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TDPAC in Molybdenum Oxide Complexes Revisited

Anastasia Burimova[1*], Katiusse Soares Souza[1], Rajendra Narain Saxena[1], Artur Wilson Carbonari[1]

[1]Nuclear and Energy Research Institute, IPEN-CNEN/SP, São Paulo, Brazil

[*] anstburimova@gmail.com

Time Differential Perturbed Angular Correlation (TDPAC) spectroscopy, utilizing Mo-99 and In-111 probe parents, has been extensively applied to investigate local effects and defects in molybdenum oxides (MoO_x) [1, 2]. However, the preparation techniques and pre-measurement treatments of samples, which induce probe incorporation, may significantly influence their stoichiometry and structural characteristics. Furthermore, due to the layered nature of MoO_3, probe atoms can occupy interstitial sites [3], complicating the interpretation of hyperfine data. In this study, we present a new series of TDPAC measurements obtained for nominal MoO_3 samples using an In generator that allows tracing probe diffusion. We critically summarize and discuss alternative interpretations of these new data sets, supporting our analysis by comparisons with complementary TDPAC experiments involving Mo-based chelates.

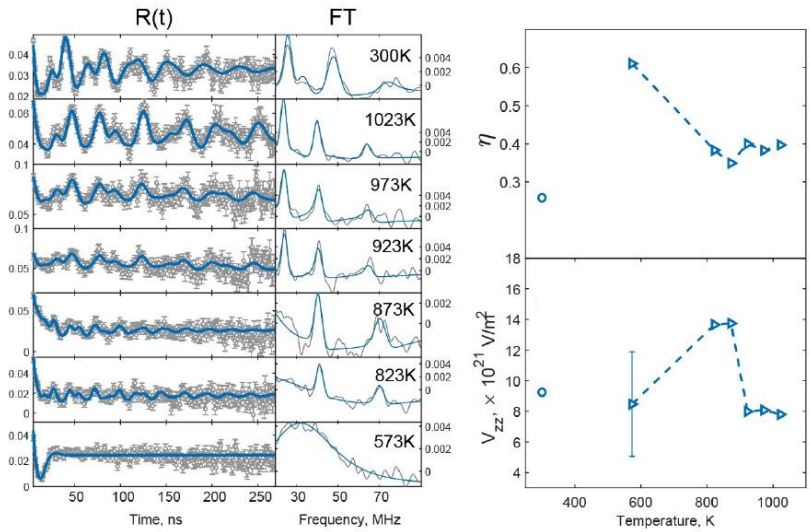


Figure 1. TDPAC R(t) of nominal α-MoO_3 collected at different temperatures with radioactive ^{111}In tracer and their Fourier Transforms (left), evolution of hyperfine parameters on heating (right). The RT data was obtained after cooling (◦).

[1] T. Butz et al., *Hyperfine Interact.* **15/16** (1983) 915.
[2] F. G. Requejo et al., *Physica Status Solidi* **116** (1989) 503.
[3] A. M. Gerami et al., *Phys.l Rev. Mater.* **7** (2023) 033603.