New computer modeling approach could improve material design across airframes

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How do jumbo jet designers develop resilient materials for modern airframes, while still bringing in their projects on time and on budget? Before they prototype a new material, they depend heavily on computer simulations to indicate how it will perform—and scientists at the National Institute of Standards and Technology (NIST) are making those simulations more effective.

A team including NIST scientists has found a way to improve the process of simulating the onset of failure in the materials used to build airplane wings. Understanding this initiation point is critical for predicting when and how wings fail. Their method shows designers how to put a particular sample through a series of stress scenarios to efficiently determine the amount of stretching that will cause it to break.

The approach, according to NIST physicist Paul Patrone, could help address one of the key factors that reduces the effectiveness of simulations—uncertainty in their prediction of the wing's strength.

"Probably the most dramatic material property that aerospace engineers and the public care about is how far a wing can bend before it breaks," said Patrone. "Historically, simulations have done a poor job at predicting this because you need detailed information about the material's atomic structure over large distances. Computers simply aren't powerful enough to simulate such systems, so we're hoping that this new approach will provide a workaround."

Developing a new high-performance composite is a laborious process. Aerospace companies dream up large numbers of candidate ingredients, narrow the list down to a promising few, and then mix those together in combinations that might give the strongest material. But an R&D department can't mix them all or run stress tests on very many. So they sometimes turn to NIST to find ways of getting effective results quickly.

One approach has been to directly simulate the force required to bend a sample, but not of an entire wing made of it—just of a few thousand atoms. "It's possible to run 50 of these simulations a week on a supercomputer," Patrone said, "and in principle, that helps engineers zero in on the combinations that are worth testing in the lab. The problem is that we have to infer the damage initiation indirectly from the simulated forces, which simply doesn't work well for such small systems."

The team's paper shows companies a better way to design these simulations. They hit upon a simple but effective idea: Simulate deforming this tiny bit of material by increasing amounts and make it possible to save the state of the simulation at any given point. The advantage of state-saving, Patrone said, is that you can see what happens if the material is allowed to relax.

"It's kind of like taking the material down a road with different forks and looking at what happens down each one," he said. "We pause the simulation at different points along the way and ask, 'If I stopped trying to bend this, what would happen? Would it stay bent, or bounce back to its original shape?' We have the ability to explore all these forks, which allows us to more precisely state when the material was first damaged."

Because a new jumbo jet can run up several billion dollars in

development costs, Patrone said, improvements like this can help companies trust the reliability of their modeling approaches before they commit to more expensive steps involving real-world materials.

"Our approach provides a new 'signal' for a material's breaking point that will hopefully improve the reliability of the simulations," he said. "It also allowed us to statistically quantify our confidence in their predictions. We need that, if simulations are to be used as a proxy for experiments."

More information: Paul N. Patrone et al. Estimating yield-strain via deformation-recovery simulations, *Polymer* (2017). DOI: 10.1016/j.polymer.2017.03.046

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