

pose. This macroinstruction code simulates fracture strengths of specimens by use of a combination of a random-number generator (for probability of failure), CARES/Life, and ANSYS finite-element modeling for specimens having randomly chosen dimensions based on a statistical distribution and parameters thereof specified by the user. A unique contribution of this macroinstruction code is that given multiple stochastic input variables, including those pertaining to the strength of the material and the geometry of the part, one can now predict the fracture strength of a complexly shaped part as a single statistical distribution, and can predict a single value of probability of failure for a given load. This capability makes it possible to directly compare predictions made by use of CARES/Life with data from tests of specimens while accounting for the significant amounts of variability that are common in dimensions of MEMS structures.

The methodology was tested by applying it to submillimeter-sized single-crystal SiC tensile specimens fabricated by

deep reactive-ion etching. The specimens had large thickness-to-width ratios (high-aspect-ratios). Some of the specimens contained, variously, elliptical or circular through-thickness holes, which served as stress concentrators. The roughness of the sidewalls left by etching was greater than that of the top and bottom specimen surfaces. There was a large amount of scatter in the measured fracture strengths (typical for ceramics), but the average fracture strength was observed to increase with greater concentration of stress. Variations in dimensions among specimens were measured. The aforementioned macroinstruction code was used to predict the fracture strengths of the specimens with the stress-concentrating holes and the variations in dimensions.

The predictions were found to correlate well with data from tests of the specimens containing circular holes but not quite as well with data from tests of the specimens containing elliptical holes. The results were interpreted as signifying, in part, that (1) the Weibull distribution, which is used in the CARES/Life

software, adequately characterizes the distribution of strengths of MEMS parts; (2) the surface areas of the relatively rough etched sidewalls likely controlled the observed failure responses; (3) the methodology enables accounting for part-to-part variations in dimensions and other properties; and (4) at least at moderate levels of concentration of stress, the methodology can be used to enable successful design of complexly shaped parts on the basis of data from tests of simply shaped specimens.

This work was done by Noel Nemeth, Laura Evans, Glen Beheim, and Mark Trapp of Glenn Research Center; Osama Jadaan of the University of Wisconsin; and William N. Sharpe, Jr., of Johns Hopkins University. 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, Innovative Partnerships Office, Attn: Steve Fedor, Mail Stop 4-8, 21000 Brookpark Road, Cleveland, Ohio 44135. Refer to LEW-18095-1.

Ion-Conducting Organic/Inorganic Polymers

Properties can be tailored through a choice of starting alkoxy silane and diamine ingredients.

John H. Glenn Research Center, Cleveland, Ohio

Ion-conducting polymers that are hybrids of organic and inorganic moieties and that are suitable for forming into solid-electrolyte membranes have been invented in an effort to improve upon the polymeric materials that have been used previously for such membranes. Examples of the prior materials include perfluorosulfonic acid-based formulations, polybenzimidazoles, sulfonated polyetherketone, sulfonated naphthalenic polyimides, and polyethylene oxide (PEO)-based formulations. Relative to the prior materials, the polymers of the present invention offer greater dimensional stability, greater ease of formation into mechanically resilient films, and acceptably high ionic conductivities over wider temperature ranges. Devices in which films made of these ion-conducting organic/inorganic polymers could be used include fuel cells, lithium batteries, chemical sensors, electrochemical capacitors, electrochromic windows and display devices, and analog memory devices.

The synthesis of a polymer of this type (see Figure 1) starts with a reaction be-

tween an epoxide-functionalized alkoxy silane and a diamine. The product of this reaction is polymerized by hydrolysis and condensation of the alkoxy silane group, producing a molecular network that contains both organic and inorganic (silica)

links. The silica in the network contributes to the ionic conductivity and to the desired thermal and mechanical properties.

Examples of other diamines that have been used in the reaction sequence of Figure 1 are shown in Figure 2. One can

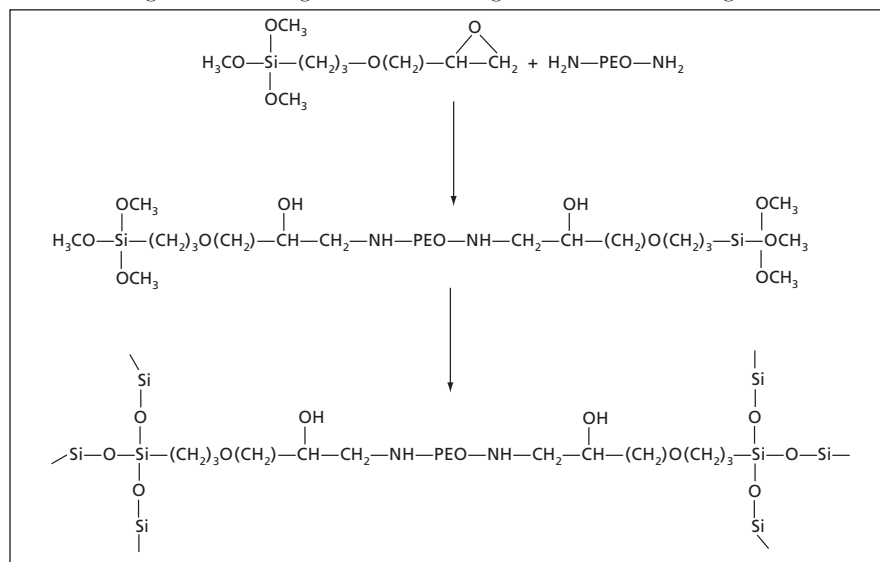


Figure 1. A **Molecular Network of Organic and Inorganic Moieties** is produced in this representative reaction sequence. The starting alkoxy silane and diamine can be other than the ones shown here.

use any of these diamines or any combination of them in proportions chosen to impart desired properties to the finished product. Alternatively or in addition, one could similarly vary the functionality of the alkoxy silane to obtain desired properties. The variety of available

alkoxy silanes and diamines thus affords flexibility to optimize the organic/inorganic polymer for a given application.

