FE-study on maximum swelling anisotropy in silica

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Abstract

Strength of silica fibers heat treated in humid air is affected by swelling strains. In the absence of externally applied stresses swelling is isotropic. Under uniaxial stress an anisotropy of swelling strains has to be expected with maximum expansion in stress direction. In order to compute the maximum possible anisotropy, a Finite Element analysis is carried out. Under the assumption of a spherical nano-pore generated by a single bond breaking event, an averaged axial swelling strain was computed that is by a factor of >2 larger than the volume swelling strain.

Contents

1. Introduction

Water penetrated into silica reacts with the silica network according to

$$\equiv\text{Si-O-Si}\equiv +\text{H}_2\text{O} \leftrightarrow \equiv\text{SiOH+HOSi}\equiv \tag{1}$$

with the concentration of the hydroxyl $S = [\equiv\text{SiOH}]$ and that of the molecular water $C = [\text{H}_2\text{O}]$. It was early shown by Brückner [1, 2], Shackelford [3] and Shelby [4] that this reaction is accompanied by volume swelling.

In Fig. 1 a volume element with a number of N Si-O bonds is shown. In a statistical sense, the number of N arbitrarily oriented Si-O-bonds can be dismantled in components oriented in the x-, y-, z-directions of a rectangular coordinate system with $N/3$ single bonds in each direction.
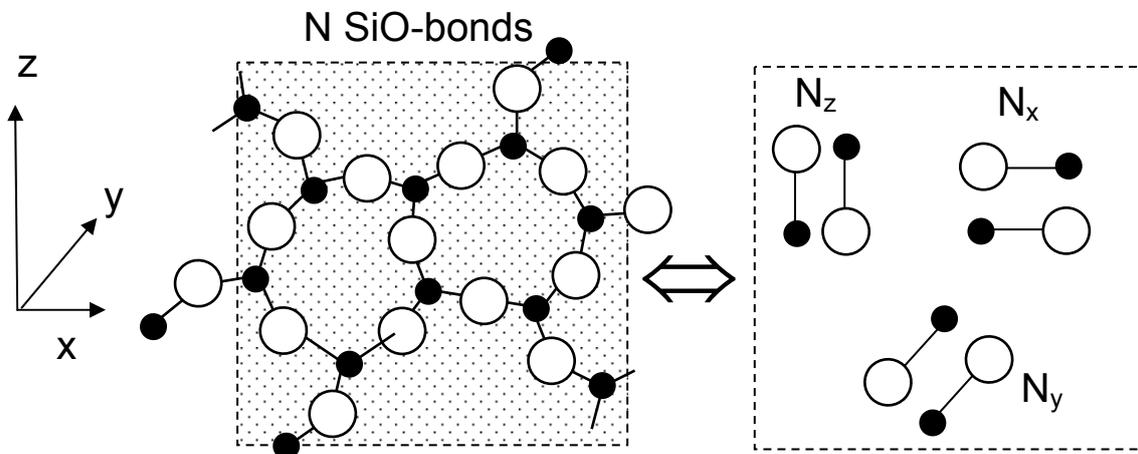
Fig. 1 Volume element containing a number of N Si-O bonds (2-dimensional representation) divided into $N/3$ bonds oriented in x-, y-, and z-directions.

Under mechanical stresses applied in z-direction, the probability of reaction events is expected to be increased for the bonds N_z. The maximum swelling strain in z-direction should therefore result when all reactions occur at bonds N_z exclusively. In a FE-study we considered this special case and looked for the maximum swelling strain $\varepsilon_{\text{sw,z}}$.

Maximum anisotropy is reached if all reaction events are located at bonds oriented in z-direction. For this situation the strain components ε_x, ε_y, ε_z, and the volume strain ε_v were determined by FE-computations.

2. Maximum anisotropy expected from FE-computations

Due to the reaction a SiO-bond may be fractured in the absence of stresses. Our coordinate system is oriented so that the z-axis agrees with the direction in which the repulsive forces between the silanols act (Fig. 2). The "nano-pore" defined by the dashed circle in Fig. 2 was modelled as a sphere of radius R in an "infinite body".

