FRACTAL ANALYSIS OF $PrFe_{1-x}Ni_xO_3(0\leq X\leq 0.3)$ PERVOSKITE SAMPLES BY USING MICROGRAPHS

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Fractal dimensions of different samples of $PrFe_{1-x}Ni_xO_3(0\leq x\leq 0.3)$ system, were computed using scanning electron micrograph (SEM). These SEM micrographs were analyzed using correlation function method. Present samples have good fractal properties. The fractal dimension increases with Ni doping, however, a saturation for fractal dimension is obtained for x=0.2.

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1. Introduction

The scientific interest during last few decades has been devoted to study the orthoferrites and related compounds because of their important technological applications, unusual magnetic and electrical properties. The orthoferrites $RFeO_3$ (R is the rare earth element) have a ABO_3 distorted type perovskite crystal structure [1]. All the transition metal elements are at the corners and are surrounded by six oxygen anions forming octahedra. These orthoferrites are anti ferromagnetic insulators. The magnetic interactions in such cases are formed as a result of the strong negative indirect exchange interaction in the network of Fe^{3+}–O–Fe^{3+}, which causes the formation of two magnetic sub lattices whose moments are almost anti parallel [2]. The small angle between the magnetic moments of these sub lattices leads to appearance of a weak ferromagnetic moment [3].

Rare-earth nickelates have the generic formula $RNiO_3$ (where *R*=lanthanide rare earth) and belong to the perovskite structural family. Compounds in which the rare earth is smaller than lanthanum are orthorhombically distorted at room temperature and display a first-order metal-semiconductor phase transition [4]. The critical temperature of the phase transition appears to be dependent on the Ni–O–Ni bond angle. Straightening out this angle stabilizes the metallic state over the semiconducting one, thus lowering metal–insulator transition temperature (T_{MI}), and can be achieved by increasing rare-earth radius[5] or by applying external hydrostatic pressure [6]. More precisely, most of these properties depend upon the microstructure of the system.

For last few decades, there are a lot of studies concerning structural heterogeneity of solid surfaces related to fractal geometry [7-11]. At molecular-size range, surfaces of most materials are fractals, in other words, geometric irregularities and defects are self-similar at different scales. Fractal dimensions, that describes such fractal materials, were found to be in the complete range $2\leq D\leq 3$: low D=2.0 values, indicate regularity and smoothness, intermediate D values indicate irregular surfaces and D values close to 3 indicate highly irregular surface. Fractal dimension can be computed using direct methods such as micrograph analysis, or using methods related to chemical and physical properties behaviour when fractal characteristics are involved.

Hence in the present paper, we shall use scanning electron micrographs (SEM) analysis method to calculate fractal dimension for $PrFe_{1-x}Ni_xO_3(0\leq x\leq 0.3)$ system.In this method, correlation function is used to compute fractal dimension.

2. Theory

Image analysis

A fractal is an object of which observed volume depends on the resolution (length scale) over several orders of magnitude and follows a power law behavior with a nontrivial exponent.

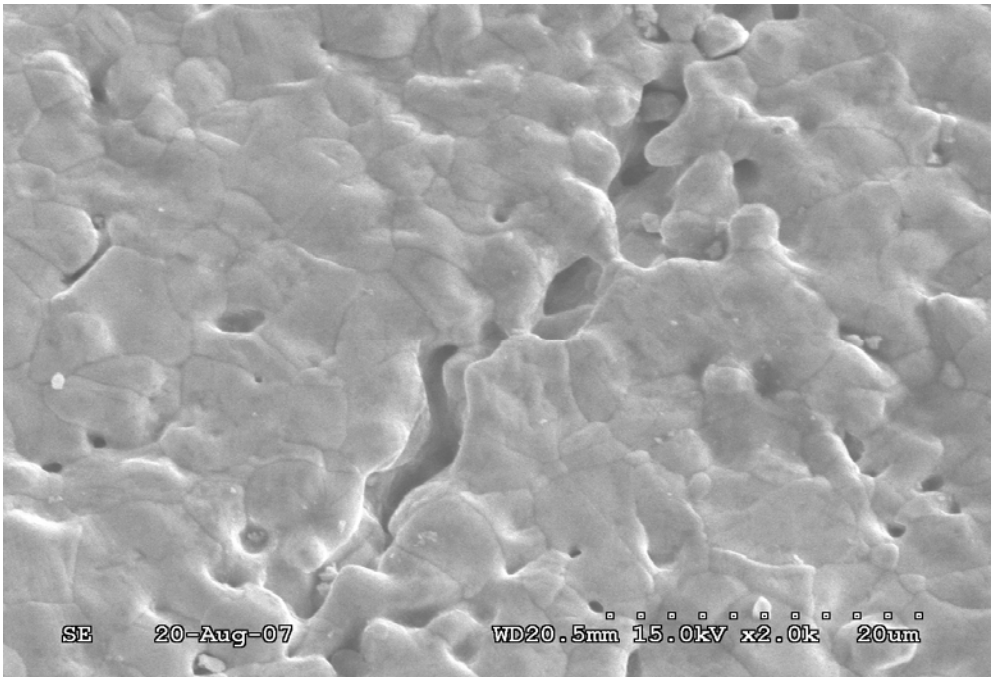

Fig. 1. Scanning electron micrograph of $PrFeO_3$ sample.

