Homoepitaxial "Web Growth" of SiC to Terminate C-Axis Screw Dislocations and Enlarge Step-Free Surfaces

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Abstract: Homoepitaxial CVD growth of thin lateral cantilevers emanating from the edges of mesa patterns dry-etched into on-axis commercial 4H-SiC substrates prior to growth is reported. Cantilevers on the order of a micrometer thick extending tens of micrometers from the edge of a mesa have been grown. The termination of vertically propagating screw dislocations, including a micropipe, that are overgrown by the cantilevers has been demonstrated, in large part because the crystal structure of the cantilevers is established laterally from the mesa sidewalls. This technique could help reduce performance-degrading dislocations in SiC electrical devices.

Introduction: The formation of SiC mesa surfaces as large 0.2 x 0.2 mm completely free of even a single atomic step was recently reported [1]. Such step-free surfaces have previously been proposed as ideal for realizing greatly improved heteroepitaxial growth of 3C-SiC and III-N films with much lower dislocation defect densities [2,3]. As better described in [1], these surfaces are produced on commercially purchased on-axis 4H- or 6H-SiC wafers by first dry etching trench patterns into the wafer surface to form an array of isolated growth mesas. Pure stepflow epitaxial growth, carried out under conditions that suppress 2D terrace nucleation, is then used to grow all initial surface steps on top of the mesa over to the edge of the mesa, leaving behind a top mesa surface that is completely free of atomic steps. However as reported in [1], the high density of screw dislocations limited the yield and size of step free mesas attained on commercial SiC substrates. Mesas that initially contain screw dislocation defects cannot be flattened due to the continual spiral of new growth steps that emanate from screw dislocations during epitaxial growth.

This paper presents significant advancements in growth and characterization of step-free mesas on commercial SiC wafers. In particular, we have observed that thin lateral cantilevers form at the edges of mesa surfaces after pure step-flow growth removes almost all atomic-scale steps from the top surface. The lateral propagation of the cantilevered surface is significantly affected by pre-growth mesa shape and crystallographic orientation. Building on these observations, we have implemented a SiC homoepitaxial lateral "web growth" process that overgrows and thus terminates the c-axis propagation of screw dislocations, thereby enabling larger-area atomically flat surfaces to be realized on commercial SiC wafers.

Experimental: All experiments used commercial 4H- and 6H-SiC wafers polished to within 0.3° of the (0001) silicon-face basal plane. Wafers were prepared and grown using the same general procedures described in [1], except that growth times, trench etch depths, and mesa geometric patterns were varied. Following epitaxial growth, wafers were characterized by Nomarski optical microscopy (NOM) and atomic force microscopy (AFM). The ability of AFM to clearly reveal 0.5 nm steps was verified (by measuring nearby non-flat mesas containing elementary screw

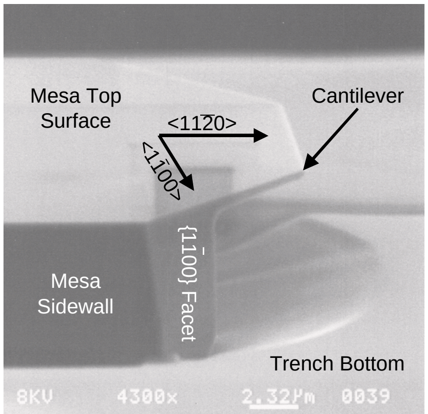

Fig. 1: SEM of thin lateral 4H-SiC cantilever emanating from mesa top after 30-min. growth.

dislocations as described in [1]) before and after measurement of step-free mesas. Following the conclusion of AFM studies, some samples were studied by scanning electron microscopy (SEM). Synchrotron White Beam X-Ray Topography (SWBXT) was also carried out to spatially map non-micropipe dislocations in the wafer [4].