In our FE-study we modelled the infinite body by a cylinder of radius $500\,R$ and half height $500\,R$, Fig. 3a. For the computations we used ABAQUS Version 6.9 on a mesh of 1246 elements and 3880 nodes. Due to symmetry only a 4th of the total body had to be modelled. As the only material parameter of relevance we used the Poisson ratio of $\nu=0.17$. In order to compute the expansion in z-direction, a constant displacement δ_0 is prescribed over a sphere part with an opening angle φ with respect to the z-axis, Fig. 3b.
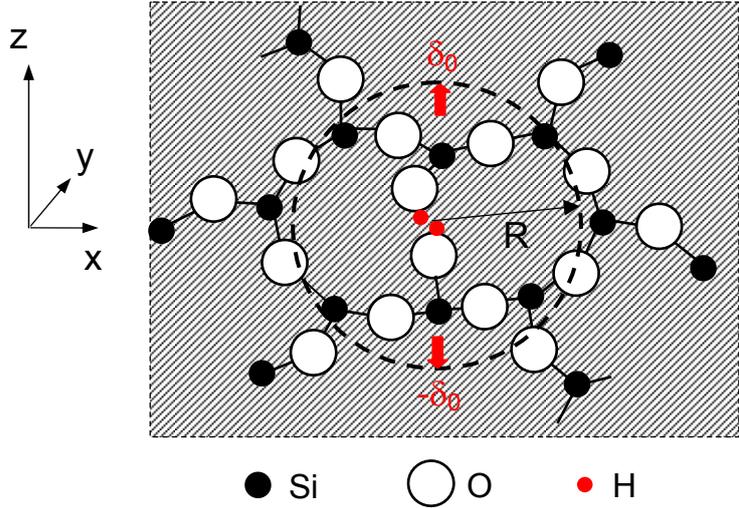
Fig. 2 Bond breaking by water/silica reaction; the two hydroxyls yield an expansive displacement δ_0 in z-direction; the volume element in which the reaction occurred is represented by the dashed circle.
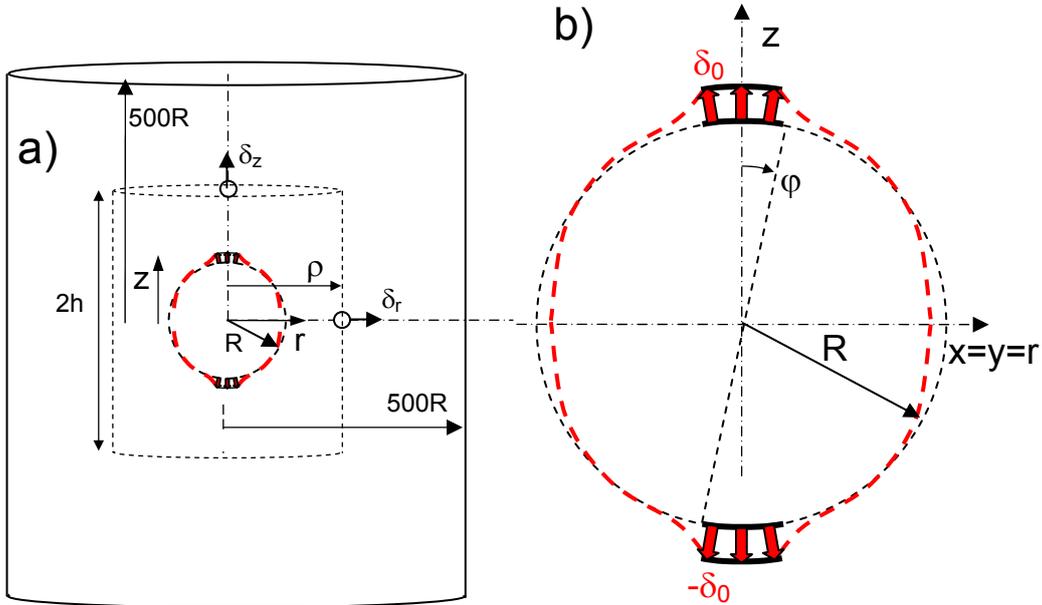
Fig 3 a) Finite Element model of a "nano pore" loaded by displacement caused by a repulsive interaction between the silanol groups, b) details of pore loading.