The most important property of fractals is the self-similarity, which is the property for a part to look like the whole. Isotropic fractals are self-similar: they are invariant under isotropic scale transformation. When object scales different on different space directions, we call it a self-affine fractal. From this point of view, rough surfaces are usually self-affine fractals [12].

Fractal dimension of a self-affine surface can be computed from the height correlation function [13]-[15]:

$$G(r) = < C(x, r) >_X \tag{1}$$

where the C(x,r) is defined as:

$$C(x, r) = [h(x)-h(x-r)]^2 \tag{2}$$

and surface is described by the function h(**x**) which gives the maximum height of the interface at a position given by x .
Thus the height correlation function G(r) obeys the following scaling relation [16]:

$$G(r) \sim r^{2a}, r << L \tag{3}$$

where, for a surface embedded in a 3-dimensional euclidean space:

$$a=3 - D\text{, with D - the fractal dimension.} \tag{4}$$

The scaling range in which equation (3) is obeyed is called the "cut-off" limits and it indicates the range of self-affinity, in other words, the range where there are correlations between surface points.

In the following, in order to compute fractal dimension of scanning electron micrographs, we shall use equations (1)-(4).

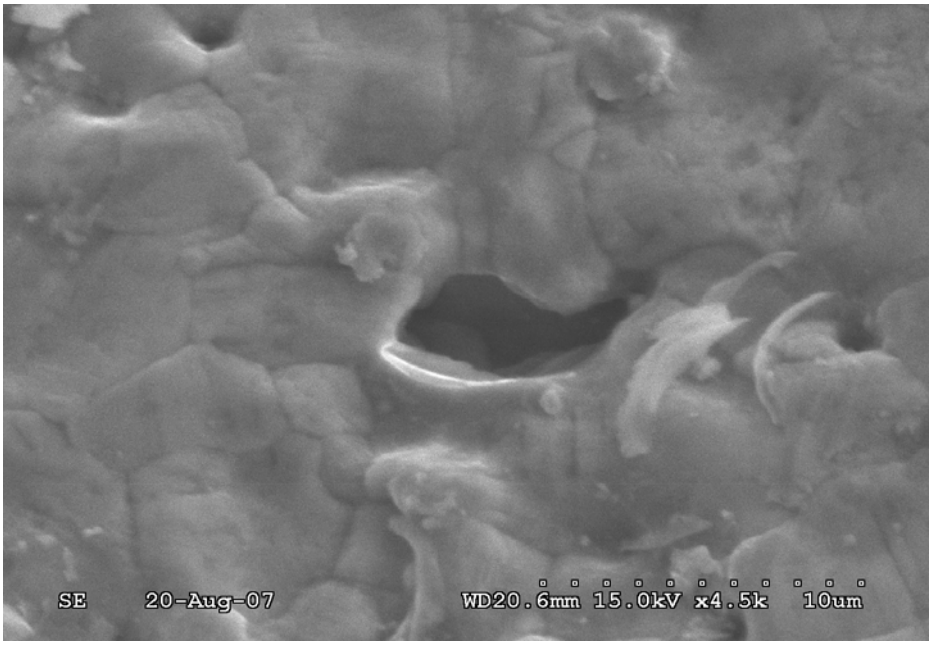

Fig. 2. SEM image of PrFe0.2Ni0.8O3 sample.

3. Experimental procedure

The single phase polycrystalline samples of $PrFe_{1-x}Ni_xO_3$($0 \leq x \leq 0.3$) were synthesized using solid-state reaction technique; the details about preparation, crystal structure, electronic structure and transport are already published elsewhere [17].

