



Reproducible Growth of High-Quality Cubic-SiC Layers

Cubic SiC could be used to improve high-power and harsh-environment electronic devices.

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Semiconductor electronic devices and circuits based on silicon carbide (SiC) are being developed for use in high-temperature, high-power, and/or high-radiation conditions under which devices made from conventional semiconductors cannot adequately perform. The ability of SiC-based devices to function under such extreme conditions is expected to enable significant improvements in a variety of applications and systems. These include greatly improved high-voltage switching for saving energy in public electric power distribution and electric motor drives; more powerful microwave electronic circuits for radar and communications; and sensors and controls for cleaner-burning, more fuel-efficient jet aircraft and automobile engines.

Silicon carbide occurs in many different crystal structures, called polytypes. Despite the fact that all SiC polytypes chemically consist of carbon atoms covalently bonded with equal numbers of silicon atoms, each SiC polytype has its own distinct set of electrical semiconductor properties. While there are more than 100 known polytypes of SiC, only two of them are commonly grown and commercially available in a form acceptable for use as an electronic semiconductor. Both of these polytypes, denoted 4H-SiC and 6H-SiC, respectively, have hexagonal crystal structure. Another polytype, denoted 3C-SiC, has cubic crystal structure and, with respect to use in electronic devices, offers significant benefits over conventional hexagonal SiC polytypes. However, all previous attempts to reproducibly grow 3C-SiC layers have yielded inferior crystals with high densities of defects that make the crystals unusable for realizing their beneficial electronic properties.

Recently, a growth process denoted step-free surface heteroepitaxy has been shown to produce greatly improved 3C-SiC single-crystal films that should enable the reproducible realization of the beneficial properties of 3C-SiC for electronic devices. In this process, the 3C-SiC films are produced on arrays of mesa surfaces that are patterned into commercially available hexagonal-SiC wafers. Figure 1 depicts the subprocesses that affect a mesa. First, reactive-ion etching is performed to form a pattern of trenches into the surface of the

wafer, thereby forming the mesas as the unetched surface areas between trenches. The cross section at the top of Figure 1 shows tightly bonded Si-C bilayers along the crystallographic basal plane, along with single bilayer height steps on the mesa surface that arise because of an unavoidable tilt angle (typically about 0.1°) that is attributable to polishing of the crystal surface at the wafer factory.

Next, pure step-flow homoepitaxy, wherein new reactants become incorporated into the crystal only at the surface steps (which are sites favorable to bond-

ing), is used to grow 4H-SiC from the surface steps on top of each mesa over to the edge of the mesa. Upon completion of this subprocess, the top surface of the mesa is free of atomic steps. That fact that all growth takes place at the steps enables replication of the hexagonal crystal structure of the substrate in this initial epilayer.

After the step-free basal-plane mesa surface of the hexagonal SiC crystal has been established, heteroepitaxial growth of a film having the cubic SiC crystal structure is then initiated by lowering the growth temperature. The lower growth tempera-

