Modelling of o-Ps "pick-off" Annihilation Process in Nanoporous Ceramics for Sensor Electronics

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Abstract – **The modelling of ortho-positronium annihilation processes in nanoporous humidity-sensitive ceramics were 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 – **"pick-off" process, nanopore size modelling and mathematical model.**

I. INTRODUCTION

Nanoporous spinel-structured $MgAl_2O_4$ 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 because significant complications in correct interpretation of the obtained data.

Early was shown, that the main channels of positron annihilation in these materials could be ascribed to positron trapping and ortho-positronium (o-Ps) decay modes, the best fitting being achieved using at least three independent components in the resolved lifetime spectra. 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 $MgAl_2O_4$ 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. THEORETICAL APPROACH OF TAO-ELDRUP MODEL

Since 20 years the relation between o-Ps lifetime and free volume size has been determined using the Tao-Eldrup model [2]. 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 was elaborated for small free volumes, like vacancies in solids, voids in polymers, bubbles forced by Ps in liquids. 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 radius.

III. EXPERIMENTAL

The studied ceramics were prepared from Al_2O_3 with specific surface area of 67 m^2/g and $4MgCO_3 \cdot Mg(OH)_2 \cdot 5H_2O$ with specific surface area of 12.8 m^2/g. The pellets are sintered in a special technological regime with maximal temperatures T_s of 1200, 1300 and 1400 °C during 2 h.

The PAL measurements with a full width at half maximum of 270 ps were performed with an ORTEC spectrometer using ^{22}Na source placed between two sandwiched samples as it was described in more details elsewhere.

IV. RESULTS AND DISCUSSION

Taking into account the model for PAL in ceramic materials, the shortest lifetime component in the studied ceramics reflects mainly the microstructure specificity of the spinel with character octahedral and tetrahedral cation vacancies. The second component with lifetime τ_2 corresponds to extended defects near intergranual boundaries. The third and fourth component with lifetime τ_3 and τ_4 is due to "pick-off" annihilation of o-Ps in the nanopores. These changes are connected with more branched structure of the open pores of the ceramics sintered at higher T_s.

The size of nanopores for spinel-structured $MgAl_2O_4$ ceramics modelling and calculation with Tao-Eldrup model using τ_3 and τ_4 lifetimes is shown in table 1.

TABLE 2

O-PS LIFETIME AS FUNCTION OF PORE SIZE

o-Ps life-time, ns	Pore size, nm					
	Geometry			Geometry		
	spherical		cubic	cylindrical		Cuboidal
	Δ= 0.166 nm	Δ= 0.18 nm	Δ= 0.18 nm	Δ= 0.19 nm	Δ= 0.18 nm	Δ= 0.18 nm
2.03						
1.98	~0.28	~0.31	~0.28	~0.25	~0.2	~0.22
1.94						
48.4	~1.60	~1.80	~1.70	~1.52	~1.4	~1.35
40.8	~1.40	~1.55	~1.45	~1.30	~1.2	~1.17
42.4	~1.45	~1.60	~1.50	~1.36	~1.3	~1.20

V. CONCLUSION

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

REFERENCES

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