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▶ To cite this version:

Hadi Loutfi, Geneviève Tastevin, Pierre-Jean Nacher, Andrey Stanislavovas, Vyacheslav Kuzmin, et al.. Gas diffusion and relaxation within ordered Al2O3 aerogels. European Magnetic Resonance Meeting EUROMAR 2023, Jul 2023, Glasgow (Ecosse), United Kingdom. https://euromar2023.org/abstract-book/. hal-04334265

HAL Id: hal-04334265

https://hal.science/hal-04334265

Submitted on 10 Dec 2023

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Gas diffusion and relaxation within ordered Al₂O₃ aerogels

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Introduction: Gas diffusion in nanoporous materials correlates with key properties for applications. NMR studies of diffusion and magnetic relaxation in ordered Al₂O₃ aerogels are jointly made [1] at low temperature in Kazan and room temperature in Paris.

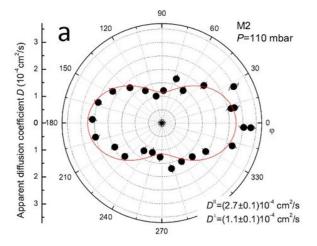
Aim: Strongly reduced ³He gas diffusion and diffusion anisotropy (Fig. a) were found in ordered aerogels at 4.2 K [1]. Data deviate from expectations within Knudsen models. This behaviour was attributed to the action of the aerogel wall attractive potential on gas atom dynamics. The hereby reported room temperature studies may confirm this scenario.

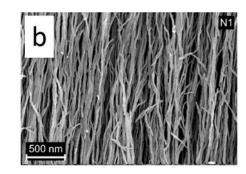
Methods: 3 He gas is laser-polarised (at ~1 mbar) for high sensitivity, then compressed into a low- or medium-density [2] aerogel sample (Fig. b). Each measurement uses a few mbar of 3 He mixed with 0-1 bar of buffer gas. NMR is performed at 1.3 mT, using pulsed gradients and CPMG sequences or small flip angles for T_2 or T_1 measurements, respectively. Experimental details for low temperature studies are given in [2].

Results: Polarisations of $\sim 50\%$ typically yield SNRs of ~ 1000 . Very long relaxation times (minutes) are achieved with no applied gradients. Changes in T_2 with gradients and timings are investigated and effective diffusion coefficients D_{eff} are inferred (Fig. c). Results on the pressure and orientation dependence of D_{eff} will be presented and discussed, as well as data for gradient-induced T_1 s.

Discussion: Hyperpolarisation provides excellent sensitivity for ³He NMR, even at low gas pressure and weak magnetic field. Polarisation is well preserved in Al₂O₃ aerogel samples thanks to slow wall relaxation on this material. Final conclusions on actual processes restricting gas diffusion are expected to be derived from data obtained with aerogels of different densities and comparison with low-temperature results and with suitable numerical models.

- [1] MARGIN project: anr.fr/Projet-ANR-19-CE30-0023
- [2] Kuzmin et al., doi.org/10.1021/acs.jpcb.2c08251





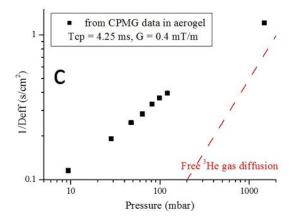


Fig. 1 a: Diffusion anisotropy of ³He gas in compressed Al₂O₃aerogel at 4.2 K [1].

b: SEM images of uncompressed aerogel [1].

c: Example of pressure dependence of diffusion coefficients in aerogel at room temperature.