MS37-P5 **Surface Structural Inhomogeneities And Fractal Properties of MnO_2 Semiconductor Thin Films**

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The significant influence of fractal layer on electrical characteristics of MDS capacitors was reported earlier. This feature as well as the developed surface microrelief ob MnO_2 films are responsible for the interest in investigating the fractal properties of this compound.The theory of scattering by a porous solid was developed by Wong [1], and the theory main formula is as follows :$I(q) \sim$ constant x q^{-D} .(Here D is the surface fractal dimension that shows fractal behavior).

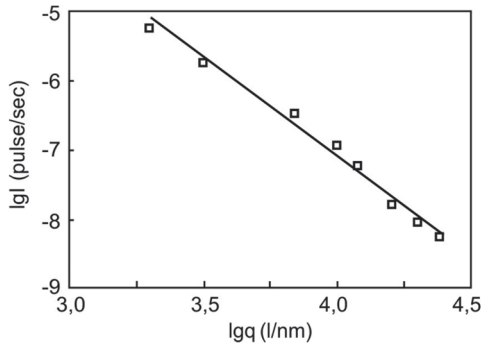

Fig. 1. Logarithmic dependence of the SAXS intensity I *vs* the wavevector q for the smiconductor layer: (▉) – experimental data; (_)- approximation to the linear range.

On the graph, the coefficient of the curved part slope, which can be closely approximated by line á, (Fig.1) is:

$$\alpha = -dlgI(q)/dlgq = 2.87 \qquad (1)$$

Comparison result (1) with the Wong's formula (1) gives (for $\alpha = D$) the value of D=2.87. Obtained D value coincides with the previously [1] found value of surface fractal dimensionality in a sintered niobium powder pellet with high accuracy, D =2,81.

References

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MS39-P1 **Peak broadening effects from nanocrystallite material: modeling of average shape.**

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Crystallite shape in powder samples has a pronounced effect on X-Ray diffraction maxima. Broadening of diffraction peaks is inversely proportional to crystallite size, and materials with nanoparticle size cause substantial broadening of the maxima [1]. In the case of anisotropic crystallite shape the broadening is diffraction-vector dependent. In order to correct for this effect in Rietveld refinement, the quadratic formalism can be used. When applied correctly this formalism results in more reliable crystal structure parameters and at the same time physically realistic average dimensions of crystallites and their crystallographic orientation [2]. The method has been demonstrated on patterns of nanosized materials by full pattern fitting and confirmed by electron microscopy [3].

Here we will show that the formalism also works very well in combination with LeBail fitting. This turns out to be important in cases where the precise atomic structure of the material is not known. Determination of crystallite size and morphology of industrially important materials such as boehmite and zeolites will be presented.

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