



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  $\mu\text{m}$  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).*

*Inquiries concerning rights for the commercial use of this invention should be addressed to NASA Glenn Research Center, Commercial Technology Office, Attn: Steve Fedor, Mail Stop 4-8, 21000 Brookpark Road, Cleveland, Ohio 44135. Refer to LEW-17186.*

## Nonlinear Thermoelastic Model for SMAs and SMA Hybrid Composites

This model captures essential mechanics with fundamental engineering property input.

Langley Research Center, Hampton, Virginia

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

can be derived, using the present model as a basis, following a mechanics-of-materials approach or other suitable approach. The present constitutive model, in combination with classical lamination theory, has been incorporated into a finite-element mathematical model and computer code to enable modeling of static and dynamic responses of panel-type SMAHC structures subjected to static and dynamic

thermal and mechanical loads. Loads that have been considered include acoustic pressures, acceleration forces, and concentrated forces. Phenomena that have been investigated include control of thermal buckling, thermal post-buckling, random vibration, and acoustic transmission/radiation responses of structures under constrained recovery. The constitutive model and structural response for-

mulation have been validated against experimental measurements of thermal buckling/post-buckling and random vibration responses.

*This work was done by Travis L. Turner of Langley Research Center. For further information, access the Technical Support Package (TSP) free on-line at [www.techbriefs.com/tsp](http://www.techbriefs.com/tsp) under the Materials category. LAR-16274*

## Liquid-Crystal Thermosets, a New Generation of High-Performance Liquid-Crystal Polymers

Liquid-crystal polymers can now be used as resins in textile composites.

*Langley Research Center, Hampton, Virginia*

One of the major challenges for NASA's next-generation reusable-launch-vehicle (RLV) program is the design of a cryogenic lightweight composite fuel tank. Potential matrix resin systems need to exhibit a low coefficient of thermal expansion (CTE), good mechanical strength, and excellent barrier properties at cryogenic temperatures under load. In addition, the resin system needs to be processable by a variety of non-autoclavable techniques, such as vacuum-bag curing, resin-transfer molding (RTM), vacuum-assisted resin-transfer molding (VaRTM), resin-film infusion (RFI), pultrusion, and advanced tow placement (ATP).

To meet these requirements, the Advanced Materials and Processing Branch (AMPB) at NASA Langley Research Center developed a new family of wholly aromatic liquid-crystal oligomers that can be processed and thermally cross-linked while maintaining their liquid-crystal order. All the monomers were polymerized in the presence of a cross-linkable unit by use of an environmentally benign melt-condensation technique. This method does not require hazardous solvents, and the only side product is acetic acid. The final product can be obtained as a powder or granulate and has an infinite shelf life. The obtained oligomers melt into a nematic phase and do not exhibit isotropization temperatures greater than the temperatures of decomposition ( $T_i > T_{dec}$ ). Three aromatic formulations were designed and tested and included esters, ester-amides, and ester-imides.

One of the major advantages of this invention, named LaRC-LCR or Langley Research Center-Liquid Crystal Resin, is the ability to control a variety of resin characteristics, such as melting temperature, vis-

cosity, and the cross-link density of the final part. Depending on the formulation, oligomers can be prepared with melt viscosities in the range of 10–10,000 poise (100 rad/s), which can easily be melt-processed using a variety of composite-processing techniques. This capability provides NASA with custom-made matrix resins that meet the required processing conditions for the fabrication of textile composites. Once the resin is in place, the temperature is raised to 375 °C and the oligomers are cross-linked into a high-glass-transition-temperature ( $T_g$ ) nematic network without releasing volatiles. The mechanical properties of the fully cross-linked, composite articles are comparable to typical composites based on commercially available epoxy resins.

LaRC-LCR can also be used in thermoforming techniques where short holding times are desired. The resin can be used to spin fibers, extrude thin films and sheets, or injection mold complex parts. Although LaRC-LCR has been developed to meet NASA's needs towards the development of a next-generation launch vehicle, other applications can be envisioned as well. The thermal and mechanical behavior of this material are ideally suited for electronic applications and may find use in flexible circuits, chip housings, and flip-chip underfills. Another area where thermal stability and chemical resistance are highly desirable is the automotive industry. Distributor caps, fuel tanks, air-intake manifolds, rocker covers, and ignition systems

are among the potential applications. The low viscosity of this resin makes this material ideal for coating applications as well. Fine powders have been used in plasma-spray applications, and well-defined thin coatings were obtained. LaRC-LCR can also be used as an adhesive. Lap-shear values of 3,435 psi (22,683 kPa) were easily obtained. In contrast, these values are  $\approx 20$  times higher than those observed in commercially available LCP resins.

*This work was done by Theo Dingemans, Erik Weiser, Tan Hou, Brian Jensen, and Terry StClair at Langley Research Center and funded under NASA's Reusable Launch Vehicle (RLV) research program.*

*This invention is owned by NASA, and a patent application has been filed. An exclusive license for its commercial development has been granted to TICONA Inc. (Summit, NJ). For further information, contact Diane Hope at the Technology Commercialization Program Office (TCPO), NASA Langley Research Center, 3 Langley Boulevard, Mail Stop 200, Hampton, VA 23681-2199. E-mail: [d.l.hope@larc.nasa.gov](mailto:d.l.hope@larc.nasa.gov). LAR-16079*



Several Products made from LaRC-LCR include films, plaques, foams, uniaxial carbon-fiber prepregs, and carbon-fiber composites.