International study identifies the process of rock formation by meteor strikes or nuclear blasts

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Coesite is a polymorph of silica that only forms under extremely high pressure—10,000 times more, on average, than normal atmospheric pressure. The presence of coesite indicates either that material has pushed up through Earth's crust from the mantle, or that a comet, meteor or meteorite struck the site. Coesite can also be created in nuclear explosions.

The mechanism whereby silica (SiO2) is transformed into coesite is poorly understood by the scientific community. It has now been elucidated by atomistic computer simulation in a study conducted by researchers affiliated with the University of São Paulo (USP) in Brazil, the Chinese Academy of Sciences in Hefei, China, and the Abdus Salam International Center for Theoretical Physics in Trieste, Italy.

The article, "Multiple pathways in pressure-induced phase transition of coesite," was published in *Proceedings of the National Academy of Sciences* (*PNAS*).

"Coesite is silicon dioxide. Its chemical composition is the same as that of quartz. The difference is that high pressure destructures the crystal lattice characteristic of quartz and compresses the silicon and oxygen atoms into an amorphous system. The result is high-density glass. Once the pressure has surpassed a certain threshold, the amorphization process becomes irreversible and the material can no longer return to a crystalline configuration," said Caetano Rodrigues Miranda, a professor at the University of São Paulo's Physics Institute (IF-USP) and lead author of the article.

There are commercial applications of the findings, but for now, the main interest is to use them as markers of high-pressure scenarios. "Coesite is the characteristic 'signature' of these scenarios," said Miranda.

In the study, the researchers resolved divergences that existed with regard to the transformation of coesite into other phases (a high-pressure octahedral phase, coesite-II and coesite-III) and arrived at a model consistent with the observational data. They also described the molecular mechanisms associated with these transformations. "It would be very difficult to reproduce in the lab the high-pressure conditions found in Earth's mantle," Miranda said. "We used a computer simulation, describing the interactions among atoms as realistically as possible, and mapping, step by step, the transformations resulting from pressure changes."

The best way to follow this evolution is via the Raman effect, observed experimentally in 1928 by Indian physicist Chandrasekhara Venkata Raman (1888-1970). The Raman effect relates to the inelastic scattering of light by matter. When a sample is excited by a laser pulse, most of the photons are scattered elastically, i.e., at the same frequency as the incident photons, by the molecules or atoms in the material. However, a small portion of the photons scatters inelastically, generally at a lower frequency. Analysis of this inelastic scattering by means of Raman spectroscopy determines the composition and structure of the material. "You could say it provides the material's fingerprint," Miranda said.

The researchers performed molecular dynamics simulations of the Raman spectrum for the different structures of coesite under various pressures. They obtained correlations between the structure of the material and the external pressure, mapping step by step the multiple paths in the transformation of coesite until it was completely amorphized, or those in the crystalline phases of silica under high pressure.

"Each structure displays a very characteristic pattern in the Raman spectrum," Miranda said. "As the structure changes owing to pressure variation, this pattern also changes. And this enables us to know which structures are present and how they are transformed under pressure. A comparison with experimental results validates the model adopted.

"Bond lengths and angles, as well as atomic vibrational modes, are variables supplied by the procedure. Although it's an amorphous structure and has a much less regular configuration than quartz, for example, which is crystalline, coesite has a characteristic fingerprint in Raman spectroscopy.

"In a crystal, the distances between lattice atoms and the angles made by the segments bonding the different atoms are always the same. This produces a clearly defined peak in the spectrogram. As the material amorphizes, the peak changes into an elongated plateau."

An interesting study performed by Miranda in parallel consisted of the "sonification" of the spectral data collected. In this case, "sonification" entailed converting the high frequencies characteristic of light into low frequencies typical of sound. "Sonification allows you to use hearing instead of sight to analyze data. From the scientific perspective, the advantage of this procedure is that when you hear sounds, you can identify small variations or more complex data more precisely. They're easier to hear than to see. In addition, there's an advantage from the artistic standpoint: music can be composed using the sound fragments obtained. So a bridge can be built between science and art," Miranda said (click to hear audio).

The discovery of coesite in the Chicxulub Crater under the Yucatan Peninsula in Mexico was significant evidence that this geological formation resulted from the impact of a comet or large asteroid. The circular crater has a diameter of more than 180 km, and is buried deep below the surface of the peninsula. It was discovered in the late 1970s by Antonio Camargo (Mexico) and Glen Penfield (United States), geophysicists who were prospecting for oil. In 1990, Penfield obtained samples of rock formed under high pressure that suggested it was an impact feature.

In 2016, scientists drilled hundreds of meters below the ocean floor into the peak ring of the crater, obtaining samples of coesite and other rocks, and all but closing the debate by supplying robust evidence that it was indeed an impact crater.

The impact that produced the crater was two million times more powerful than the largest nuclear device ever tested, a 58-megaton hydrogen bomb known as Tsar Bomba, detonated by the Soviet Union in 1961.

The date of the impact, estimated at slightly less than 66 million years ago, converges with the hypothesis that worldwide climate disruption in this period caused a mass extinction event in which 75 percent of plant and animal species on Earth suddenly became extinct, including all non-avian dinosaurs. The impact would have caused a mega-tsunami and a colossal shock wave, followed by earthquakes, volcanic eruptions, wildfires and other phenomena on a global scale, including a cloud of dust and aerosols covering the entire planet for over a decade.

More information: Wei Liu et al, Multiple pathways in pressure-induced phase transition of coesite, *Proceedings of the National Academy of Sciences* (2017). DOI: 10.1073/pnas.1710651114

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