# Modelling of nanopore size distribution in humidity-sensitive ceramic materials

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***Abstract*** **The modelling of nanosize pore distribution in nanoporous humidity-sensitive is performed using the Tao-Eldrup model. It is shown that this model is adequate for modelling "pick-off" annihilation processes in ceramic materials for sensors applications and calculation of the size of their nanopores.**

***Keywords*** **nanopore size modelling, "pick-off" process, mathematical model.**

## I. INTRODUCTION

Nanoporous humidity-sensitive nanosstructured $MgAl_2O_4$ ceramics are known to be perspective materials for sensors electronics [1]. Because of significant complications in the microstructure of these ceramics, the further progress in this field is dependent on the development of new characterization techniques, which can be used in addition to traditional ones. This concerns, in part, the positron annihilation lifetime (PAL) spectroscopy, the method recently applied to ceramics.

The main channels of positron annihilation in these materials could be ascribed to positron trapping and ortho-positronium (o-Ps) decay modes. In terms of this model, the largest component is responsible for a so-called o-Ps "pick-off" annihilation. To study of o-Ps "pick-off" annihilation processes in ceramics, the mathematical model is needed for adequate describing and modelling nanostructured pores in this humidity-sensitive materials. Such model can be Tao-Eldrup model.

## II. TAO-ELDRUP MODEL

It assumes that o-Ps trapped inside the spherical free volume may decay pontaneously by three quantum annihilation or by "pick-off" process. The Tao-Eldrup model [2] was elaborated for small free volumes, like vacancies in solids, voids in polymers, bubbles forced by Ps in liquids. In that case the spacings of energy levels in small voids are much larger than thermal energy and thus only the lowest level is populated; positronium wavefunction for this state is spherical Bessel function. In order to simplify the calculations, the well of finite depth is substituted by infinitely deep one but broadened by, which is needed to reproduce the value of in finite well depth and radius:

$$P = 1 - \frac{R}{R+\Delta R} + \frac{1}{2\pi}\sin\left(\frac{2\pi R}{R+\Delta}\right). \qquad (1)$$

The results of calculation for cubic geometry can be compared to spherical (or cylindrical) ones for $a = 2(R+\Delta)$.

## III. PAL MEASURING AND NANOPORE SIZE MODELLING

Taking into account the model for PAL in ceramic materials, the third and fourth component with lifetime $\tau_3$ and $\tau_4$ is due to "pick-off" annihilation of o-Ps in the nanopores [3]. The size of nanopores for spinel-structured $MgAl_2O_4$ ceramics modelling and calculation with Tao-Eldrup model using $\tau_3$ and $\tau_4$ lifetimes is shown in table 1.

TABLE I

O-PS LIFETIME AS FUNCTION OF PORE SIZE

| o-Ps life-time, ns | Geometry/Pore size, nm | | |
|---|---|---|---|
| | spherical | cubic | cylindrical |
| 2.03-1.94 | ~0.31 | ~0.28 | ~0.2 |
| 48.4 | ~1.80 | ~1.70 | ~1.4 |
| 40.8 | ~1.55 | ~1.45 | ~1.2 |
| 42.4 | ~1.60 | ~1.50 | ~1.3 |

The size of nanopores for $MgAl_2O_4$ ceramics in spherical, cylinder, cubical and cuboidal approximation was modelling and calculated using Tao-Eldrup model in accordance with Fig. 1. The values of the lifetime of the third and fourth components were used for calculation of the nanopores size.

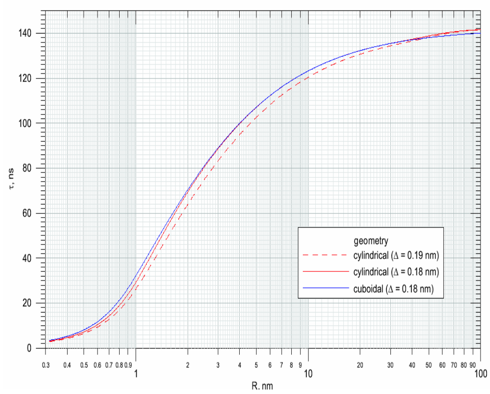


Fig. 1. o-Ps lifetime as function of pore size in the range of large free volumes for capillaries with circular and square cross section

## IV. CONCLUSION

Thus, the Tao-Eldrup model can be application to modeling and calculation of nanopore size in ceramic materials for sensors electronics.

## V. ACKNOWLEDGEMENTS

This work has been supported from Lviv Polytechnic National University (Grant for young scientist GLP 13/3).

## VI. REFERENCES

[1] Traversa, E.: "Ceramic sensors for humidity detection", Sens. and Actuat. B. vol. 23, 1995, pp. 135-156.

[2] Zaleski, R.: "Positronium lifetime vs. temperature and free volume size", Lublin (2002) p.20.

[3] Klym, H., Ingram, A.; "Unified model of multichannel positron annihilation in nanoporous magnesium aluminate ceramics", Journal of Physics: Conf. Ser., 2007, v. 79, p. 012014-1-6.