

Universidade de São Paulo Instituto de Física de São Carlos

Semana Integrada do Instituto de Física de São Carlos

13^a edição

Livro de Resumos

São Carlos
2023

Ficha catalográfica elaborada pelo Serviço de Informação do IFSC

Semana Integrada do Instituto de Física de São Carlos
(13: 21-25 ago.: 2023: São Carlos, SP.)

Livro de resumos da XIII Semana Integrada do Instituto de Física de São Carlos – Universidade de São Paulo / Organizado por Adonai Hilário da Silva [et al.]. São Carlos: IFSC, 2023.
358p.

Texto em português.

1.Física. I. Silva, Adonai Hilário da, org. II. Título.

ISSN: 2965-7679

PG33

Incorporation of niobium into photonic glasses: new structure/function relations uncovered by advanced magnetic resonance techniques

HERNÁNDEZ, Laureano Javier Ensuncho¹; BRADTMÜELLER, Henrik²; ECKERT, Hellmut¹

laureanoensuncho@usp.br

¹Instituto de Física de São Carlos – USP; ²Universidade Federal de São Carlos - UFSCar

While niobium-containing oxide glass are used in several technological applications, especially for high-resolution augmented reality devices, the exact structural role of niobium (Nb), which can serve either as a network modifier or as a network former, in these glasses is still ill-understood. Solid-state nuclear magnetic resonance (NMR) has been proven to be a powerful tool for structural elucidation of glasses, due to its element-selectivity, inherently quantitative character, and its focus on local order. (1) From the NMR point of view, Nb features one of the most NMR-sensitive nuclei (⁹³Nb) which is 100% natural abundant. Nevertheless, it suffers from a large nuclear quadrupolar moment, and the ⁹³Nb NMR spectra are dominated by strong quadrupolar interactions, resulting in excessive line broadening and poor resolution. These challenges can be addressed by techniques involving fast Magic angle spinning (MAS), wideband excitation methods and dipolar recoupling techniques. (2) Here, we report results on glasses from the structurally more simple niobium phosphate glasses in the system $xNb_2O_5 - (1 - x)NaPO_3$. Advanced NMR experiments have been used to characterize the local environments of sodium, phosphorus and niobium with the aim of obtaining new structural insight towards the development of new structure-function correlations. As first results, ⁹³Nb MAS NMR and Raman spectroscopy suggest that Nb is pentavalent and six-coordinated.

Palavras-chave: NMR. Phosphate glass. Niobium

Agência de fomento: FAPESP (2022/01937-5)

Referências:

- 1 ZHANG, R. *et al.* Structural studies of Bi₂O₃–NaPO₃ glasses by solid state nuclear magnetic resonance and x-ray photoelectron spectroscopy. **Journal of Physical Chemistry C**, v. 121, n. 18, p. 10087-10094, 2017.
- 2 KOPPE, J.; HANSEN, M. R. Minimizing lineshape distortions in static ultra-wideline nuclear magnetic resonance of half-integer spin quadrupolar nuclei. **Journal of Physical Chemistry A**, v. 124, n. 21, p. 4314-4321, 2020.