This work was done by James D. Kinder and Mary Ann B. Meador 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, Innovative Partnerships Office, Attn: Steve Fedor, Mail Stop 4-8, 21000 Brookpark Road, Cleveland, Ohio 44135. Refer to LEW-17592-1.

MoO₃ Cathodes for High-Temperature Lithium Thin-Film Cells

Cycle lives of these cathodes exceed those of LiCoO₂ and LiMn₂O₄ cathodes.

NASA's Jet Propulsion Laboratory, Pasadena, California

MoO₃ has shown promise as a cathode material that can extend the upper limit of operating temperature of rechargeable lithium thin-film electrochemical cells. Cells of this type are undergoing development for use as energy sources in cellular telephones, wireless medical sensors, and other, similarly sized portable electronic products. The LiCoO₂ and LiMn₂O₄ cathodes heretofore used in these cells exhibit outstanding cycle lives (of the order of hundreds of thousands of cycles) at room temper-

ature, but operation at higher temperatures reduces their cycle lives substantially: for example, at a temperature of 150 °C, cells containing LiCoO₂ cathodes lose half their capacities in 100 charge/discharge cycles.

The superiority of MoO₃ as a cathode material was demonstrated in experiments on lithium thin-film cells fabricated on glass slides. Each cell included a layer of Ti (for adhesion to the glass slide), a patterned layer of Pt that served as a cathode current collector, a cathode

layer of MoO₃, a solid electrolyte layer of Li_{3.3}PO_{3.8}N_{0.22} ("LiPON"), and an anode layer of Li. All the layers were deposited by magnetron sputtering except for the Li layer, which was deposited by thermal evaporation.

These cells, along with similar ones containing LiCoO₂ cathodes, were subjected to several tests, including measurements of specific capacity in charge/discharge cycling at a temperature of 150 °C. The results of these measurements, plotted in the figure, showed that whereas specific capacity of the cells containing LiCoO₂ cathodes faded to about half its initial value after only 100 cycles, the specific capacity of the cells containing the MoO₃ cathodes faded only slightly during the first few hundred cycles and thereafter not only recovered to its initial value but continued to increase up to at least 5,500 cycles.

This work was done by William West and Jay Whitacre of Caltech for NASA's Jet Propulsion Laboratory. Further information is contained in a TSP (see page 1).

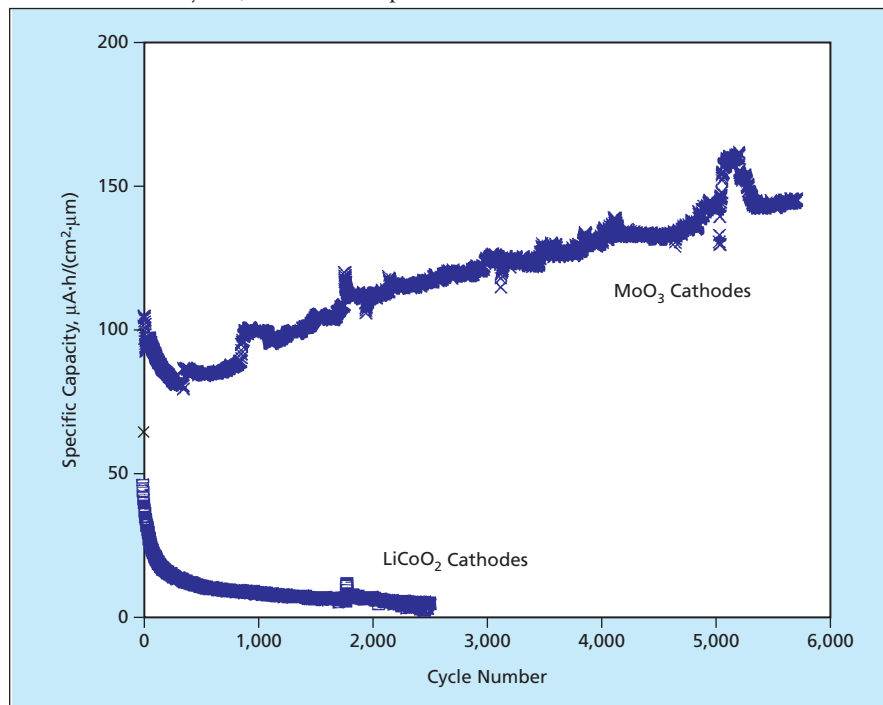
In accordance with Public Law 96-517, the contractor has elected to retain title to this invention. Inquiries concerning rights for its commercial use should be addressed to:

*Innovative Technology Assets Management
JPL*

*Mail Stop 202-233
4800 Oak Grove Drive
Pasadena, CA 91109-8099
(818) 354-2240*

E-mail: iaoffice@jpl.nasa.gov

Refer to NPO-41099, volume and number of this NASA Tech Briefs issue, and the page number.



The Specific Capacities and Cycle Lives of cells containing LiCoO₂ and MoO₃ cathodes at a temperature of 150 °C were measured in charge/discharge cycling at a current density of 0.7 mA/cm².