

Supporting Information

One-Step, Catalyst-Free, Scalable *in situ* Synthesis of Single-Crystal Aluminum Nanowires in Confined Graphene Space

Yanan Chen^{1, (a)}, Yanbin Wang^{1, (a)}, Shuze Zhu², Chaoji Chen¹, Valencia A. Danner¹, Yiju Li¹, Jiaqi Dai¹, Hongbian Li¹, Kun (Kevin) Fu¹, Teng Li², Yang Liu³, Liangbing Hu^{1,*}

¹Department of Materials Science and Engineering, University of Maryland College Park, College Park, Maryland, 20742

²Department of Mechanical Engineering, University of Maryland College Park, College Park, Maryland, 20742

³Department of Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina, 27606

(a) Contributed equally to this work.

Email: binghu@umd.edu

Morphology of Al nanowires

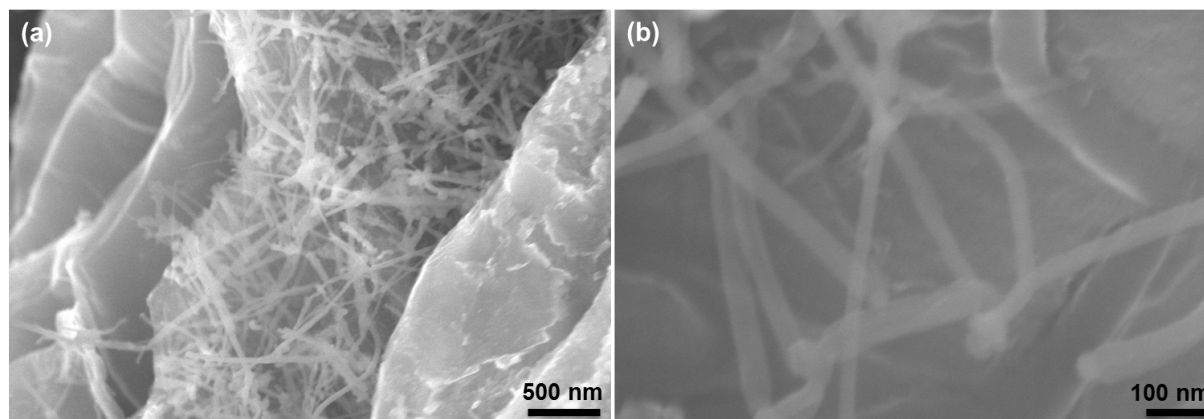


Figure S1. (a) SEM image of Al nanowires, (b) shows the morphology at a higher magnification.