2.1 Local strains along symmetry axes

The displacements in axial and radial directions, δ_z and δ_r, were determined first for the symmetry axes as a function of distances z and r. Figure 4a gives the displacement ratio δ_r/δ_z for $\varphi=3.5°$ as a function of the distance r/R (note reciprocal scaling of the abscissa).

In Fig. 4b the ratio δ_r/δ_z is plotted as a function of the angle φ given in Fig. 3b. For angles $<45°$ the expansion in z-direction is accompanied by a reduction in y- and x-directions. For angles $>45°$ all directions show expansion.
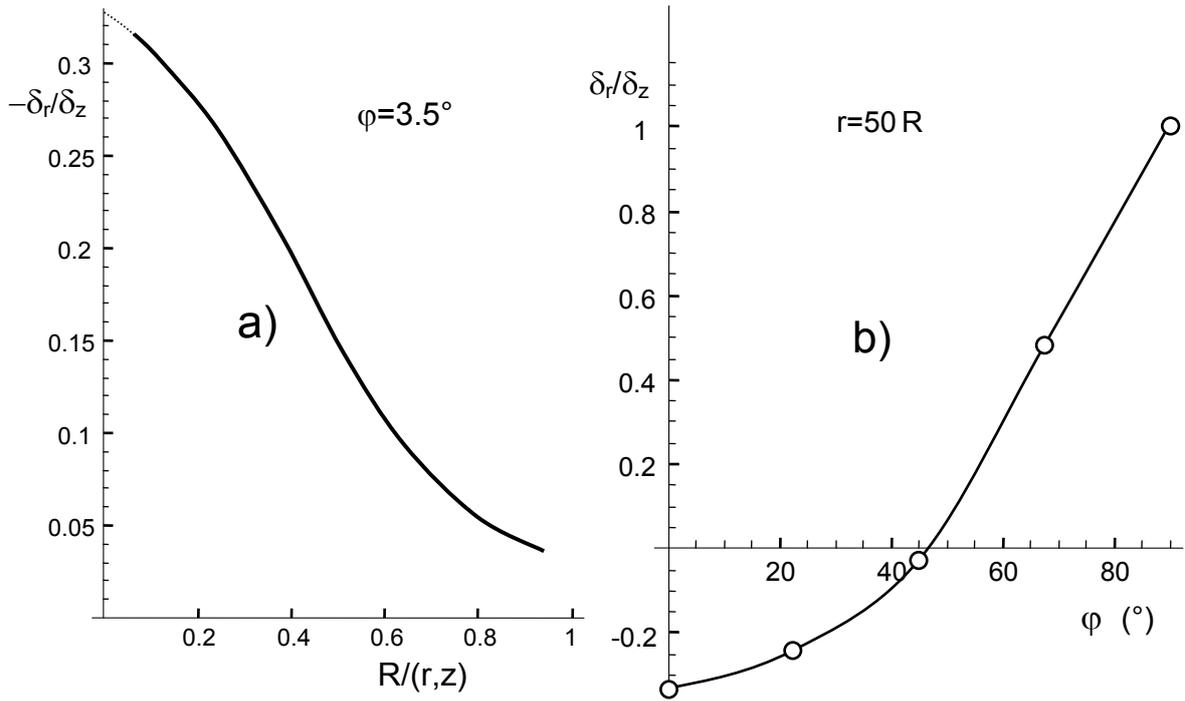
Fig. 4 a) Ratio of transversal and axial displacements plotted against the reciprocal distance for $\varphi=3.5°$, b) displacements in y- and x-directions normalized on the axial strain vs. the angle φ.

