

Supporting Information

Defect Dynamics in Self-Catalyzed III-V Semiconductor Nanowires

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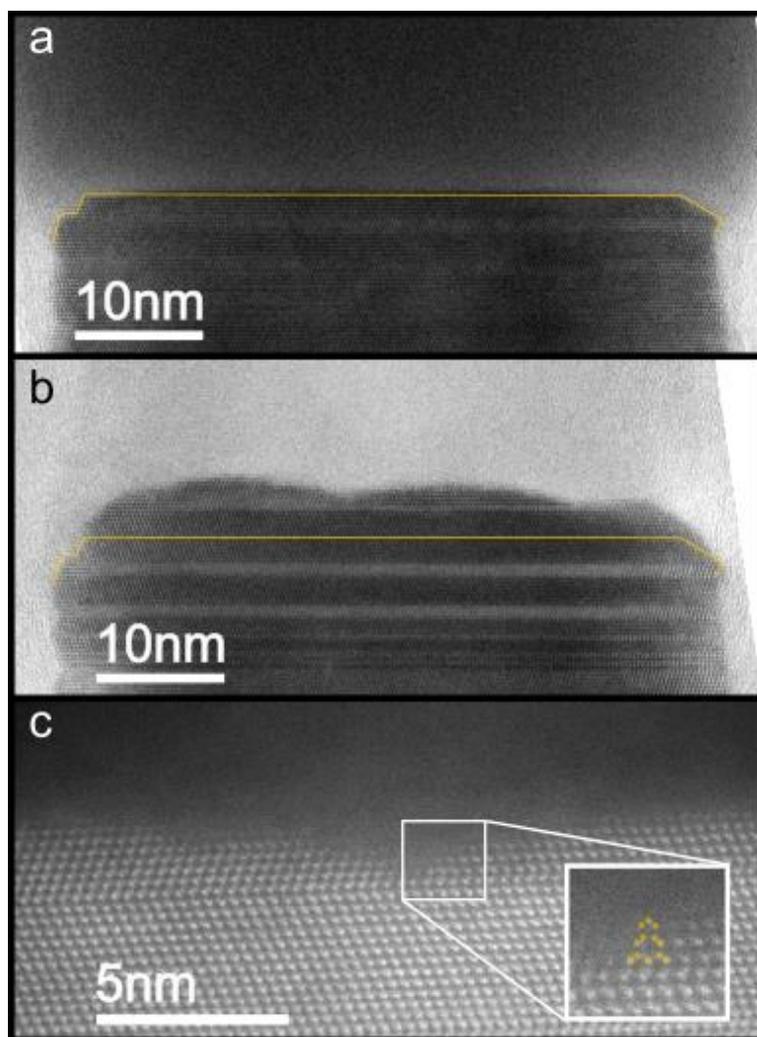


Figure S1. In situ observation of 3ML defect formation during droplet consumption. A GaAsP NW with Ga catalyst droplet was heated in situ under TEM observation. The temperature was increased to 350°C and then decreased to 250°C to simulate droplet consumption during growth. The yellow line marks the original NW/droplet interface. a) The NW and droplet before heating, b) after temperature cycling. Two islands have nucleated, one of which is twinned with respect to the original NW surface, which meet in the center of the NW. A video of the two islands forming and meeting is shown in Supporting Information Movie S1. c) ADF-STEM image showing a 3ML type defect at the island boundary, highlighted in the inset.

Information on Supporting Information Movie S1

Video was acquired using a JEOL 2100 TEM with a OneView camera at 60fps. Scale bar 10 nm.