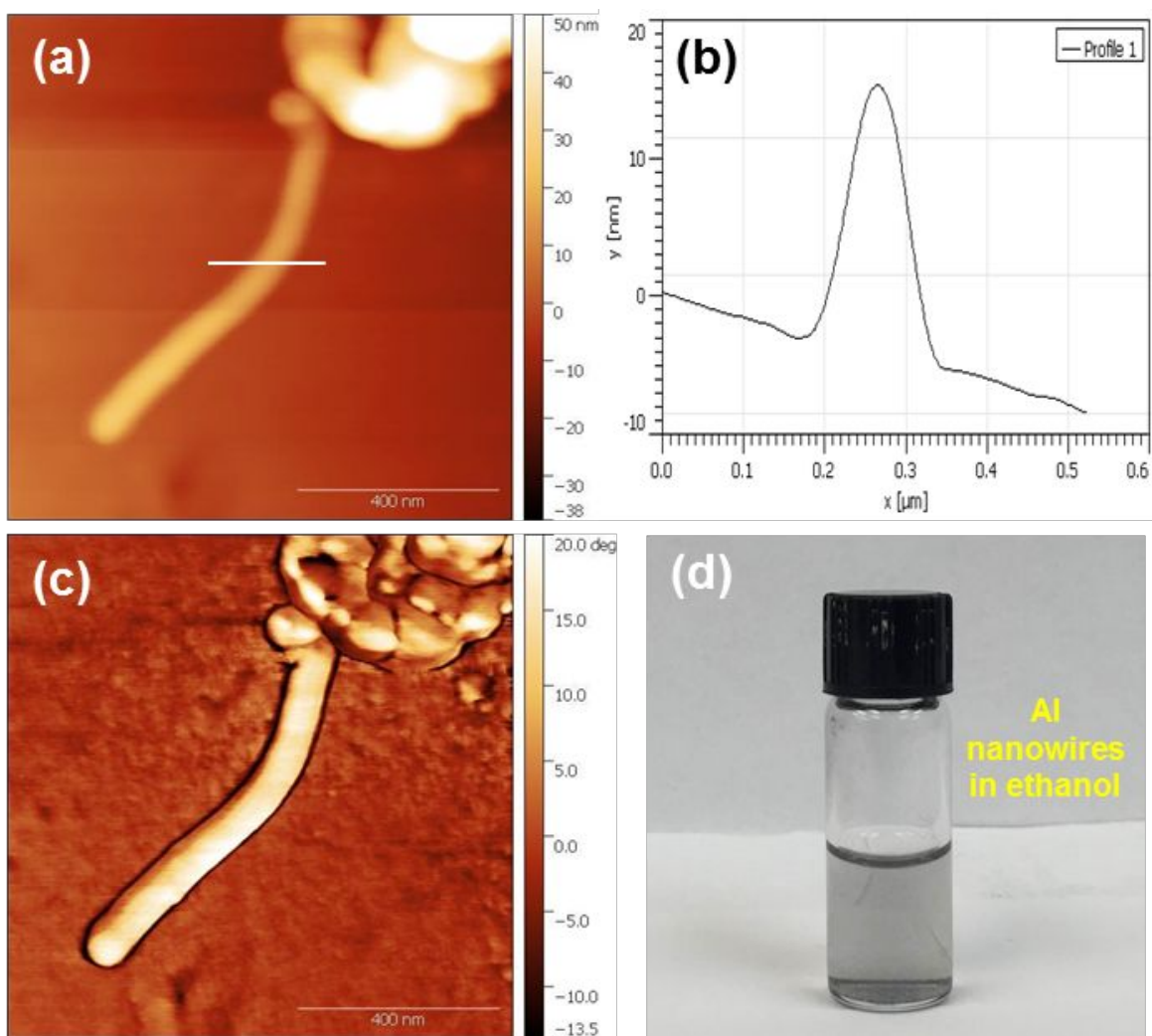


Figure S2. (a, b) AFM image of a single Al nanowire showing the height profile. (c) AFM Phase image of the single Al nanowire. (d) Al nanowires disperse uniformly in ethanol by sonication the RGO-Al nanowires film for 15 minutes.

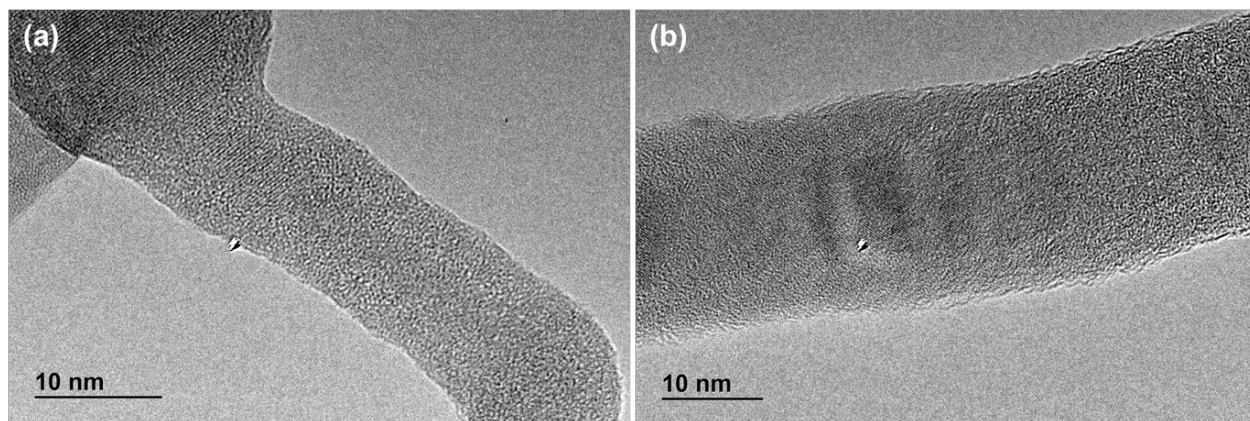


Figure S3. HRTEM images of single-crystal Al nanowires.