Figure 5a shows the axial displacements, δ_z normalized on the sum of the displacements in all 3 directions as a function of the distance from the pore centre for $\varphi \to 0$. Due to rotational symmetry with $\delta_x=\delta_y=\delta_r$ this ratio reads

$$\frac{\delta_z}{\delta_x + \delta_y + \delta_z} = \frac{\delta_z}{\delta_x + 2\delta_r}$$

It should be noted, that the denominator does not agree with a volume change since the individual values are determined at different locations.

In Fig. 5b the same results are plotted versus $\sin(\varphi)$ showing a nearly linear dependency. A numerical representation of the FE-results is

$$\frac{\delta_z}{\delta_z + 2\delta_r} \cong 3 - \tfrac{8}{3}\sin\varphi \qquad (2)$$

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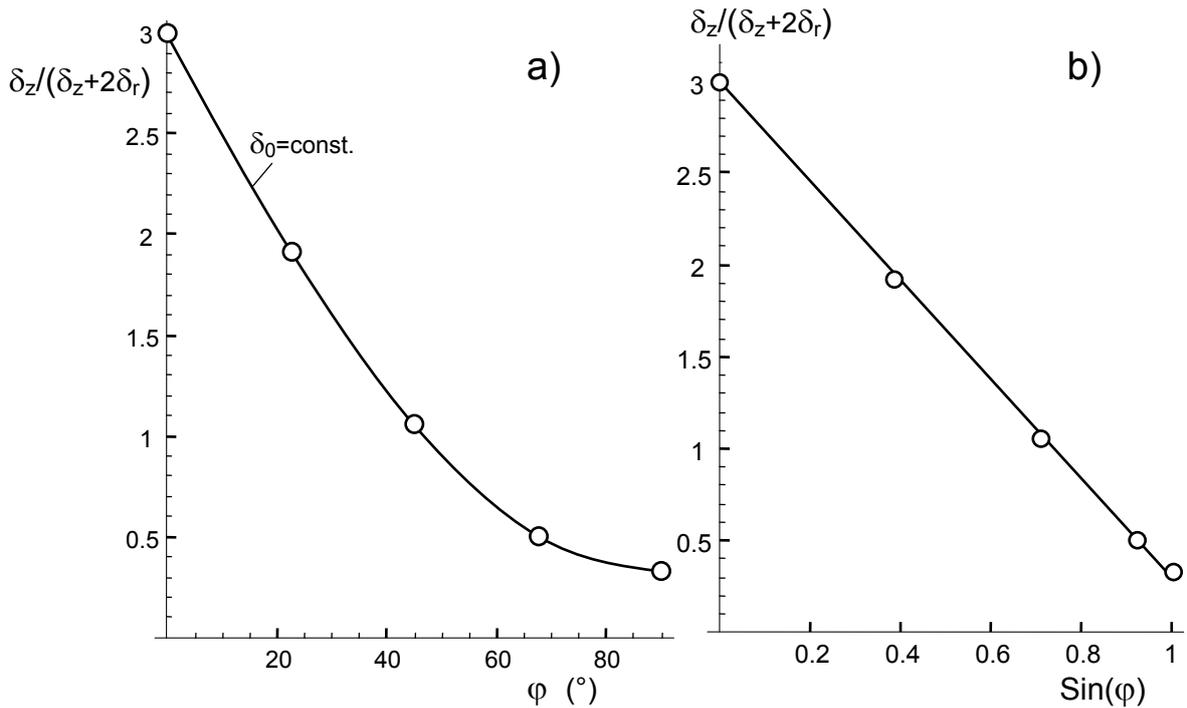
Fig. 5 "Anisotropy" of the displacements in axial and radial directions vs. angle φ defined in Fig. 3b.