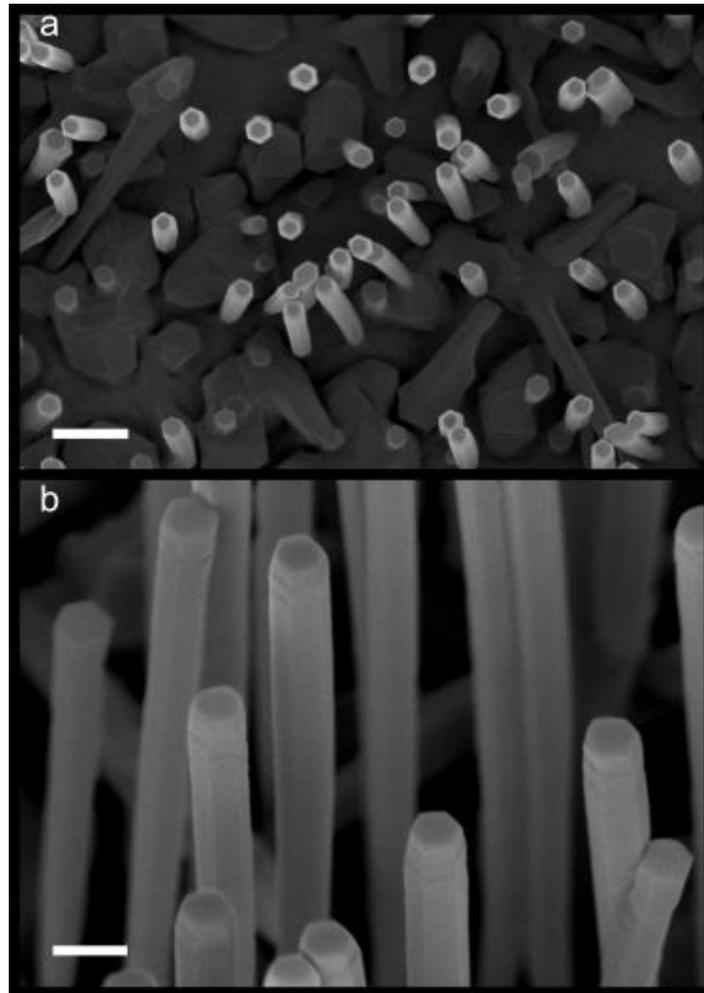


Figure S2. a) In-lens SEM top view image of nanowires still on substrate from the same batch as those used in the study here. This image shows that most of the NWs have a good hexagonal shape with a few having not-perfect shape. Scale bar is 500 nm. b) In-lens SEM image of a side view of nanowires on the substrate. The tips are seen to not be perfectly flat. Scale bar is 200 nm.

