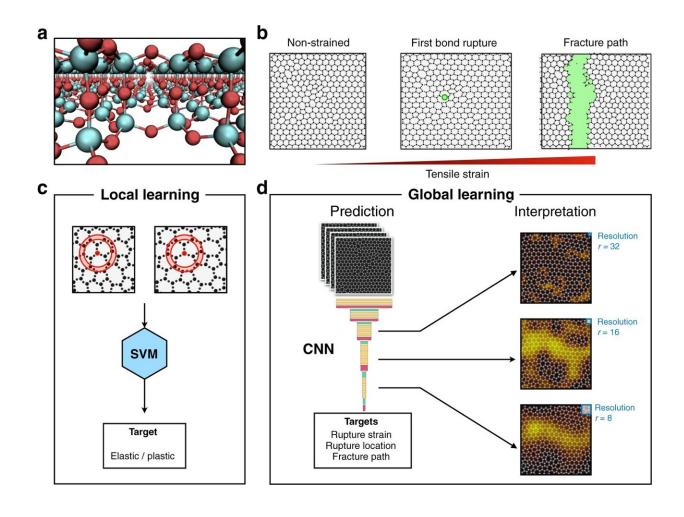


## Using AI to predict when and where glass will break

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Schematic of system and algorithms. a) Perspective view of the silica glass bilayers: silica atoms are colored in cyan and oxygen ones in red. b) Schematic representation of the fracture formation under increasing tensile strain from left to right: non-strained (left panel), first plastic event corresponding to a bond breaking (central panel) and crack path (right panel). c) Local learning approach that uses Support Vector Machine to predict the elastic/plastic nature of



individual atoms. d) Global learning approach which uses a ResNet model to predict rupture strain, location and the full crack path. The approach also allows for the interpretation of the model decisions using attention maps (right side of panel). Credit: *Nature Communications* (2022). DOI: 10.1038/s41467-022-30530-1

The ability to predict when materials will fracture is of immense importance for industrial applications—companies can use this information to maintain devices and components more efficiently and cost effectively. A research team from FAU and the University of Milan has demonstrated that artificial intelligence can predict when quartz glass will fracture based on information learned from images of its atomic microstructure. The researchers have published their results in the journal *Nature Communications*.

Glass is a non-crystalline solid and in contrast to solid crystalline materials, its atoms are not arranged consistently. This makes it more difficult to predict when glass will break: where there is no defined order, it is difficult to detect the first signs of disorder—an important sign that the crystalline material will soon fracture. Thanks to the latest developments in deep learning with artificial intelligence, researchers can now reliably predict when glass is likely to break.

Scientists are not yet able to explain how the AI system achieves its results and which parameters are being considered and focused on, which is a common problem in <u>artificial intelligence</u> research. "Neural networks are <u>black boxes</u>," explains Prof. Dr. Stefano Zapperi from the University of Milan who was a guest researcher at FAU for one year after receiving the Humboldt Prize. "This is an important limitation in scientific research which is tasked with explaining the causes of a specific phenomenon."



To solve this problem, the researchers are using a method to identify the areas of the microstructure image most often used by the <u>neural</u> <u>networks</u> to predict the fracture.

"Neural networks try to imitate the brain. We also don't always understand how the brain reaches a certain result. But in humans, at least we can observe behavior such as eye movement, which may explain how a certain decision is reached," explains Michael Zaiser, Professor of Material Simulations at FAU and co-author of the study. "We took a similar approach to our problem and investigated points that attracted the attention of the neural network, essentially following what it is looking at."

This method allowed the researchers to investigate local parameters that influence fracturing behavior. "Thanks to this method, we were able to identify and better understand aspects that cause glass to break and not only predict when glass is likely to fracture but also gain fundamental insights into the mechanics of glass materials," says Stefano Zapperi. "The strategy that we have developed can be applied to further applications," adds Michael Zaiser "for example in designing related materials with better fracture resistance."

**More information:** Francesc Font-Clos et al, Predicting the failure of two-dimensional silica glasses, *Nature Communications* (2022). DOI: 10.1038/s41467-022-30530-1

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