2.2 Strain distributions over cylinder contours

In Section 2.1 only the displacements on the symmetry axes were taken into account. In the following considerations the displacement distributions over the surface of cylinder elements are given which result for a purely axial displacement δ_0, i.e. for $\varphi \rightarrow 0$. Figure 6a gives a schematic illustration. Figure 6b represents the displacement distributions for a cylinder contour with $h=\rho=16R$.
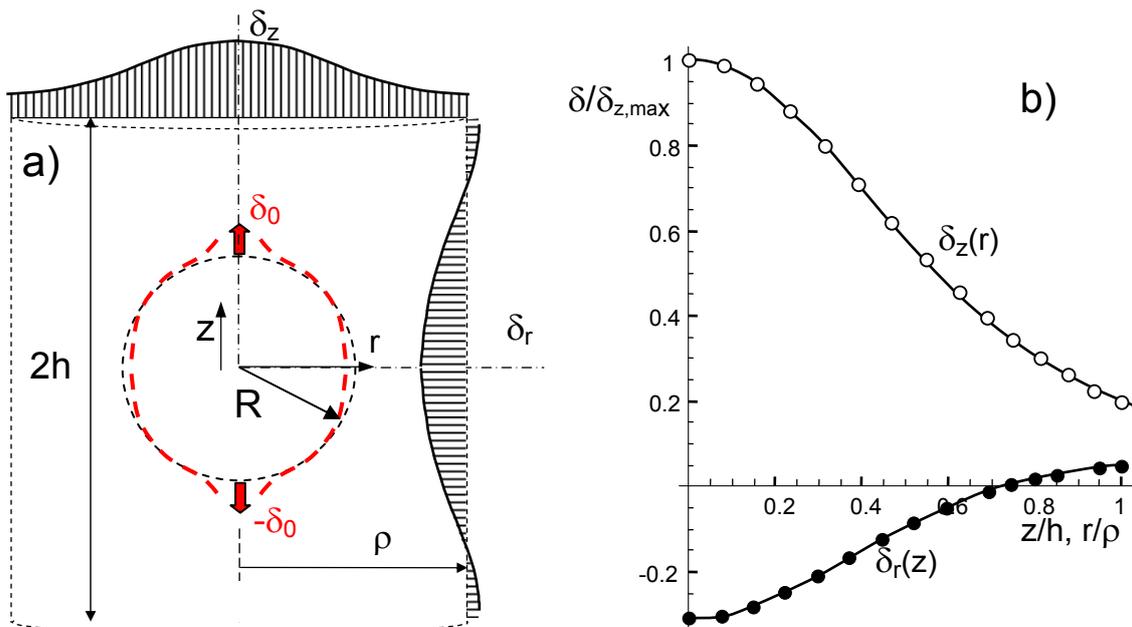
Fig. 6 a) Axial displacements acting on the "nano pore", b) displacement distributions δ_z and δ_r at the cylinder contours in a distance of $h, \rho = 16 R$.

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3. Volume expansion strain and anisotropy ratio

The volume change in axial direction is given by

$$\Delta V_z = 2\pi \int_0^\rho \delta_z(r)\, r\, dr \tag{3}$$

In radial direction it holds

$$\Delta V_r = 2\pi r \int_0^{h=\rho} \delta_r(z)\, dz \tag{4}$$

On a cylinder contour with $\rho = h$ the average displacement in z-direction reads

$$\bar{\delta}_z = \frac{2}{\rho^2} \int_0^\rho \delta_z(r)\, r\, dr = \frac{\Delta V_z}{\rho^2 \pi} \tag{5}$$

Consequently, the average strain in z-direction is obtained as

$$\bar{\varepsilon}_z = \frac{\bar{\delta}_z}{h} \underset{\rho=h}{=} \frac{\bar{\delta}_z}{\rho} = \frac{\Delta V_z}{\rho^3 \pi} \tag{6}$$

Since the cylinder volume in the absence of swelling is

$$V_0 = \rho^2 \pi h \underset{\rho=h}{=} \rho^3 \pi \tag{7}$$

the volume welling strain results as

$$\varepsilon_v = \frac{\Delta V_z + \Delta V_r}{\rho^3 \pi} \tag{8}$$

The anisotropy ratio $\bar{\varepsilon}_z / \varepsilon_v$ is obtained by combining eqs.(6) and (8):

$$\frac{\bar{\varepsilon}_z}{\varepsilon_v} = \frac{\Delta V_z}{\Delta V_z + \Delta V_r} \tag{9}$$