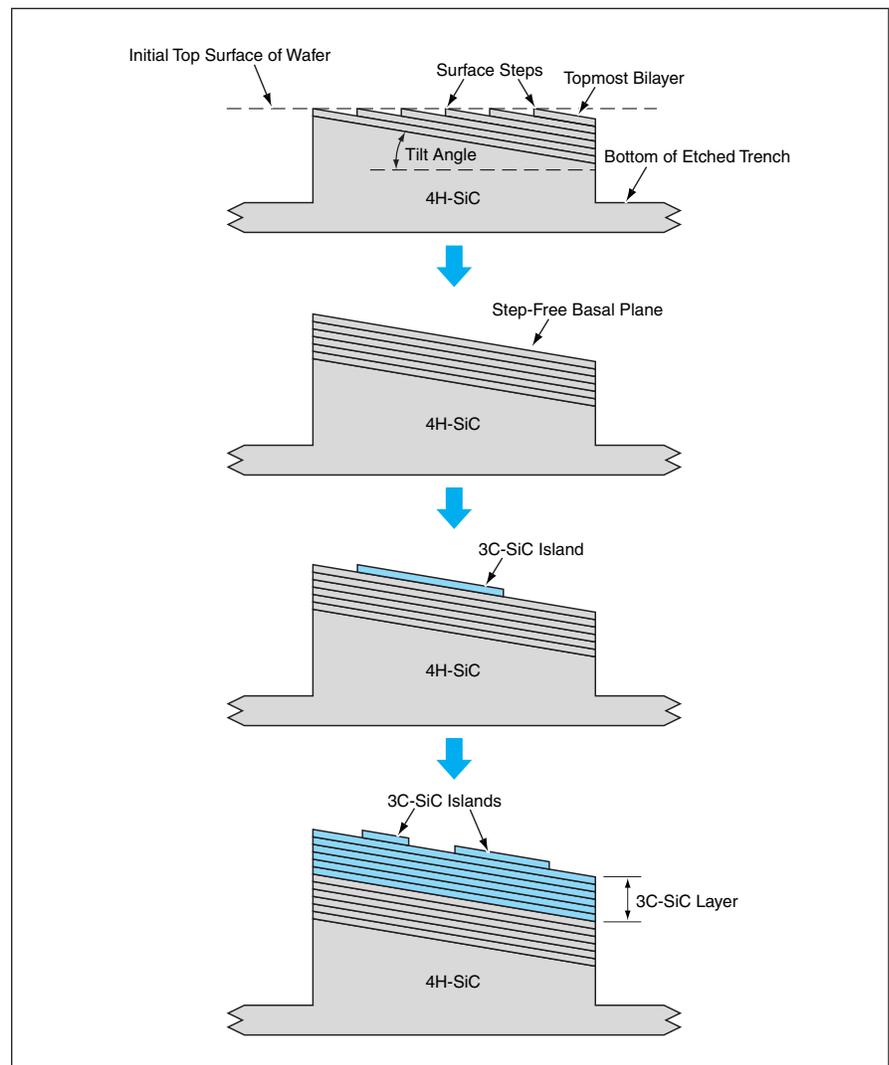


Figure 1. These Schematic Cross Sections of a mesa on a hexagonal-SiC wafer depict the process of growing 3C-SiC by step-free surface heteroepitaxy.

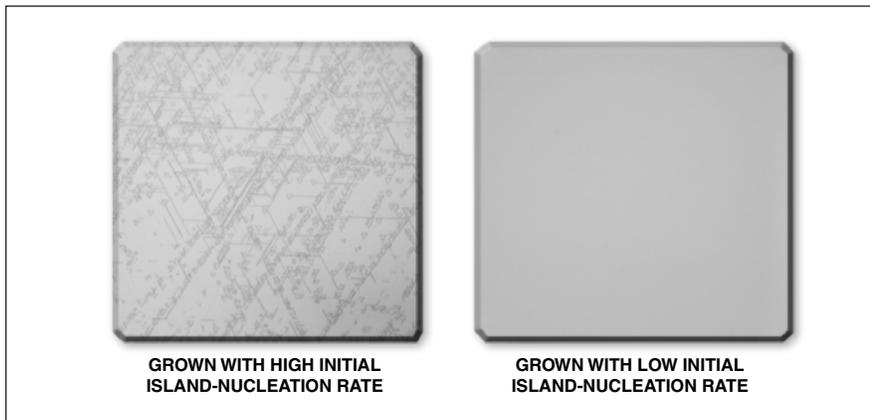


Figure 2. 3C-SiC Films were grown on flattened mesas, then thermally oxidized to reveal crystal defects. The defect-free film shown on the right was made by use of step-free surface heteroepitaxy.

ture enables the growth of 3C-SiC on the basal plane via nucleation of 3C-SiC islands, followed by lateral step-flow expansion. Well-behaved thermodynamic control of polytype occurs in the absence of surface steps, so that the film grows in the cubic crystal structure rather than a hexagonal crystal structure. In experiments, the step-free interface between the hexagonal and cubic polytypes was found to eliminate the double-positioning boundary defects commonly found in previous 3C-SiC heterofilms. However, it was also discov-

ered that the initial 3C-SiC bilayers must be nucleated slowly to obtain 3C-SiC films free of stacking-fault defects.