Results: Figs. 1 and 2 show results from 4H-SiC mesas (between 5-10 µm tall prior to growth) where epitaxial growth was carried out at 1650 °C for 30 and 60 minutes, respectively. As described in [1], numerous mesa surfaces were documented by AFM to be completely free of even a single atomic step. Elementary screw dislocations were observed responsible for the vast majority (> 95 %) of mesas where steps remained, and resulting growth hillocks were in all cases observable by NOM. A thin lateral cantilever on the order of a micrometer thick is observed in Fig. 1 emanating from the top of the mesa sidewall. The cantilever appears to seamlessly extend the mesa surface. It should be noted that there is no cantilever overhanging the corner region of the square (pre-growth) mesa shape, which appears to have evolved into a small {1$\bar{1}$00} growth facet. NOM and SEM data indicate that the vertical non-cantilevered portion of the mesa sidewall also expands laterally during growth, albeit at a much slower rate than the cantilevers.

Fig. 2 shows (a) pre-growth NOM and (b) post-growth SEM taken from a cross-shape (pre-growth) mesa. The epitaxially grown thin lateral cantilevers have completely spanned (or "webbed") the arms of the cross-shaped mesa, forming a seamless nearly hexagonal-shaped "tabletop" sitting on top of a cross-shaped support structure. The formation of this structure indicates that enhanced lateral web growth occurred at the inside (i.e., concave) corners of mesa shapes, which combined with hexagonal growth faceting to produce the result shown in Fig. 2. We have descriptively named such features "webbed cantilevers". In addition to web growth, Fig. 2 shows that some growth also occurred to somewhat expand the cross-shaped support structure.

To explain the formation of the thin lateral cantilevers, we propose the following: In the absence of steps and 2D nucleation on the top of a large step-free surface, vertical epilayer growth in the c-axis direction ceases. Nevertheless, growth reactants in the CVD system continue to impinge on the large top surface areas and become mobile surface adatoms that migrate across the step-free surface. These mobile adatoms eventually arrive at the mesa edge and flow off the top surface onto the mesa sidewall. The favorable bonding (i.e., high bond density) of the mesa sidewall promotes rapid incorporation of adatoms into the crystal before they migrate more than a few micrometers below the top edge of the mesa sidewall. Cantilevers are generally not observed on mesas that contain screw dislocations prior to epitaxial growth, because screw dislocations readily provide steps for incorporating top surface adatoms into the crystal resulting in vertical growth of the mesa top surface and preventing realization of a step-free top surface.

To further study the growth of webbed cantilevers, pre-growth mesa shapes resembling V's of various sizes, aspect ratios, and crystallographic orientations were etched into another on-axis 4H-SiC wafer to a height of nearly 20 um. The epitaxial growth time was increased to 6 hours to facilitate complete webbing of larger structures.

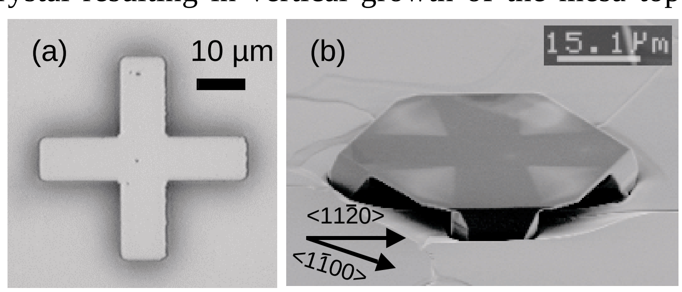

Fig. 2: (a) Pre-growth optical photo of cross-shaped mesa. **(b)** Post-growth SEM of “webbing” formed following 60-minute growth.

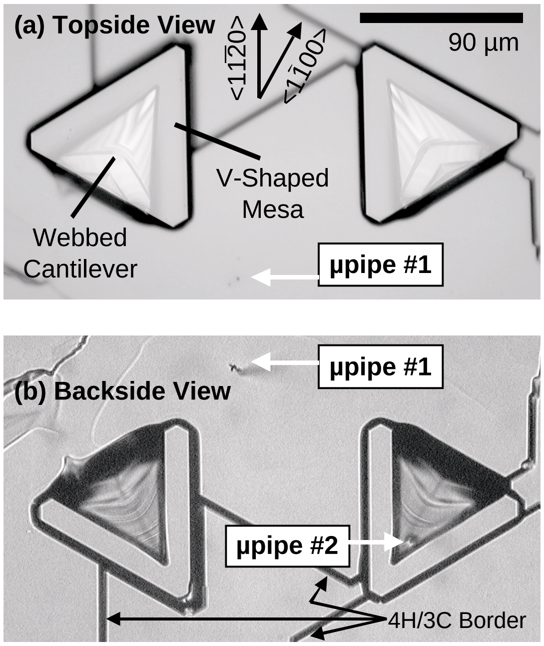

Fig. 3: Optical microscope **(a)** top view of web growth fully spanning two V-shaped mesas following a 6-hour epitaxial growth, and **(b)** view of the same mesas looking through the polished backside, showing micropipe #2 beneath the web growth of the right mesa.

