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Optical model of porous glasses using genetic algorithms

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ABSTRACT

Porous surfaces on glasses have been proved to be effective in suppressing light reflection due to the continuous variation in the refractive index with thickness. The porous structures were fabricated on BK7 glass by neutral-solution leaching process, and broadband transmittance was measured by a spectrometer. An optical model was applied to determine gradient refractive index profiles of porous glasses using a genetic algorithm. Scanning electron microscopy (SEM) analysis of the nanostructure variants will be shown, along with spectral transmittance that is matched to theoretical models. This model has potential applications in tracking optical properties according to the depth of nanostructures measured by SEM, or obtaining gradient refractive index profiles of porous glasses by the measured transmittance. Therefore, it is useful to optimize experimental condition for special optical properties of porous glass.
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1. Introduction

Since the application of conventional antireflective (AR) coatings is limited by the availability of proper materials, the gradient-index antireflective (GIAR) nanostructures have attracted an increasing interest, and offer an alternative to thin-film coatings for high power laser systems [1]. These advanced diffractive optical elements are investigated from the view points of manufacture [2–7] and design not only in the performance of antireflection for wide range of spectrum and wide incident angle range [2] but also in high laser damage threshold [8–11]. GIAR nanostructures were first found in the cornea of night-flying moths, and so was called the “moth-eye” effect [12]. The GIAR surfaces have the gradient refractive index from the incident medium to the substrate, shown schematically in Fig. 1 [13]. The different distribution functions have been introduced to describe the graded-index profile, including linear, parabolic, cubic, Gaussian, quintic, exponential, exponential-sine, and Klopfenstein [14–19]. Porous surface is one form of GIAR structures by introducing porosity to glass or other substrate surface. Among various preparation of GIAR nanostructures, neutral-solution leaching process [6] is the low-cost and non-toxic method. Thus, this technique is applied in the preparation of GIAR porous glass. However, to the best of our knowledge, few people have considered combining the graded index (GRIN) and textured surface structures [20], and gradient refractive index profiles of porous glasses have not been studied before.

In this paper, porous glasses were made by simply immersing borosilicate glasses in a hot neutral-solution. Different solution concentration and leaching time caused different surface porosity and optical property. Then, a theoretical model is used to study the refractive index profile of GIAR nanostructure by simulated as a sequence of sub-layers, which is based on the effective medium theory (EMT). The effective refractive index and thickness of each sub-layer are calculated using a genetic algorithm, and then the gradient refractive index profiles of porous glasses are determined. This approach has potential applications in tracking optical properties according to the depth of nanostructures measured by SEM, or obtaining its depth information by the transmittance measured, and this property may be useful to optimize experiment condition for special optical properties of porous glass.

2. Experimental

For the leaching method, porous surfaces are formed by selective solution of some of the elements present in the glasses without destroying the skeleton structure of glass. Because the refractive index of glass is lowered by the porosity on optical surfaces, the amount of light transmitted can be increased. It is required, however, that the pore size was substantially smaller than the wavelength of the light and the pore distribution must be homogeneous in order not to affect the light transmittance and cause scattering [21].

Before leaching, BK7 glasses were cleaned with acetone and ethanol under sonication, which was followed by rinsing with deionized (DI) water. After drying in atmosphere, the glasses were immersed in hot Na_2HPO_4 solution. Finally the glass substrates

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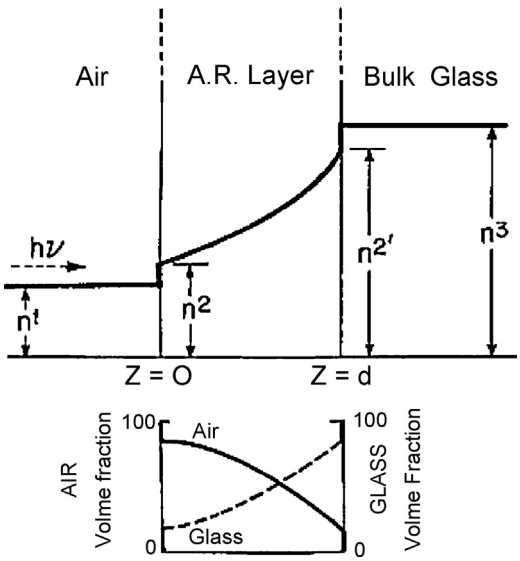

Fig. 1. Schematic of index of refraction, n, and volume fraction air/glass for GIAR film [13].

Table 1
Experimental parameters.

Test	Na_2HPO_4 (mol/L)	Leaching time (h)
(a) Test 1	0.03	13
(b) Test 2	0.035	13
(c) Test 3	0.035	26

were rinsed with DI water. The leaching parameters were listed in Table 1.