A cylinder contour of $\rho = h = 16\,R$ may be considered. In this case, the evaluation of eq.(9) results in

$$\frac{\bar{\varepsilon}_z}{\varepsilon_v} = 2.07 \tag{10}$$

A Poisson's ratio ν for swelling strains can be defined via

$$\nu = -\frac{\bar{\varepsilon}_r}{\bar{\varepsilon}_z} \tag{11}$$

Since the volume strain is

$$\varepsilon_v = \bar{\varepsilon}_x + \bar{\varepsilon}_y + \bar{\varepsilon}_z = \bar{\varepsilon}_z + 2\bar{\varepsilon}_r \tag{12}$$

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eqs.(10) to (12) yield

$$\frac{\bar{\varepsilon}_z}{\varepsilon_v} = \frac{\bar{\varepsilon}_z}{\bar{\varepsilon}_z + 2\bar{\varepsilon}_r} = \frac{1}{1 + 2\dfrac{\bar{\varepsilon}_r}{\bar{\varepsilon}_z}} = \frac{1}{1 - 2v} = 2.07 \Rightarrow v = 0.258 \tag{13}$$

The resulting Poisson's ratio is similar to those found for ceramics and metals.

4. Influence of the chosen geometry

In order to show the effect of the *finite* body that had to be modelled for the FE-computations, we computed the strains on cylinder contours in different distance from the pore. Figure 7 shows the ratios $\bar{\varepsilon}_z / \varepsilon_v$ and $\bar{\varepsilon}_r / \bar{\varepsilon}_z$.

It can be seen that the results are rather independent of the chosen cylinder contour. For $\bar{\varepsilon}_z / \varepsilon_v$ the maximum variation within the range of $16R \le h, \rho \le 100\,R$ is less than 2%. This weak dependency clearly indicates that the theorem of Saint-Venant is sufficiently fulfilled, i.e. that

$$R \ll h, \rho \ll 500R \tag{14}$$

When (14) holds, the validity of Saint-Venant's theorem suggests that special details of the pore-shape cannot have a noticeable influence on $\bar{\varepsilon}_z / \varepsilon_v$ and $\bar{\varepsilon}_r / \bar{\varepsilon}_z$.
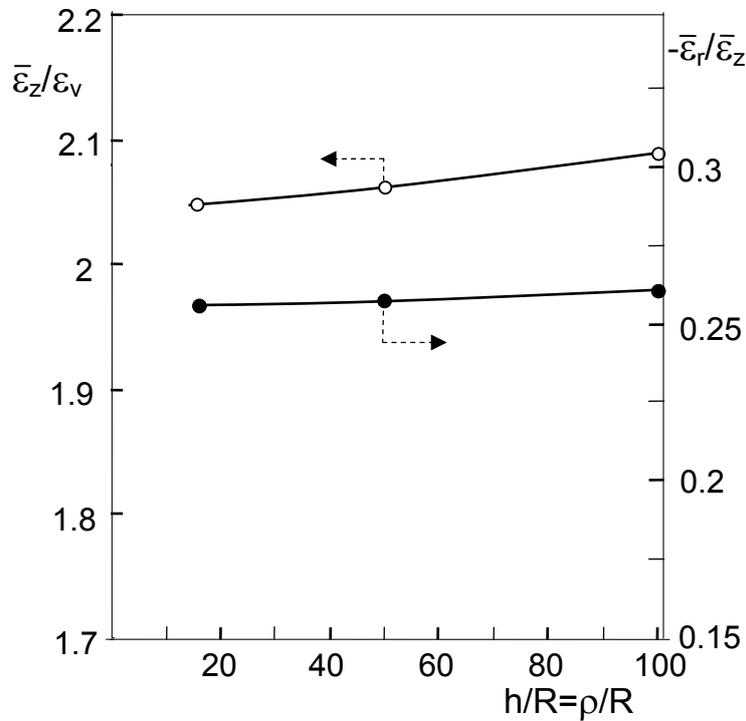
Fig. 7 Strain ratios $\bar{\varepsilon}_z / \varepsilon_v$ and $-\bar{\varepsilon}_r / \bar{\varepsilon}_z$ vs. h/R or ρ/R.

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