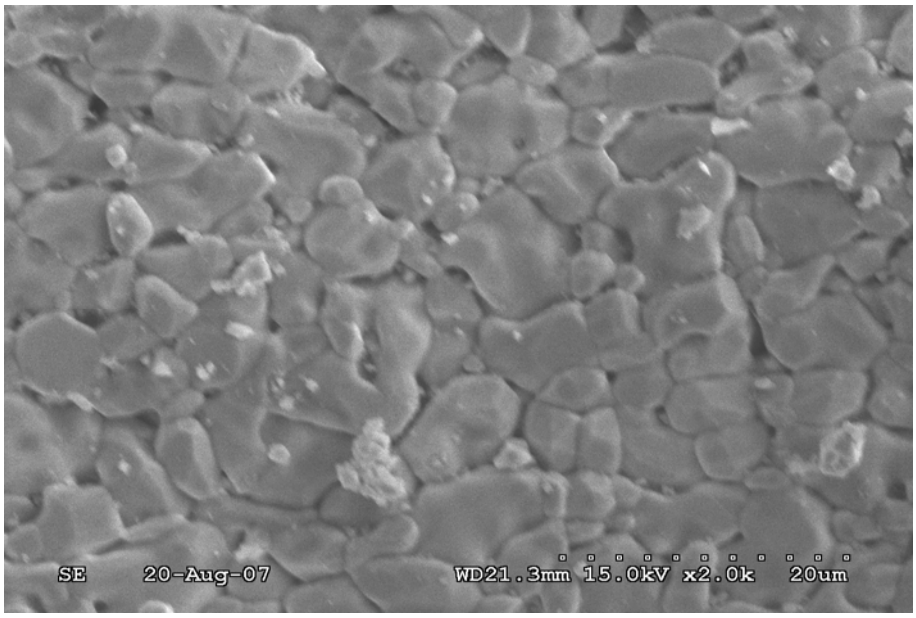

Fig. 3. SEM image of $PrFe_{0.3}Ni_{0.7}O_3$ sample.

The morphology and the size of the products was carried out using high resolution FE-SEM (FEI NOVA NANOSEM-600).

4. Results and discussion

Scanning electron micrographs for $PrFe_{1-x}Ni_xO_3(0\leq x\leq 0.3)$ are presented in Fig.1-3.Log-log plot of height correlation function computed from equations (1)-(4) from SEM image versus squared distances curve is presented in Fig. 4 (sample $PrFe_{0.7}Ni_{0.3}O_3$, x=0.3). Similar curves can be computed for the other samples. Computing slopes of log-log plot of height correlation functions versus squared distances curves with a least square method one can obtained fractal dimensions in Table I. Good determination coefficients (0.97-0.99) were found meaning that for correlation distances of 0.23-1.12 μm (x=0), 0.1-0.42μm (x=0.1) and 0.04-0.31 μm (x=0.2) samples have shown very good fractal properties.

Table 1. Computed Fractal dimensions $PrFe_{1-x}Ni_xO_3(0\leq x\leq 0.3)$ system.

x	SEM analysis
0	2.32±0.02
0.1	2.41±0.01
0.2	2.47±0.04
0.3	2.45±0.03

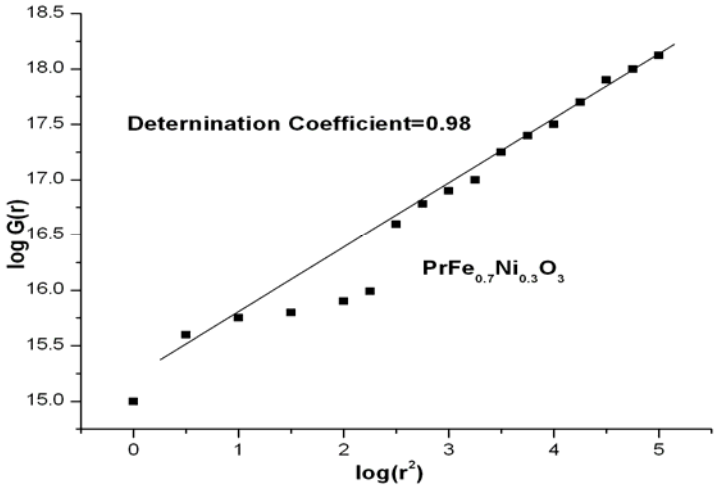

Fig. 4. Log-log curve of height correlation function versus squared distance for x=0.3

Results presented in Table I show good fractal properties of the samples and good agreement between fractal dimensions computed from the two methods. The intermediate fractal dimensions obtained (D= 2.3-2.5), show that the pore size distribution is not so steep, that means that there are more and more the wider pores of the microporosity regime when fractal dimension decreases.

Another remark is that fractal dimension increases with Ni doping, but a maximum for fractal dimension is obtained for x = 0.2.A similar behavor was also obtained for cobaltate system [18].

4. Conclusions

Polycrystalline bulk samples of $PrFe_{1-x}Ni_xO_3(0\leq x\leq 0.3)$ were synthesis by solid state reaction.Fractal properties at molecular level were observed for the present system. The fractal dimension increases with Ni doping, however, a saturation for fractal dimension is obtained for x=0.2.

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