Stretch goals: Elastic conductors reach a new milestone

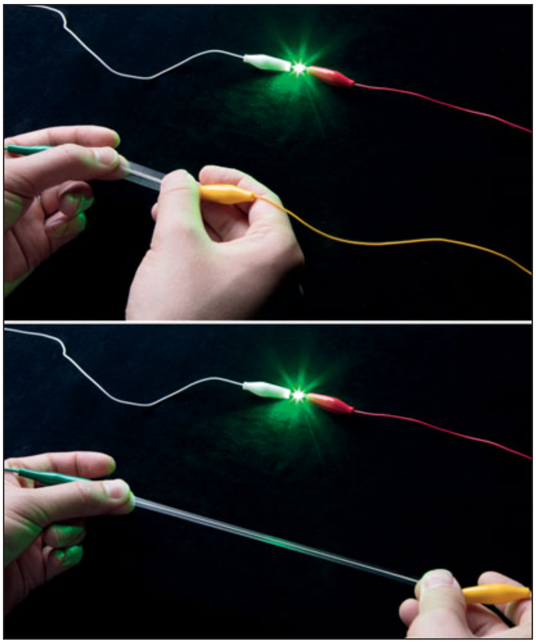
Sensitive elastic conductive materials that can withstand high strains due to stretching are critical for next-generation wearable devices and robotics. Printable elastic conductors are promising candidates for generating large-area, stretchable sensor/actuator networks. These conductors are typically composite materials comprising elastomers laced with metal nanoparticles. Although these composites can deliver high performance, their widespread use has been hampered by various processing challenges.

Now, researchers at The University of Tokyo have fabricated a new elastic composite material that retains its high conductivity even when stretched to five times its original length. This new material is made by printing an ink containing fluorine rubber, fluorine surfactant, silver flakes, and methylisobutylketone as the solvent. It can be printed in various patterns on textiles and rubber surfaces, and can be used as stretchable wiring for wearable devices with sensors.

Remarkably, the silver flakes—which are used as a low-cost conducting filler—transform into silver nanoparticles upon printing and heating of the ink (temperatures between 80°C and 150°C were studied). Electron microscopy revealed silver nanoparticles between two and ten nanometers in diameter, about 1000 times smaller than the original flakes. "We did not expect the formation of Ag nanoparticles," says lead researcher Takao Someya.

As reported in *Nature Materials* (doi:10.1038/NMAT4904), these printable elastic composites exhibit conductivity higher than 4000 S cm^{-1} at 0% strain, and 935 S cm^{-1} when stretched up to 400%—the highest conductivity reported to date for this amount of stretching.

The high performance of the conductor resulted from self-formation of silver nanoparticles one-thousandth the size of the Ag flakes that were formed after the conductive composite paste was printed and heated. The researchers say that the *in situ* formation of silver nanoparticles in the elastomer matrix improves the conductivity due to enhanced percolation between the silver flakes and the suppression of crack formation through nanoparticle reinforcement. Furthermore, by adjusting the molecular weight of the fluorine rubber, the team could control the distribution and population of nanoparticles, while the surfactant and heating accelerated particle formation and influenced their size.



A new elastic composite conductor demonstrates high conductivity that is maintained even while the material is stretched. For example, a light-emitting diode (top) continues to shine brightly even when stretched to five times its original length (bottom). Courtesy of Takao Someya, The University of Tokyo.

To test the viability of the elastic conductors, the researchers fabricated fully printed stretchable pressure and temperature sensors to sense weak forces and measure heat close to the body and the temperature of the room. These sensors were wired with the printable elastic conductors on textiles by laminating onto surfaces using a hot-pressing technique. The team showed that the sensors took precise measurements even when stretched by 250%.

This is enough to accommodate high-stress flexible areas, such as elbows and knees on conformable, form-fitting sportswear, or joints on robotic arms that have been designed to surpass human capabilities and thus undergo higher strain, the researchers say. The team is now exploring substitutes for silver flakes to reduce the cost, such as copper, and alternative polymers.

"We saw the growing demand for wearable devices and robots and felt it was very important to create printable elastic conductors to help realize the development of products," Someya says.

Aditi Risbud

2D electrocatalytic MOF sets efficiency record for water splitting

A two-dimensional nickel/iron metal–organic framework (2D NiFe-MOF), fabricated by researchers at the University of New South Wales in Sydney, Australia, has established a new record for efficient electrocatalytic water splitting. Published recently in *Nature Communications* (doi:10.1038/ncomms15341), this work expands the capabilities of MOFs to new applications in energy conversion and storage.