Figure 2 shows two 0.2-by-0.2-mm mesas topped with 3C-SiC films nearly 2 μm thick and thermally oxidized to reveal stacking-fault defects. As indicated in the figure, the mesas were grown with different initial island-nucleation rates. It has been suggested that what is needed during the initial stages of growth to obtain a defect-free 3C-SiC film is the single-island growth mode, in which a single 3C island nucle-

ates and expands laterally to cover the mesa before a second interfering 3C island nucleates. It has been further suggested that the multiple-island growth mode, depicted at the bottom of the figure, is acceptable after the initial bilayers of the 3C-SiC film have been grown in the single-island mode. In experiments, it was found that 4H-SiC/3C-SiC atomic lattice spacing mismatch was at least partially relieved, without generating stacking faults that threaded to the surface of the film.

The step-free surface heteroepitaxy process is believed to be applicable to growth of heterofilms of materials other than 3C-SiC. Further growth and characterization experiments are in progress, including experiments on the fabrication of prototype 3C-SiC devices and attempting step-free surface heteroepitaxy of GaN films on 4H- or 6H-SiC substrates.

This work was done by Philip G. Neudeck and J. Anthony Powell of Glenn Research Center. Further information is contained in a TSP (see page 1).

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Nonlinear Thermoelastic Model for SMAs and SMA Hybrid Composites

This model captures essential mechanics with fundamental engineering property input.

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A constitutive mathematical model has been developed that predicts the nonlinear thermomechanical behaviors of shape-memory alloys (SMAs) and of shape-memory-alloy hybrid composite (SMAHC) structures, which are composite-material structures that contain embedded SMA actuators. SMAHC structures have been investigated for their potential utility in a variety of applications in which there are requirements for static or dynamic control of the shapes of structures, control of the thermoelastic responses of structures, or control of noise and vibrations. The present model overcomes deficiencies of prior, overly simplistic or qualitative models that have proven ineffective or intractable for engineering of SMAHC structures. The model is sophisticated enough to capture the essential features of the mechanics of SMAHC structures yet simple enough to accommodate input from fun-

damental engineering measurements and is in a form that is amenable to implementation in general-purpose structural analysis environments.

SMAs exhibit thermoelastic martensitic transformations. The interaction of temperature and stress applied to an SMA can be used to exploit the shape-memory effect. An SMA can easily be deformed in the low-temperature (martensitic) state and, if not mechanically constrained or restrained, can be returned to its original shape and size by heating through its reverse-transformation temperature range; recovery in this mode is denoted free recovery. If recovery of the original size and shape is completely prevented by mechanical constraint, then the heating results in a large stress and the recovery is said to be constrained. If the SMA is neither completely free nor constrained but, instead, disposed to perform work by deforming under load, then the

recovery is said to be restrained.

The model expresses the nonlinear thermoelastic nature of an SMA in the form of an effective coefficient of thermal expansion (CTE). This form enables representation of shape-memory behavior, on the basis of either (1) measurement of the effective CTE or (2) inference of thermal strain from measured values of the recovery stress and the modulus of elasticity. The model captures the thermoelastic nonlinearity of the SMA implicitly and provides a simple means of including nonlinear thermoelastic effects of a matrix material in an SMAHC structure. The model can predict constrained and free recovery implicitly and the combination of this model with a model of nonlinear elasticity can predict restrained recovery.

The constitutive equations for a given SMA, SMAHC, or a larger structure that incorporates an SMAHC as a substructure