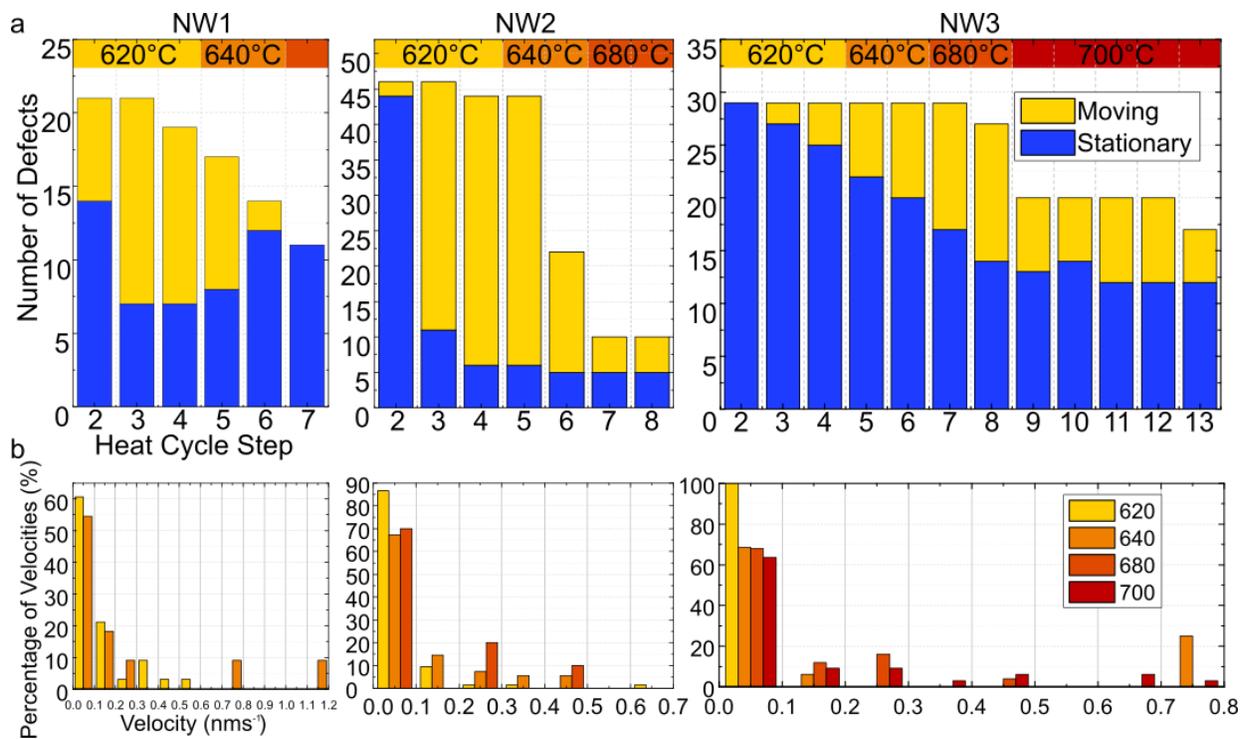


Figure S3. a) Number of defects observed in each NW (blue stationary, yellow mobile) at different heat cycle steps. b) Histograms of defect velocities for each NW normalized to total number of velocity measurements made for each temperature cycle step.

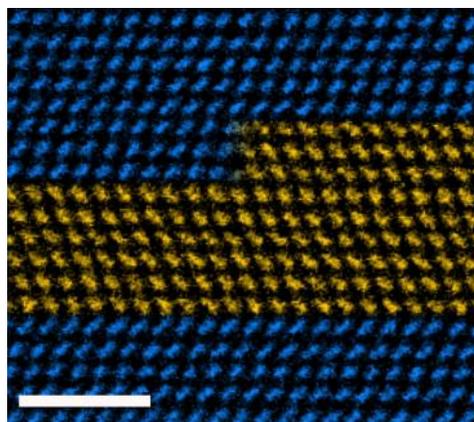


Figure S4. ADF image of an example of a 3ML step facet seen in the central area of a NW. After all stages of heating, the step facet is not seen to move. Scale bar is 2 nm.