Fig. 3(a) shows the post-growth optical micrograph of two V-shaped mesas where complete webbing of the interior portions of the mesas by thin cantilevers was achieved. Optical interference fringes, visible in the webbed regions, indicate that the webbed regions are thin but not uniform in thickness due to growth on the underside of the webbing. Fig 3(b) is an optical micrograph of the same two mesas viewed looking through the polished wafer backside, showing that the webbing of the right Fig. 3 mesa overgrew a substrate micropipe. The additional lines in Figs 3(a) & 3(b) are 3C/4H polytype boundaries arising from uncontrolled nucleation and growth in the trenches between the mesas. The nucleation of 3C-SiC in trench bottoms between mesas was likely aided by plasma etch damage, while steps from screw dislocations enabled growth of 4H in trench bottoms. Otherwise, the relative abundance of 3C-SiC in trench bottoms with steps would be inconsistent with the relative absence of 3C-SiC on large step-free mesa surfaces.

Numerous webbed and non-webbed mesas on the sample were characterized by AFM. AFM characterization of webbed regions was made difficult due to sinusoidal optical interference measurement artifacts generated by the interaction of the AFM laser with the thin SiC webbing. These artifacts are evident in both scans of Fig. 4, which show AFM scan data from two different AFM instruments of the webbed surface directly over micropipe #2 of Fig. 3. Fig. 4(a) was measured with a DI3000 AFM in tapping mode, while Fig. 4(b) shows the same region measured with a Park Scientific Auto Probe LS AFM in contact mode. The inconsistency between the two Fig. 4 measurements indicates that the sinusoidal undulations are measurement artifacts. Similar AFM measurement artifacts have been previously observed [1,5].

Despite the presence of optical interference undulations, the DI3000 AFM was nevertheless able

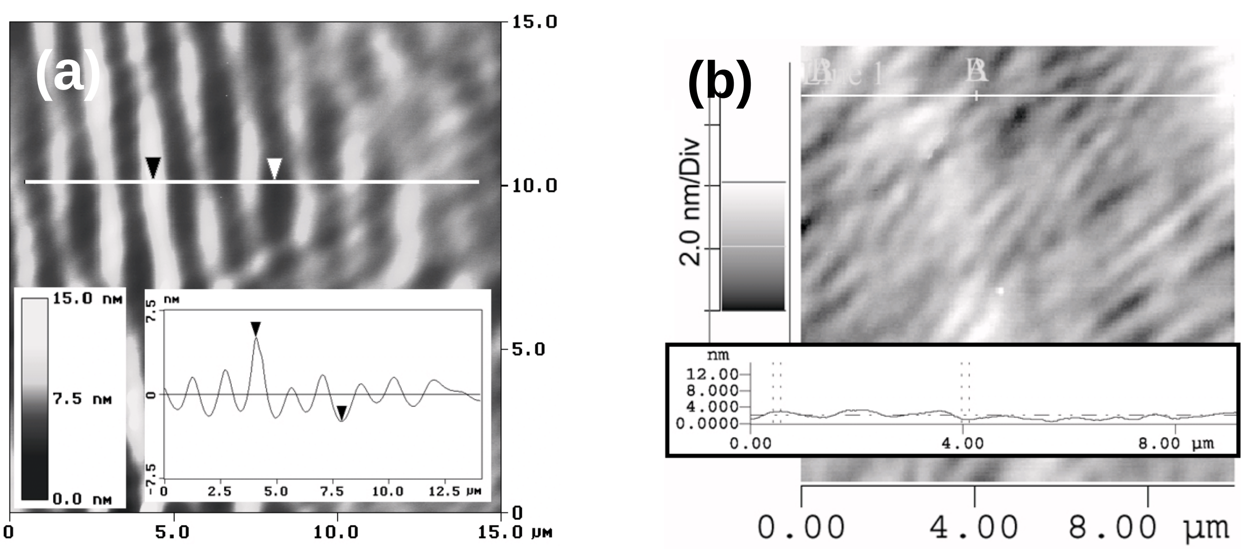

Fig. 4: AFM data of webbed region above Fig. 3 micropipe #2 measured by (a) DI3000 in tapping mode, and (b) Park Scientific LS in contact mode. Both scans show different undulation characteristics (see insets) due to AFM measurement artifacts, but no steps were detected.

