Building Batteries from the Microstructure Up
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Tires squeal before a loud crash. Car parts, antifreeze and glittering glass litter the street. Nearby, an iPad hits a sidewalk. Cracks erupt like a spider web across its screen.

We understand pretty well how everyday brittle materials – ones that crack after even tiny deformations – break. But scientists have a hazier picture of another vital fracture phenomenon: how brittle particles in lithium-ion batteries crack. These batteries power our modern world; they are ubiquitous in iPhones and electric cars alike. Their high power and ample charge capacity also make them contenders for large-scale energy storage. For example, Tesla Motors founder Elon Musk unveiled a system in April that can store solar energy in large household batteries to provide power day and night. Electric utilities can use similar devices to make renewable energy a more dependable option for millions of users. The battery market exceeds $100 billion annually, with lithium-ion grabbing an increasing share.

Despite our growing need for them, however, lithium-ion batteries aren't as safe or efficient as they could be. Recall the news stories about Tesla cars erupting into flames after minor collisions? And on a smaller scale, damage during manufacturing robs us of storage performance and prematurely shortens battery life.

What if the same techniques we use to model cracks in glass also could help make lithium-ion batteries safer and more powerful?

If we look deep inside them, we can see what's going on. There are two sides, the anode and cathode, represented by minus and plus signs. Each is made of a skeleton of particles, and lithium ions (Li^+ for chemistry folks) flow in one direction or the other, depending on whether the battery is charging or discharging. The cathode microstructure is made of millions of spherical particles of a brittle metal oxide containing materials such as lithium, cobalt, nickel and manganese.

The particles must be sandwiched between two metal sheets before the battery can be rolled into the familiar cylindrical shape. They're laid in a wet paste onto the sheet and pressed to the desired thickness.

This is where the problem begins: Because the cathode particles are so brittle, some crack under the pressure. The battery works by exchanging lithium ions between the cathode and anode and sending electrons to the outer plates. When particles crack and split, their interconnectivity weakens. If electrons have a harder time travelling through the cathode skeleton to the outer plate, then the battery doesn't store and supply as much power.

Cracks in the battery particles can get worse as the battery is used. During charging and discharging, the cathode particles correspondingly shrink and grow, causing some small cracks from the initial pressing to enlarge, splitting the particles. This is one reason battery life gets worse with age.

The standard method for computationally modeling battery microstructure geometry portrays each particle individually but at a low accuracy. Because there are millions of them, it's difficult to do more, and so these models imprecisely predict or represent events like particle cracking.

But by using computational failure models that simulate cracks on larger objects – like window panes and iPad screens – we can identify and predict loading cases that make lithium-ion battery particles fail. For our study, we have great experimental data of the cathode microstructure at different stages of manufacturing. We're also preparing an experiment to load individual particles and record their failure pressures and crack patterns. Comparing these tests to numerical models helps us fine-tune their input parameters. We can then evaluate how likely particular loads are to crack particles. With this information, we can evaluate alternative materials and manufacturing processes to reduce particle splitting, making batteries more powerful and efficient.

There's a great opportunity to improve lithium-ion batteries by developing and applying numerical models that simulate failure by cracking. This also improves mechanical modeling in a number of fields, enhancing technology development. Creating more powerful batteries will have far-reaching impacts on the consumer electronics and automotive industries of today and will enable development of industries we've never imagined tomorrow.