The researchers attributed this discrepancy to the existence of grain boundaries. They first constructed four typical grain boundaries observed in Li_3OCl and evaluated their corresponding energy. The results suggested that the formation of grain boundaries was more favorable in Li_3OCl than in perovskite oxides such as $SrTiO_3$. At normal battery operating temperatures (~0–150°C), all of these grain boundaries exhibited 0.05–0.30 eV higher Li-ion migration energy barriers than the grain-boundary-free bulk counterpart, which suggested that the grain boundaries impeded Li-ion migration. Because previous simulations do not take the grain boundaries into consideration, the simulations overestimate the true Li-ion conductivity in real Li_3OCl samples.

The researchers further developed a polycrystalline model and elucidated the relationship between Li-ion conductivity and the grain size of Li_3OCl. This relationship can guide future experimental studies by choosing the optimal conditions for the synthesis of solid electrolytes, as the grain size is closely related to the preparation methods.

Feng Lin of Virginia Polytechnic Institute, who was not involved in the study, says, "For practical polycrystalline solid electrolytes, grain boundaries are complicated due to dynamic evolution of local crystal orientation, defects, and secondary phase impurities. This study provides a nice nucleation point for future elaborate studies considering these practical factors, and will lead to better design of solid-state Li-ion batteries to eliminate the challenges related to ionic conductivity, area specific resistance, lithium dendritic growth, etc."

"Our approach provides valuable fundamental insights into the role of grain boundaries, which we are extending to other high-performance materials including LISICON and garnet-type solid electrolytes," Islam says.

Tianyu Liu

Bio Focus

Health monitoring reaches new heights with human trials of ingestible sensor

A sci-fi concept of an ingestible capsule to monitor human health is becoming a reality with the first human pilot trials, as reported in a recent issue of *Nature Electronics* (doi:10.1038/s41928-017-0004-x). This milestone is a joint effort between teams of Australian researchers at RMIT University, Monash University, and CSIRO.

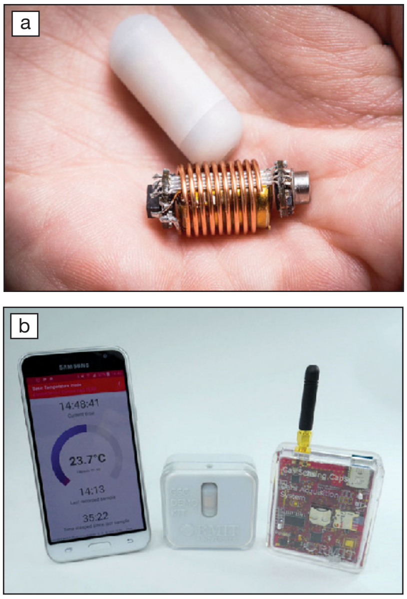
This research presents a turning point in the history of direct human health monitoring. The designed and tested ingestible capsule monitors oxygen (O_2), hydrogen (H_2), and carbon dioxide (CO_2) gases in the gut. The inside of the capsule consists of thermal conducting and semiconducting sensors that detect these gases.

Kourosh Kalantar-Zadeh, distinguished professor at RMIT University and director of the Centre for Advanced Electronics and Sensors, who is a lead researcher in this study, says, "H_2 appears in the pathway of most of the microbiome species of the gut." The microbiome (around 1.5 kg) and the human body are in a symbiotic relationship. The health of a human gut heavily relies on the correct performance of the microbiome. Kalantar-Zadeh says, "Correct function means a healthy H_2 profile." The H_2 profile changes in the range of detectability when the ecosystem of the microbiome changes, which makes it important to measure and monitor its profile in the gut. The O_2 levels vary in each organ, so its measurement provides information about the location of the capsule in the body. Oxygen gas content variation and its relation to the presence in an organ was confirmed through an ultrasound imaging technique.

In order to create benchmark profiles, the fiber content in the diet was varied in the trials to identify the effects of different fiber diets on the gas profiles. With the intake of a high fiber diet, the capsule resided in the stomach, small intestine, and large bowels for 12, 7, and 4 hours, respectively. A low fiber diet could retain the capsule for a longer period and the capsule remained in the stomach, small intestinal transit, and large intestine for 13, 5.5, and 54 hours, respectively. On the fourth day of the trial, dietary fiber was introduced to help release the capsule. The researchers conducted these tests on four healthy volunteers. The gas profiles were successfully obtained while modulating gut microbial fermentative activities with different fiber content in their diets. Experiments were successful in evaluating the small and large intestinal transit times.

Christopher J. Bettinger of Carnegie Mellon University praises this study. "Real-time monitoring of biomarkers in the GI tract is an exciting prospect. In this work, the authors create an ingestible microelectronic sensor that can monitor dissolved gases in the GI tract. The authors use chemical signatures to understand the composition of the microbiome. This device could be useful in many applications related to metabolic health," Bettinger says.

Rahim Munir



(a) Sensor-loaded capsule and the underlying sensor; (b) photo of the equipment including the phone app, capsule, and the data acquisition system. Credit: Prof. Kourosh Kalantar-Zadeh, RMIT University.