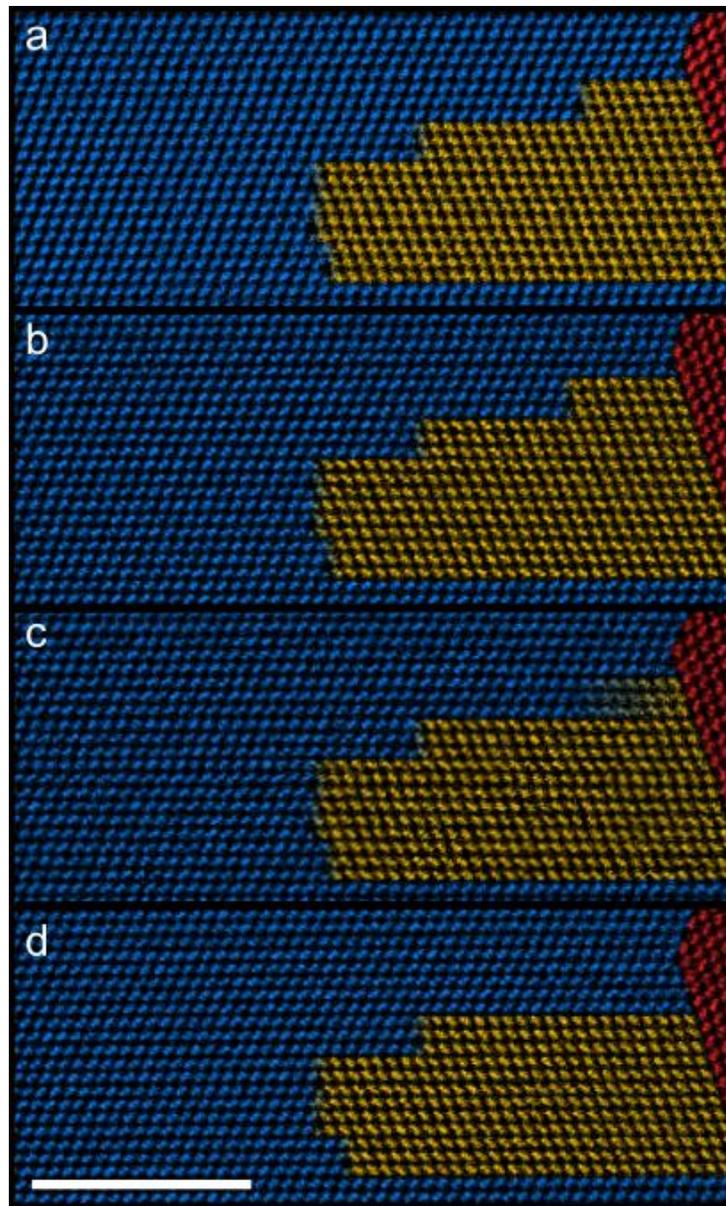


Figure S5. ADF images showing an example of a type 4 configuration where even at high temperatures most of the $\{112\}$ twin facets do not move, only the top one does. Images are taken after heating cycles in Table 1 a) before heating b) cycle 8 c) cycle 12 d) cycle 13. Scale bar is 5 nm.