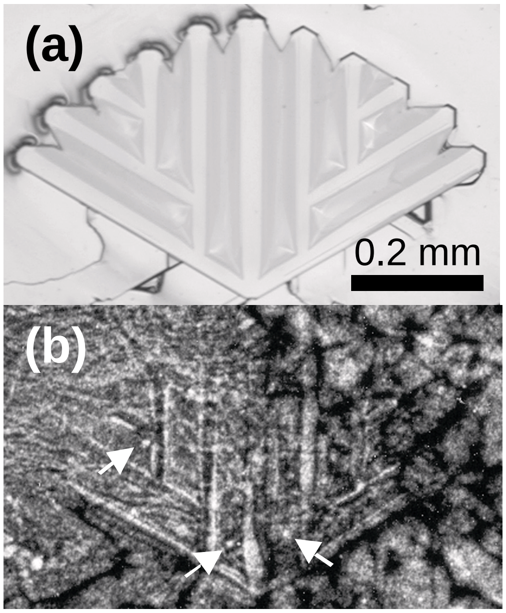

Fig. 5: Post-growth **(a)** optical micrograph, and **(b)** X-ray topograph of largest mesa/web structure, with examples of overgrown substrate screw dislocations denoted by arrows.

to resolve 0.25 nm (i.e., single Si-C bilayer) steps on the surfaces of other webbed regions, including the large web illustrated in Fig. 5. The 0.25 nm steps are consistent with stepheights measured during recent studies of 3C-SiC heteroepitaxial layers unintentionally nucleated on 4H-SiC mesas under nearly identical epitaxial growth conditions [6]. Thus we hypothesize that such steps arise from unintentional 2D nucleation of 3C-SiC following formation of large step-free webs. Therefore, while the rate of 3C-SiC nucleation is small enough to enable step-free surface and cantilever formation, it is not zero.

For the right mesa/webbing of Fig. 3, however, no such steps were observed in a series of AFM scans that covered the majority of the mesa/webbing surface. The complete absence of hillocks and steps, which are always observed when screw dislocations are present, indicates the successful overgrowth of the micropipe screw dislocation defect [1,6]. The absence of steps indicates that defect-free merging of cantilevers from each arm of the V-shape occurred. In contrast, when cantilevers from separated mesa shapes (such as side-by-side squares) merged, steps originating from the coalescence zone were observed, indicating generation of crystal defects.

Fig. 5 illustrates the largest web growth test structure on the wafer. The size of the fully webbed surface is more than 4 times the top surface area of the pre-growth mesa. AFM analysis revealed some 0.25 nm steps on the surface of this mesa, indicating that 2D nucleation of 3C-SiC occurred on the very large basal plane surface. However, no screw dislocation hillocks or 0.5 nm or 1.0 nm steps consistent with post-epitaxial growth 4H-SiC stepheights were observed by AFM. Therefore, the screw dislocations evident in the Fig. 5(b) back-reflection topograph appear confined to the substrate, having been imaged by the penetration of the X-ray beam through the thin webbing.

Summary: The homoepitaxial growth of thin lateral cantilevers emanating from step-free 4H-SiC mesa surfaces was accomplished. Web growth was obtained at concave mesas corners, permitting the realization of seamless webbed structures that can significantly enlarge the step-free surface area produced by selected mesa shapes. The lateral webbing overgrows c-axis screw dislocations (including micropipes), enabling step-free surfaces to be formed on top of these defects. Thus, with proper selection of pre-growth mesa shape, it is possible to overcome the area limitation that SiC substrate screw dislocations previously imposed on realizing step-free surfaces. This approach could be used to reduce or eliminate performance-degrading dislocations from SiC devices.

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