The surface and cross section morphology of the leached glass was examined using a Zeiss scanning electron microscope (SEM) (JSM-6360LA), and the UV–vis–NIR transmittance spectrum of the glasses was recorded using a spectrophotometer (Perkin Elmer Company, Lambda 900).

3. Results

As shown in Fig. 2, the uniform porous surface with pore size of approximately 30–50 nm and ~60 nm depth after leaching for 13 h. As solution concentration increased to 0.035 mol/L, the pore size is about 30–80 nm and the average leaching depth is ~148 nm as shown in Fig. 3. When the leaching time increases to 26 h, pore size of nanostructures is 30–80 nm, which is approximately 260 nm depth (Fig. 4.).

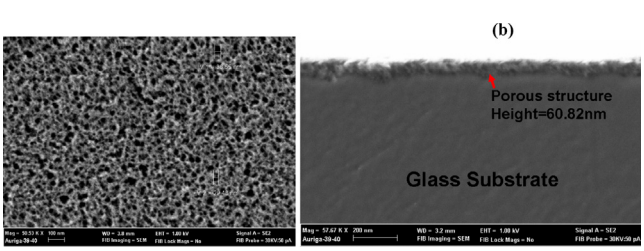

Fig. 2. SEM micrograph of glasses leached for 13 h (test 1). (a) Elevation view of porous structure and (b) cross-sectional view of porous structure.

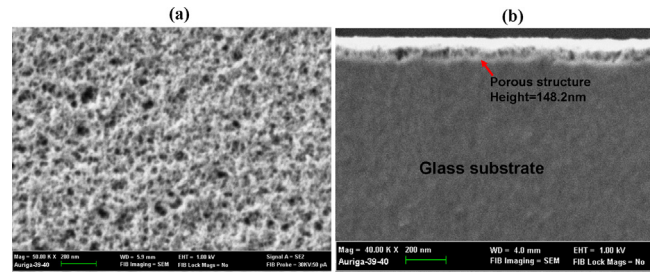

Fig. 3. SEM micrograph of glasses leached for 13 h (test 2). (a) Elevation view of porous structure and (b) cross-sectional view of porous structure.

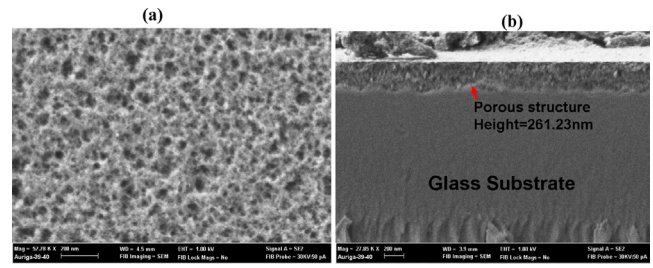

Fig. 4. SEM micrograph of glasses leached for 26 h (test 3). (a) Elevation view of porous structure and (b) cross-sectional view of porous structure.

4. Discussion

4.1. Theoretical model

The antireflective property of the porous structure originates from the tunability in the effective refractive index n_{eff}. Based on the effective medium theory, the effective refractive index n_{eff} can be calculated by [22]:

$$n_{eff} = [n_c^2 f + n_{air}^2(1-f)]^{1/2} \quad (1)$$

where n_c and n_{air} are the refractive index of the material and air, respectively, and f is the filling factor, which is an average data determined by the size and the distribution of pores. The porous layer has a lower n_{eff} due to the existence of air in the interstitial space. In addition, as the glass is gradually leached downwards, the effective refractive index of the porous layer will vary gradually from the top to the bottom of the glass. It is the reason of broadband antireflection effect of graded porosity.

In the simulation, the substrate is BK7 glass ($n_3 = 1.52$) and the ambient medium is air ($n_1 = 1.0$). The GIAR structure is modeled by 200-layer homogeneous sub-layers. The refractive-index profile is shown in Fig. 5. The differences of refractive index (Δn_i) of every adjacent layers and thicknesses (Δz_i) of each sub-layer are all optimized by iterative genetic algorithm computational method [23], which have previously been applied to the optimization of a variety of optical coatings. The genetic algorithm process is an

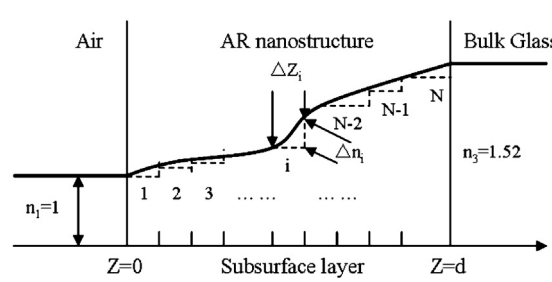

Fig. 5. Schematic drawing of optimization of the GIAR profile.

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