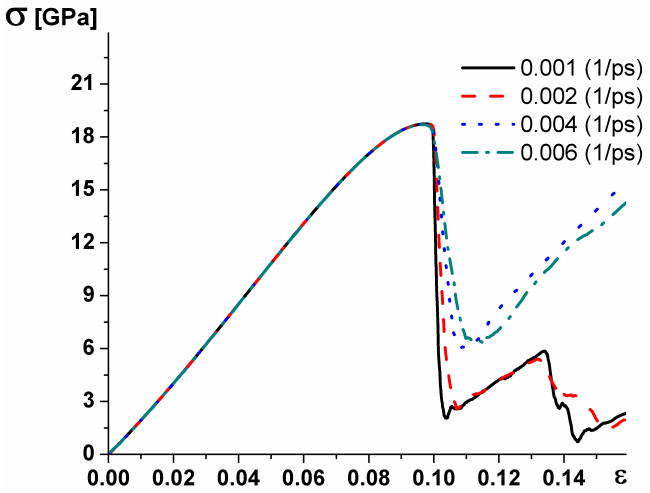


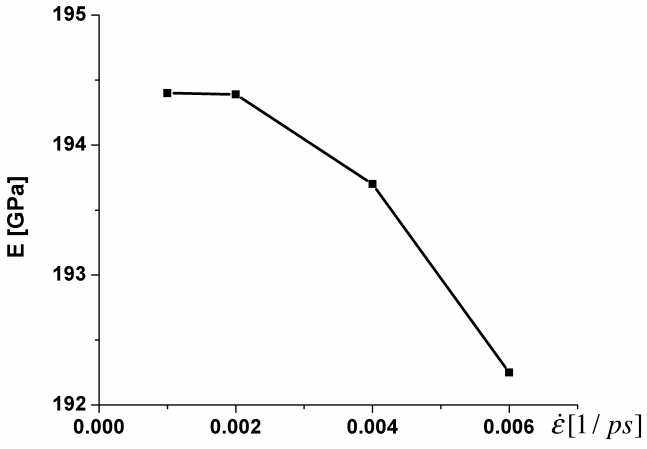
Supplementary Figure. 1. Different ZnO NWs used for simulations. Cross-section of the ZnO NWs that are used for this study are shown, where each NW is numbered in correspondence with the NBs listed in table 1.



Supplementary Figure. 2. Different ZnO NBs used for simulations. Cross-section of the ZnO NBs that are used for this study are shown, where each NB is numbered in correspondence with the NBs listed in table 2.



Supplementary Figure. 3. Effect of strain-rate on mechanical response of ZnO NWs. Stress-strain curve for 1.9 nm NW with different strain-rate is plotted, which shows strain-rate-independence for elastic part. Different curves were captured at higher strain-rates that are in correspondence with the dynamic response of nanostructures.



Supplementary Figure. 4. Variation of elastic modulus with strain rate for 1.9 nm NW. The elastic modulus slightly decreases by increasing strain rate. The similar behaviour was observed for Ni NW. However, strain rate induces amortization in Ni NWs, whereas we did not observe such transformation.

Supplementary Table. 1. Electromechanical properties of ZnO NWs as a function of their size.

No.	Diameter (nm)	$E^{\mathrm{T}}(GPa)$	$E^{\mathrm{C}}(GPa)$	$\tilde{e}_{33}(C/m^2)$
1	0.38	212.55	220.93	0.6
2	0.98	275.21	249.28	1.6545
3	1.633	227.92	206.43	1.59429
4	2.29	210.19	190.69	1.56252
5	2.94	199.65	185.54	1.54449
6	3.59	194.4	177.04	1.53172
7	4.245	190.67	173.82	1.523
8	4.9	188.05	171.43	1.51581
9	5.55	185.7	169.7	1.51062
10	6.2	183.92	168.15	1.50876
11	6.857	182.82	167.07	1.50149
12	19.31	172.6	158.56	1.485

Supplementary Table. 2. Electromechanical properties of ZnO NBs as a function of their size.

No.	$x_1(nm)$	$x_2(nm)$	$E^{\mathrm{T}}(GPa)$	$E^{\mathrm{C}}(GPa)$	$\tilde{e}_{33}(C/m^2)$
1	0.813	0.94	106.52	68.52	2.322
2	1.463	1.501	159.34	154.89	2.025
3	2.063	2.112	172.22	162.23	1.904
4	2.437	2.626	175.95	162.26	1.87
5	3.087	3.189	177.43	163.74	1.864
6	3.737	3.658	177.96	163.62	1.639
7	9.896	9.958	175.31	160.38	1.50