# Study explains role of certain types of oxide in the structure and development of specialty glass

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Non-homogeneous glass with color elements concentrated in certain regions. Credit: Nilanjana Shasmal/CeRTEV

A study conducted at the Center for Research, Education and Innovation in Vitreous Materials (CeRTEV) in São Carlos, São Paulo state, Brazil, shows for the first time that including niobium oxide ($Nb_2O_5$) in silicate glass results in silica network polymerization, which increases bond density and connectivity, enhancing the mechanical and thermal stability of specialty glass.

The study was reported in an article published in the journal *Acta Materialia*.

The first author of the article, Henrik Bradtmüller, is a postdoctoral researcher at the Federal University of São Carlos's Center for Exact Sciences and Technology (CCET-UFSCar). His supervisor is Edgar Dutra Zanotto, director of CeRTEV and last author of the article. CeRTEV is hosted by UFSCar.

"Our study combined experimental observations using nuclear magnetic resonance spectroscopy and Raman spectroscopy with computational modeling. Besides the results mentioned, we found that higher levels of niobium led to $Nb_2O_5$, clustering, and heightened electronic polarizability, with a significant impact on the optical properties of the glass," Bradtmüller said.

It is worth recalling that Raman spectroscopy provides precise information on the molecular structure of materials, while nuclear magnetic resonance (NMR) spectroscopy additionally explores the magnetic properties of their atomic nuclei.

"Our strategy based on these two observational techniques plus computational modeling can be used to study functional elements of many other types of glass, including optical materials, bioactive glass and glassy fast-ion conductors. This will facilitate the development of innovative glass formulations adapted for various applications," Bradtmüller said.

Alongside the everyday applications of ordinary glass in containers, windows and so on, high-quality glass has also become almost ubiquitous in today's world, Bradtmüller noted. It is present in the microscopes and telescopes used by scientists, for example, in the optical fibers used to carry data and power, and in the glass-ceramic orthotic devices increasingly used in medicine. "In recognition of the role played by glass in contemporary society, the United Nations declared 2022 to be the International Year of Glass," he said.

For advanced high-tech applications, materials scientists are using machine learning software and other computational resources to design glass with customized properties, but to do so they require reliable databases and structural parameters that take into account the physicochemical complexity of glass.

This is the relevance of the study by Bradtmüller and colleagues. "Glass intermediate oxides play a strategic role in this new technological moment. They don't form glass under standard cooling in the laboratory, but they can make a positive contribution in the presence of other oxides by helping to build oxygen bridges and giving glass the properties of interest. Niobium oxide is a good example," he explained.

Glass that contains niobium (Nb) is valued for its non-linear optical properties, with potential applications in optoelectrical devices, and for mechanical properties relevant to the fabrication of bioactive materials. "Although studies had been conducted using $Nb_2O_5$ before our own, the structural role of Nb remained obscure, owing mainly to lack of systematic spectroscopic characterization data. We set out to fill this knowledge gap in our study," he said.

"We discovered through spectroscopy that the addition of Nb causes 'polymerization' of the silica-oxygen network, increasing the connectivity of the glass's components. This clarified the role of Nb as a 'network former'. Another highlight of the study is our demonstration that a new NMR technique we developed in 2020 using other materials is applicable to glass. This technique, which is called W-RESPDOR, can be used to measure the distance between two elements—in this case, lithium and Nb, which has such a challenging nucleus that it had never been measured with similar techniques."

Computational modeling showed that lithium ions are randomly distributed in silica-based glass at the nanometric scale (5–10 nanometers), while Nb tends to form clusters at higher concentrations of $Nb_2O_5$, he explained, adding that this kind of structural arrangement had never been reported in the literature and is an original contribution of the study.

"In a broader perspective, the study points to an experimental and computational strategy to investigate the role played in glass by intermediate oxides with active nuclei for NMR spectroscopy," Zanotto said.

**More information:** Henrik Bradtmüller et al, Structural impact of niobium oxide on lithium silicate glasses: Results from advanced interaction-selective solid-state nuclear magnetic resonance and Raman spectroscopy, *Acta Materialia* (2023). DOI: 10.1016/j.actamat.2023.119061

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