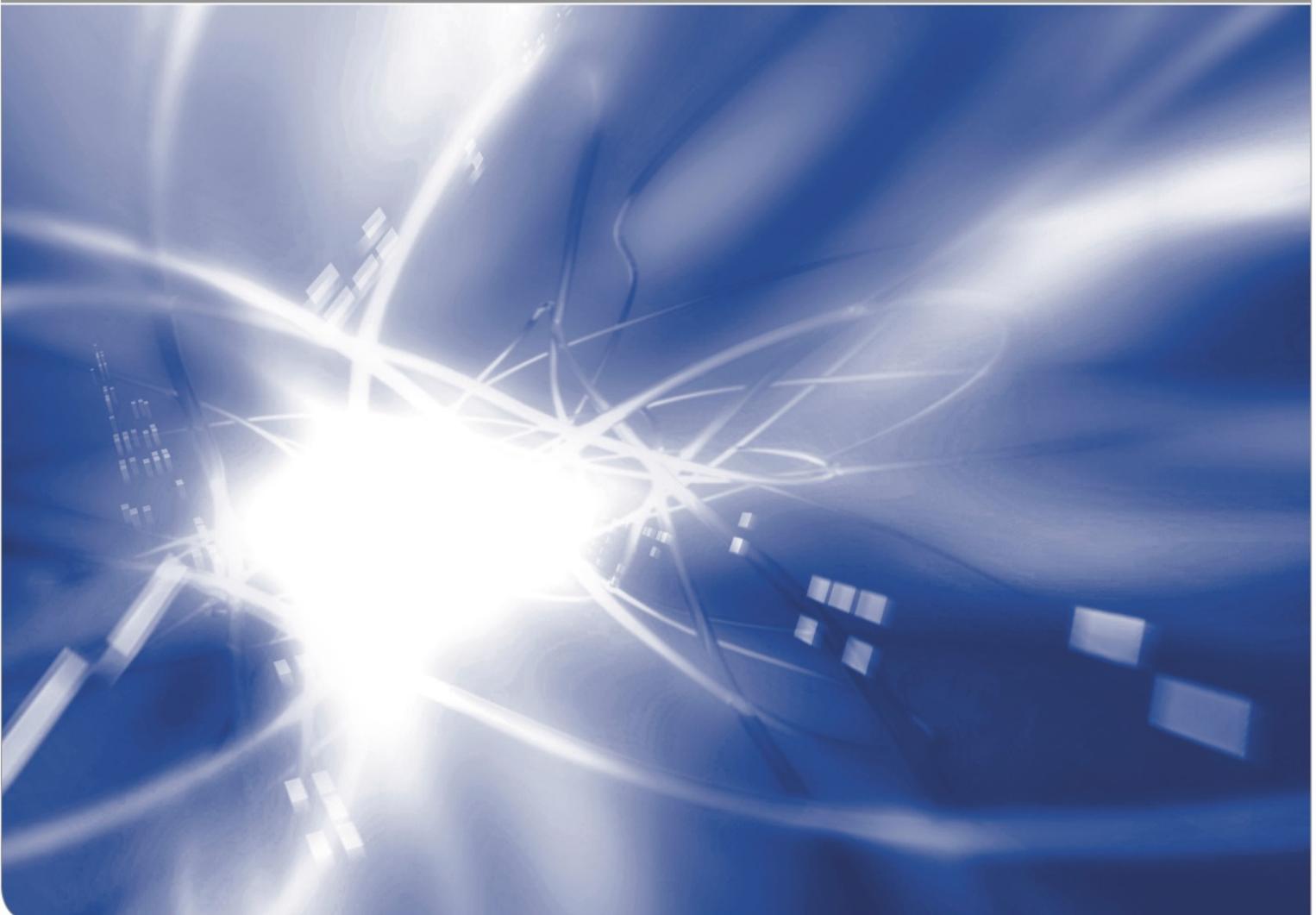# Consequence of Damage in Silica on Young's Modulus

Theo Fett, Günter Schell

Karlsruhe Institute for Technology

Institute for Applied Materials

Abstract

Water diffusion into silica glass results in a thin zone near the surface of the glass. In this zone the water reacts with the SiO_2 structure and "damages" the originally intact SiO_2 rings. The consequence is a reduced Young's module. This effect can be described by use of continuum damage mechanics according to Kachanov and Lemaitre.