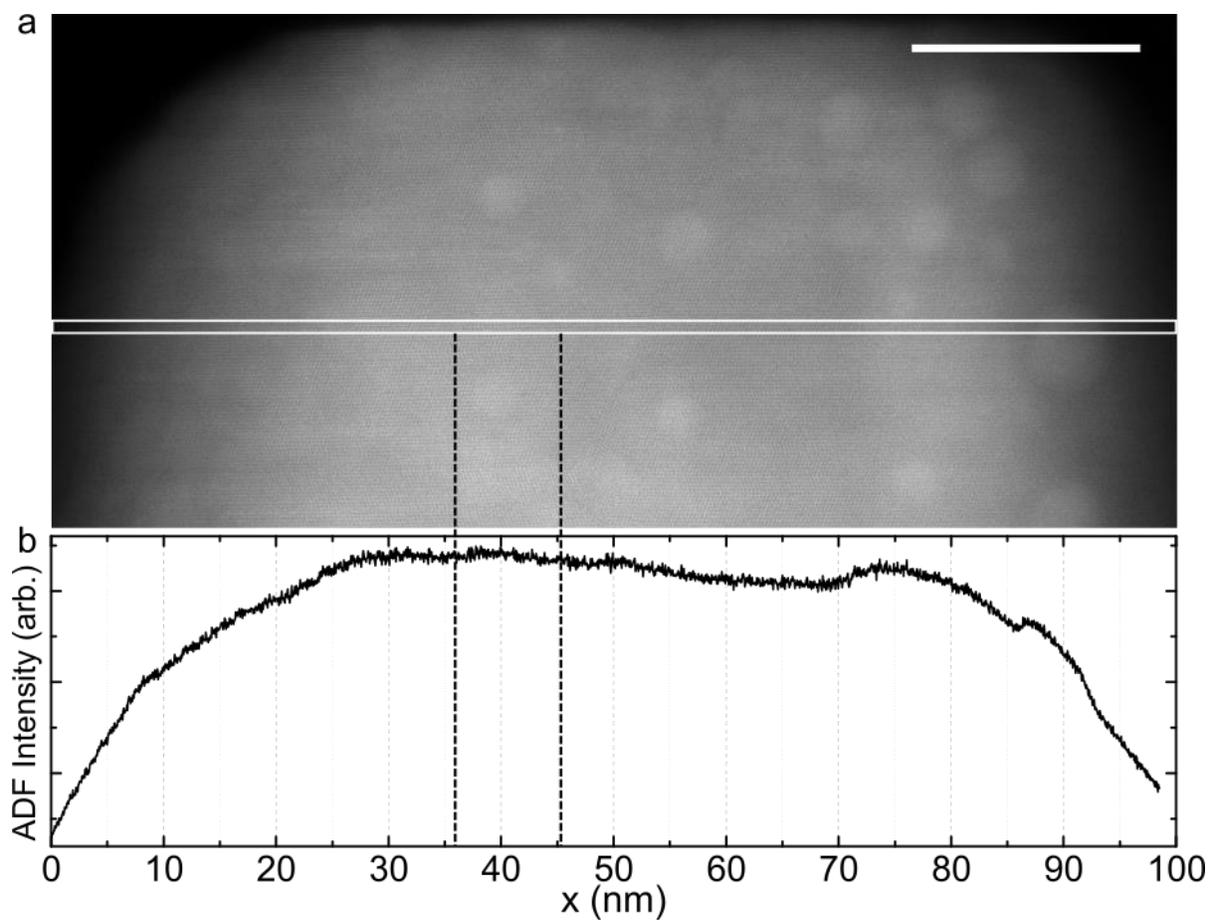


Figure S6. a) ADF image of NW3 from Figure 3b before any heating cycles. The dashed lines indicate approximately where the defect in Figure 4 starts and ends. The white box indicates the region an intensity profile is taken from and is shown in b). The position where the NW thickness becomes uniform due to the approximate hexagonal shape can be estimated from the point at which intensity flattens out, which in this example is around 30 nm and 75 nm from the left-hand side of the image. Scale bar is 20 nm.

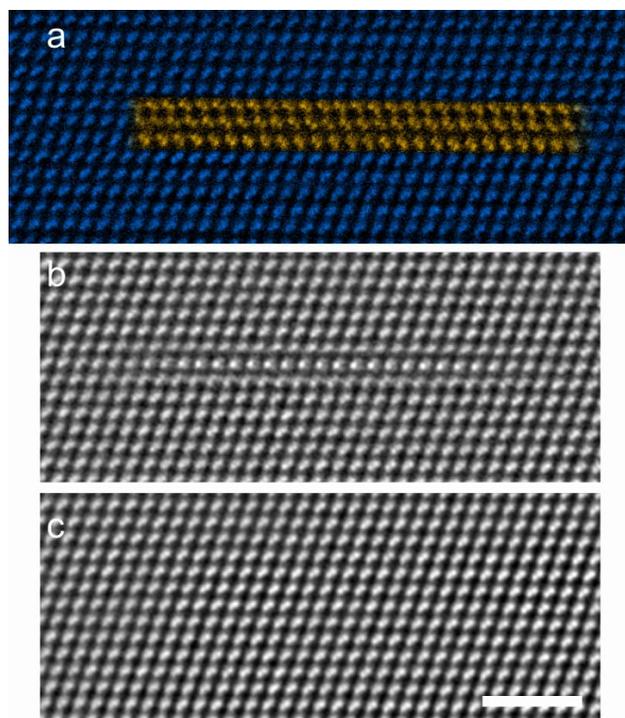


Figure S7. a) Image of an area with a 3ML high twinned region bounded by $\Sigma 3 \{112\}$ twin facets at each end before any heating. b) First frame from Supporting Information Movie S2 with the region appearing blurred as the defects move. c) Final frame from Supporting Information Movie S2 which shows no blurred region and so complete removal of the defects. Scale bar is 2nm.

Information on Supporting Information Movie S2

A 768x768 pixel image was recorded with a dwell time of 2 μ s/pixel and temperature set to 570 °C. A series of 618 images was acquired over a time period of around 15 mins. The images were aligned using SmartAlign software,^[1] a band FFT filter applied and then a rolling average of 70 frames applied. The area was cropped to that shown in Supporting Information Movie S2 with movie width 11.3nm. The initial movie frame does not show each defect on axis due to time taken to focus the image when raising temperature which has caused the defects to start moving. The movie shows the gradual progression of atomic columns being blurred from the defects being in motion, to not blurred showing complete removal of the defects. The motion of the defects is much slower compared to those shown in the main text because of the lower temperature used.

