Available online at www.sciencedirect.com

SCIENCE DIRECT®

Surface Science 579 (2005) 37–46

SURFACE SCIENCE

www.elsevier.com/locate/susc

Wavelet analysis of the surface morphologic of nanocrystalline TiO_2 thin films

Yuan Lin, Xu Rui Xiao *, Xue Ping Li, Xiao Wen Zhou

Key Laboratory of Photochemistry, Center for Molecular Sciences, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100080, China

Received 4 August 2004; accepted for publication 20 January 2005

Abstract

Surface morphologies of nanocrystalline TiO_2 thin films were studied by analyzing the surface profile of AFM images using wavelet transform method. Based on characterizing the fractal feature and computing the image details at different orientations and resolutions, the surface textures of nanocrystalline TiO_2 thin films before and after chemical treatment were examined. The results reveal that titanium isopropoxide treatment leads to an increase of surface roughness. The related mechanism of modification of the microstructure by chemical treatment associated with the improvement of the photocurrent response is discussed.

Keywords: Atomic force microscopy; Surface structure, morphology, roughness and topography; Titanium oxide; Semiconducting surfaces; Surface chemical reaction; Fractal surface

1. Introduction

Nanocrystalline porous TiO_2 thin films have attracted a great deal of attentions in photovoltaic conversion applications [1,2]. Solar cells based on the dye-sensitized nanocrystalline TiO_2 films have been studied extensively recently [3–9]. In these solar cells, nanocrystalline TiO_2 thin films used as photoelectrodes offer a larger surface area for adsorption of dyes and the pathway for transportation of electrons from photo-excited dyes to the conducting substrates. Recent studies reported that the porous microstructure of the nanocrystalline films have a great influence on the photovoltaic behaviors of the dye-sensitized solar cells [10]. Chemical treatment has been proved to be an effective method to optimize the porous microstructure for improving the photovoltaic behaviors of the solar cells [4]. Our previous work showed that chemical treatment resulted in the increase

* Corresponding author. Tel.: +86 10 82615031; fax: +86 10 82617315.
E-mail address: A1703@iccas.ac.cn (X.R. Xiao).

0039-6028/$ - see front matter
doi:10.1016/j.susc.2005.01.033

of the photocurrent response of nanocrysyalline TiO_2 films [11]. In order to examine the effect of the chemical treatment, it is important to characterize the surface texture of nanocrystalline TiO_2 films. Quantitative analysis of the surface texture is essential to understand the physical processes taken place during the chemical treatment and the mechanism for improving the photocurrent response of nanocrystalline TiO_2 films.

Recently, wavelet transform (WT) as a new technique has been used extensively in the signal and image processing [12–14]. WT has the advantage of fast computation with localization in both space and frequency domains. It is well-adapted in the analysis of the surface roughness providing an insight into the stochastic properties of a fractal surface [15,16]. Based on using the algorithm of multiresolution signal decomposition (MRSD), WT can offer the image information directly at different resolutions enabling interpretation and hierarchical analysis of the image details from a lower-to-higher resolution [17]. In this work, we use WT method with the MRSD algorithm to study the surface textures of nanocrystalline TiO_2 films before and after chemical treatment including the analysis of the surface fractal feature and the details of the surface morphologic images.

2. Computation methods

2.1. Wavelet transform (WT)

Wavelet transform is to represent the analysis of a signal with a family of functions which are the dilation and translation of the basis wavelet function $\psi(t)$ [12] i.e.

$$\psi_{a,b}(t) = \frac{1}{\sqrt{|a|}}\psi\left(\frac{t-b}{a}\right) \tag{1}$$

$$W_f(a,b) = \int_{-\infty}^{+\infty} f(t)\overline{\psi_{a,b}(t)}\,\mathrm{d}t \tag{2}$$

where a ($a \neq 0$) and b are the dilation (scale) and translation (position) parameters respectively. Eq. (2) is used to describe the continuous wavelet transform (CWT).

If the parameters a and b are chosen to be $a = a_0^j$ and $b = kb_0a_0^j$, ($j,k \in Z, a_0 = 2$ and $b_0 = 1$ in general) the discrete wavelet as another type of wavelet is derived in Eq. (3) and the discrete wavelet transform (DWT) is expressed in Eq. (4). To take the advantage of easy computation, in this work, the signal processing is performed by using DWT

$$\psi_{j,k}(t) = a_0^{-j/2}\psi(a_0^{-j}t - kb_0) \tag{3}$$

$$C_f(j,k) = \int_{-\infty}^{+\infty} f(t)\overline{\psi_{j,k}(t)}\,\mathrm{d}t \tag{4}$$

2.2. Multiresolution signal decomposition

Multiresolution signal decomposition (MRSD) is proposed as a widely used algorithm for carrying out DWT [12,17]. The multiresolution decomposition processes of a signal consist on applying orthogonal wavelet based filter to decompose the original signal C^0 into two parts of the low-frequency (approximation) C_n^1 and high-frequency (detail) D_n^1 components. The low-frequency component obtained at the first scale level C_n^1 can be further decomposed into low-frequency and high-frequency components of the second scale level i.e. C_n^2 and D_n^2 respectively. The procedure is repeated until the desired scale level of signal components is achieved. The low frequency and high frequency components at the position n can be expressed as:

$$C_n^k = \sum_{j=n-N}^{n} C_j^{k-1} h_{j-n} \tag{5}$$

$$D_n^k = \sum_{j=n-N}^{n} C_j^{k-1} g_{j-n} \tag{6}$$

$k = 1, 2, \ldots$

where N is the sampling number, n is sampling position, k is the scale level, h and g are the low-pass filter and high-pass filter respectively [17]. The relations of the filters h and g to the basis wavelet function ψ are written as:

$$h_i = \int_{-\infty}^{\infty} 2^{-1}\psi(2^{-1}x)\phi(x-i)\,\mathrm{d}x \tag{7}$$