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<td>Dayeh, Shadi A.; Liu, Xiao Hua; Dai, Xing; Huang, Jian Yu; Picraux, S. T.; Soci, Cesare</td>
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Rocking chair defect generation in nanowire growth
Shadi A. Dayeh, Xiao Hua Liu, Xing Dai, Jian Yu Huang, S. T. Picraux et al.

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Rocking chair defect generation in nanowire growth

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We report the observation of a different defect generation phenomenon in layer-by-layer crystal growth. Steps at a nanowire liquid-solid growth interface, resulting from edge nucleated defects, are found to cause a gradual multiplication of stacking faults in the regions bounded by two edge defects. In the presence of a twin boundary, these generated defects continue to propagate along the entire nanowire length. This rocking chair generation mechanism is a unique feature of nanoscale layer-by-layer growth and is significantly different from well-known defect multiplication mechanisms in bulk materials.

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Semiconductor nanowire (NW) growth is seeded by a liquid eutectic particle in an epitaxial layer-by-layer fashion.1,2 Such crystal growth at the nanoscale is distinguished by a single nucleation event for each succeeding atomic layer.2,3 Perfection is governed by interface properties that determine the driving forces for nucleation of a certain crystal phase4 or formation of defects.5 Therefore, nucleation, propagation, and interaction of defects in NWs can be dramatically different from those in bulk materials. We report here new defect generation mechanism in layer-by-layer crystal growth. This generation mechanism is mediated by atomic steps at the liquid-solid interface, which result from surface nucleated defects. When a new layer nucleation event switch between steps of surface nucleated defects, a gradual generation of stacking faults (SFs) in the regions bounded by these surface nucleated defects emerges. This rocking chair defect generation mechanism is a unique feature of NW layer-by-layer growth and contrasts well-known defect multiplication mechanisms in bulk materials such as Frank-Reed, cross-glide, climb or grain boundary-emission.6

Layer nucleation in a vapor-liquid-solid (VLS) grown NW emerges at the triple-phase-boundary (TBP) as illustrated in Figure 1(a).4,5 In the presence of SFs or twin boundaries (TBs), it is energetically favorable to nucleate a new layer at the interface between the SF or TB with the TBP (Figure 1(b)).8 In the case of a SF, nucleation is pinned at the SF/TPB (Figure 1(b)) until the SF exits the NW at the opposite edge, whereas for a single TB running parallel to the NW growth direction, nucleation is pinned at the TB/TPB throughout the NW length.8 With high supersaturations in the growth seed, nucleation of a new SF from the surface of the NW becomes possible. In the presence of two SFs in the NW, the probability of nucleation of a new layer at either SF is equal. As nucleation switches to the preexistent SF (SF1 in Figure 1(c)), fast ledge propagation—characteristic of VLS growth—encounters an atomic step at SF2, and a new fault forms within a couple atomic distances of SF2 (Figure 1(c)). We observe this mechanism in GaAs NWs and expect its applicability to other NW systems. The GaAs NWs were grown by metal-organic chemical vapor deposition (MOCVD) in a horizontal reactor (Aixtron 200) on GaAs(111)B substrates using 40 nm diameter Au colloids at a temperature of 430 °C, pressure of 50 mbar and a V/III ratio of 14.25.9 Structural characterization was performed using a high-resolution trans-mission electron microscope (HR-TEM, 300 keV FEI Tecnai F30) and Gatan Digital Micrograph software was used to identify defects in the GaAs NWs.

FIG. 1. Perspective view of nucleation and ledge flow in NWs at their faceted surface and triple-phase boundary (a) in the absence of defects (b) at the triple-phase intersection with stacking fault, marked by blue arrow, (c) and at triple-phase intersection with one of two SF2 leading to a new stacking fault (dashed red line) near SF2. (d) HRTEM image of a GaAs NW with multiple surface-nucleated SFs and a TB marked by dashed lines. In any region bounded by two faults, a successive increase in the density of SFs (numbered ≥ 2) outgoing from the surface-nucleated SFs or SF/TB is observed.
Figure 1(d) shows a HRTEM image of a GaAs NW showing three surface nucleated stacking faults (SN-SFs) and a surface nucleated twin boundaries (SN-TB) illustrating this mechanism. Multiple SFs are generated in regions bounded by SN-SFs or a SN-SF/SN-TB. In the first ~70 (111) bi-layers to the left of TB (red dashed line), there are no additional generated SFs. When SF3 emerges (green dashed line), successive nucleation of multiple SFs is observed (green and red arrows numbered in sequence of formation). All regions bounded by SN-SFs show a consistent behavior: SFs emerge near SN-SF and SN-TB and their density increases periodically toward the center of the bounded region between them.

In the postulated SF generation mechanism (Figures 1(c) and 2(a)–2(c)), the nucleation energy for the next layer is lowest at TBP intersection of the SF and NW surface (blue arrows in Figures 1(b) and 2(c) and stars in Figures 2(a)–2(c)) and this leads to one additional bi-layer, above blue star in Fig. 2(a) that stacks to preserve the underlying structure. Following a nucleation event at SF1 (Figure 2(b)), fast ledge propagation on the (111) surface encounters a surface-nucleated stacking faults running in [112] direction and are therefore preserved as the NW kinks from a [111] to a [112] orientation. (c) HRTEM image showing that the generated defects prevail in the newly kinked wire. (c) HRTEM image showing that SN-SF1 annihilates just before the kink (marked “c” in panel (a)).

Additional TEM analysis showing three surface nucleated stacking faults running in [112] direction and are therefore preserved as the NW kinks from a [111] to a [112] orientation. (b) HRTEM image showing that the generated defects prevail in the newly kinked wire. (c) HRTEM image showing that SN-SF1 annihilates just before the kink (marked “c” in panel (a)).

In summary, we reported the observation of a new defect generation mechanism in semiconductor NWs. This mechanism stems from the characteristic layer-by-layer growth at a liquid-solid growth interface. Steps that are formed by surface nucleated defects lead to the generation of additional SFs in regions that are bounded by those defects.

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