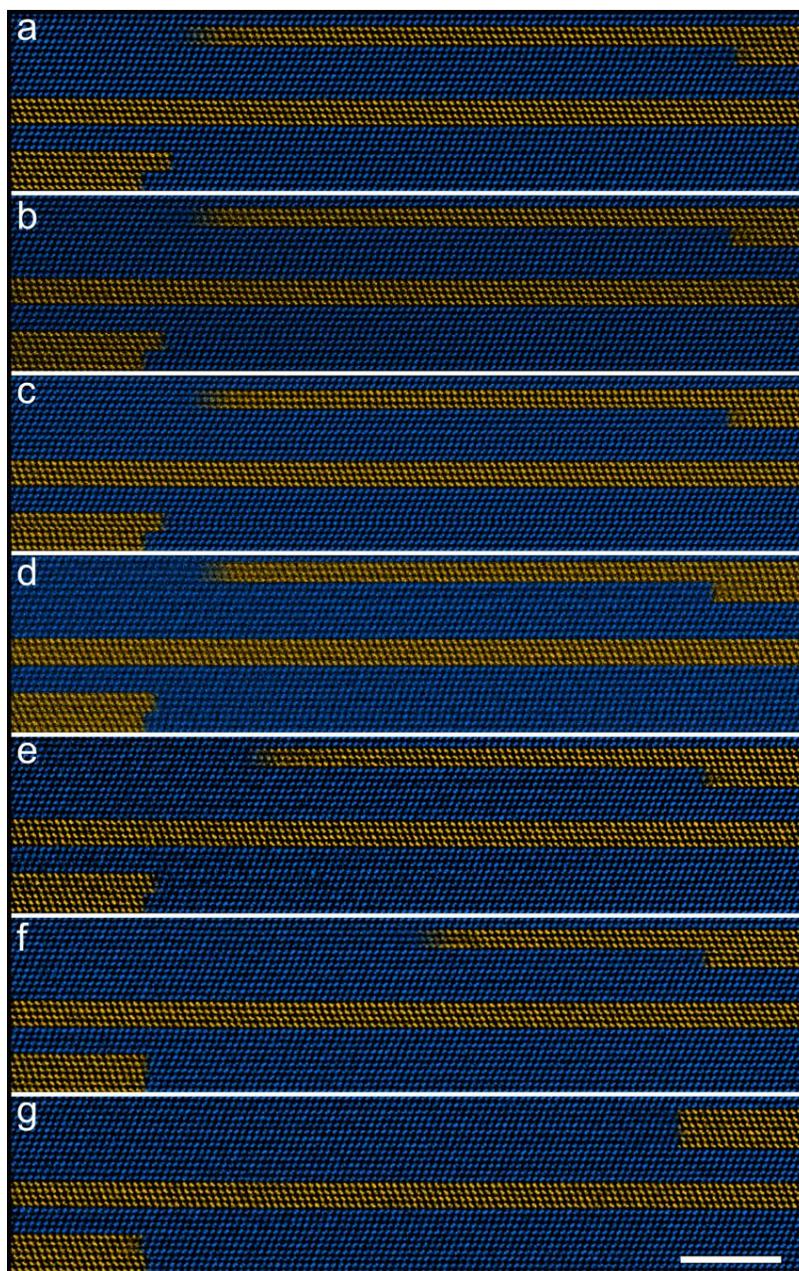


Figure S8. ADF images to show more steps of defect motion progress from figure 5. a) is before any heat cycles, b-g) show snapshots after heating cycle steps 3-8 from Table 1. Scale bar is 5 nm.

References

- [1] L. Jones, H. Yang, T. J. Pennycook, M. S. J. Marshall, S. Aert, N. D. Browning, M. R. Castell, P. D. Nellist, *Advanced Structural and Chemical Imaging* **2015**, *1*, 8.