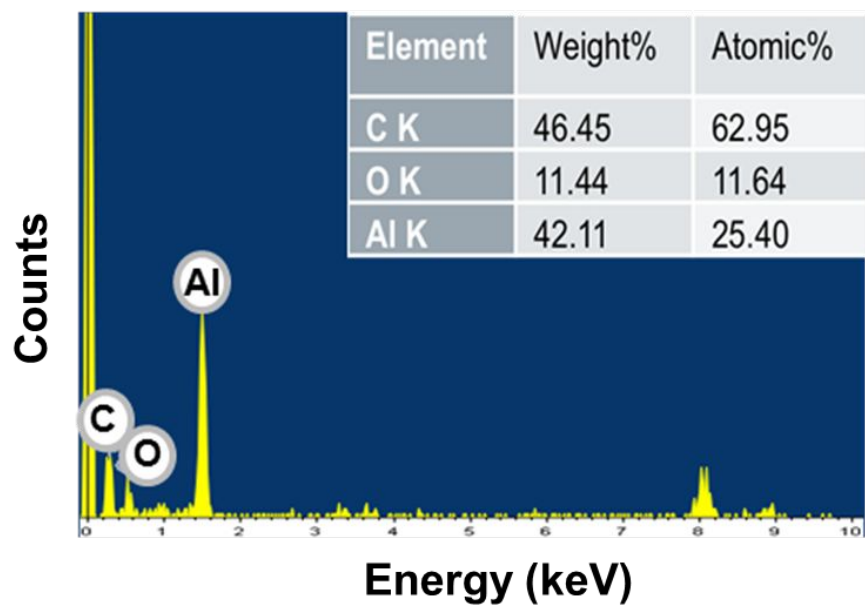


Figure S4. EDS on Al nanowire spot using TEM with 25.4% Al, 62.95% C and 11.64% O in atoms.

Molecular dynamics simulations

The artificial points have equal nearest neighbor spacing of approximately $l = 0.19$ nm (representing the Al-O bond length in the crystal of Al_2O_3), whose radius is $R_v = 2.5$ nm. The spherical cap was suddenly removed has a height of 0.1 nm, and a basal radius of about 0.8 nm. A spherical Al nanoparticle with radius of 2.3 nm is placed inside this artificial sphere (Figure S5).

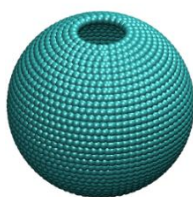


Figure S5. Atomistic model of artificial sphere containing spherical Al nanoparticle (not shown).

For 300K case, the result is shown as in Figure S6. No significant squirting of Al atoms is observed.

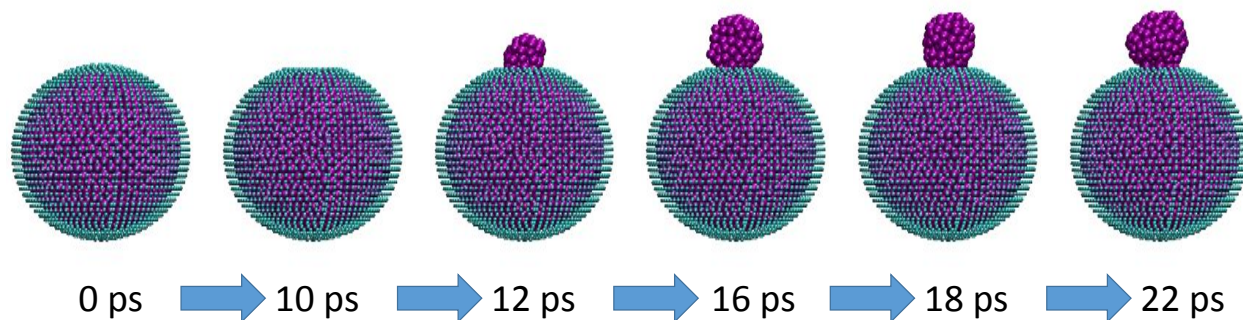


Figure S6. With the temperature of 300 K, Al nanoparticle begins to squirt Al atoms through the vent, but there are not enough Al atoms coming out from the vent for initiating the formation of long nanowire, in contrast to that of 1300 K.

Reference

(1) Rappe, A. K.; Casewit, C. J.; Colwell, K. S.; Goddard, W. A.; Skiff, W. M. UFF, a Full Periodic Table Force Field for Molecular Mechanics and Molecular Dynamics Simulations. *J. Am. Chem. Soc.* **1992**, 114 (25), 10024–10035.