Scientists have only recently begun to develop MOFs, which are structures formed by linking metal clusters in a porous network using organic ligands, for applications such as electrocatalysis. "MOFs are generally believed to be poor electrocatalysts," says Chuan Zhao, whose group published the work. Traditional MOFs are usually insulating, lack diverse pore sizes to facilitate the transfer of materials, and degrade in water. Researchers must engineer MOFs that allow for the movement

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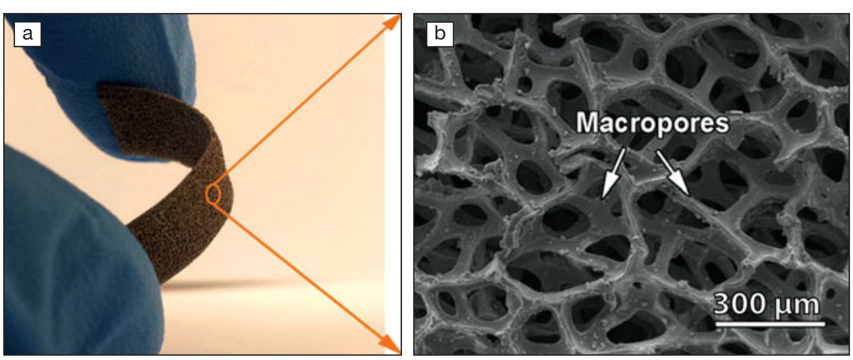
of charge, reactants, and products if these MOFs are to be used as electrocatalysts.

To create a MOF with these properties, Zhao's group devised a novel fabrication method that gave them control over many different factors. According to Sheng Chen, a research fellow in the Zhao group, "Our *bottom-up* growth method enabled us to manipulate the structure and morphology of the MOFs." Because of its 2D nature, more of the metal sites in the ultrathin NiFe-MOF are exposed and available as sites for catalysis during the electrochemical reaction. The NiFe-MOF designed by Zhao's group also has many different types of pores, like the intrinsic micropores and macropores between MOF layers (as seen in the Figure). This diversity in pore size allows electrolytes and gas molecules to diffuse through the MOF during catalysis. Thirdly, growing the NiFe-MOF directly on the electrode gives researchers more control over the final MOF-electrode architecture. This is the first demonstration of a 2D MOF being fabricated directly on a substrate. Lastly, this *bottom-up* approach is much simpler than other methods for creating 2D MOFs. "This synthetic approach is facile, universal, and adaptable for a range of MOFs and substrates," says Zongping Shao of Curtin University in Perth, Australia, who was not connected with the publication.

All of these factors combine to give this 2D NiFe-MOF its versatility and high performance. Electrocatalytic water splitting combines an oxygen evolution reaction at the anode with a hydrogen evolution reaction at the cathode. Zhao and Chen's 2D NiFe-MOF performs both of these reactions efficiently, significantly mitigating the energy losses caused by the slow kinetics of these reactions. Furthermore, an electrochemical cell with the 2D NiFe-MOF as both the cathode and anode showed excellent catalytic activity, producing a current density of 10 mA cm^{-2} at a voltage of 1.55 V. This activity is higher than that of most bifunctional catalysts, and is close to the activity demonstrated in standard precious-metal-based catalysts that are used as a benchmark for performance.

These results are only in their infancy, but researchers are excited about what this could mean for future MOF applications. "This could open up a new avenue for further tailoring and utilizing MOFs as high-performance electrocatalysts," Shao says. He would also like to see a more thorough understanding of how the substrate might affect the catalytic activity of the NiFe-MOF. Looking forward, Zhao says his group hopes to "expand MOF applications beyond water splitting" potentially addressing "challenging problems such as electro-reduction of carbon dioxide to generate liquid fuels."

Lauren Borja



(a) Optical and (b) scanning electron microscope image of the 2D nickel/iron metal–organic framework. Courtesy of Nature Publishing Group.

Universal fragment descriptor predicts materials properties

Luck as a means for scientific discovery is highly inefficient given that the possible number of materials is estimated to be around 10,100. Also, enormous piles of data are currently stored in vast repositories with no meaningful connections to each other. A group of researchers from The University of North Carolina at Chapel Hill (UNC) and Duke University has taken a significant step toward realizing a knowledge-based structure–property relationship that can predict properties given a few fundamental parameters of a material. They do this by applying machine learning techniques to such data, as reported in a recent issue of *Nature Communications* (doi:10.1038/ncomms15679).

At the heart of their approach is what they call a "universal fragment descriptor," which is essentially a labeled graphical representation of the unit cell of an inorganic material. For a given crystal, all the nearest neighbors are identified and a graph is constructed with atoms as the nodes and the bonds as edges. This infinite graph is then broken down to the simplest fragments that capture the local topology in a matrix. Combined with several chemical and physical properties of each atom, these graphs form property-labeled materials fragments (PLMFs) or a "colored graph" in graph theory terminology. The schematic for this construction is given in the Figure.

"Methodologically, we could apply this technique to any material, even amorphous solids," Olexandr Isayev of UNC, one of the researchers, told *MRS Bulletin*. "So far we are cautious to limit this method to stoichiometric materials. We are working now to extend this to include vacancies and doping, for example."

To test the predictive power of this new approach, the researchers used rigorous fivefold cross-validation as well as perspective prediction conformation with density functional theory calculations and experiments. In cross-validation, a data set is randomly partitioned into five

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