The amount of damage can be estimated from literature data on sound velocity measurements.

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1 Damage by hydroxyl generation

When a hydroxyl has been formed, the initial silica ring is broken and the mechanical cohesion is weakened. Such "defects" in the glass structure can be treated by using the damage variable D of continuum damage mechanics (Kachanov [1], Lemaitre [2]). This parameter is proportional to the density of micro-defects.

According to the postulate of strain equivalence by Lemaitre [3], the effective elastic modulus, E, decreases with increasing damage

$$E = E_0(1-D) \tag{1.1}$$

where E_0 is the modulus of virgin glass.

The elastic strain ε is according to the hypothesis by Lemaitre

$$\varepsilon = \frac{\sigma_0}{E} = \frac{\sigma}{E_0} \tag{1.2}$$

The stress term is indicated here by a subscript "0" that means the stress related to the total cross-section.

The damage variable D can be determined from modulus measurements via eq.(1.1). The occurrence of this effect is in principle known from measurements on NaO-SiO$_2$ glass as the results by Ito and Tomozawa [4]. To the authors' knowledge, so far no measurements on fused silica are available. Therefore, a simple linear relation is tentatively used where the density of defects is assumed to be proportional to the concentration of the hydroxyls S:

$$D = S/S_{max} \tag{1.3}$$

from which the Young's modulus results

$$E = E_0(1-S/S_{max}) \tag{1.4}$$

The quantity S_{max} stands for the maximum hydroxyl content in a special loading case, at which damage $D=1$ and mechanical disintegration of the glass ring structure is reached and, consequently, Young's modulus disappears.

Apart from the equi-triaxial loading case with $\sigma_x = \sigma_y = \sigma_z$ (including the case of disappearing stresses), the elastic modulus must become a tensor with components depending on the degree of loading multiaxiality. Since this possibility would make the further treatment very difficult [3] and non-transparent, we assume in the following considerations that the damage remains isotropic and is considered be of scalar nature. This is equivalent to the assumption of pore-like defects. Then also E remains isotropic.

Due to damage, the load-carrying cross-section is reduced and, consequently, the effective stress increased. If σ_0 is the nominal stress, the effective stress is given by

$$\sigma = \frac{\sigma_0}{1-D} \qquad (1.5)$$

2 Experimental evidence for modulus reduction in silica

In literature, there is experimental evidence for modulus decrease with increasing hydroxyl content. This can be seen from measurements of Young's modulus as a function of water content. Measurements on longitudinal sound velocities in silica specimens with different water content were reported by Fraser [5] and Le Parc et al. [6]. Their results are shown in Fig. 1a and additionally with normalized ordinate scaling in Fig. 1b. Individual fits for the two data sets were made resulting for Fraser [5] in

$$v \cong 5974 - 0.025\,S \qquad (2.1)$$

From LeParc et al. [6] we obtain

$$v \cong 5959 - 0.0318\,S \qquad (2.2)$$

When we normalize the results of the two test series on their individual values for $S{=}0$, we get the representation in Fig. 1b. A common straight-line fit of these data yields

$$\frac{v}{v_0} = A - B\,S \qquad (2.3)$$

with the parameters

$$A{=}1\ [0.99974,\ 1.00026]\ ,\ \ B{=}{-}5.13\ [4.18,\ 6.08]$$

(90%-CI in brackets). The dependency of eq.(2.3) is introduced in Fig. 1b as the straight line.

Since the longitudinal sound velocity depends on Young's modulus E and density ρ by $v = \sqrt{E/\rho}$, we obtain for small S with $\rho/\rho_0 \approx 1-(0.84/2)S$ according to measurements by Shelby [7]:

$$\frac{E}{E_0} = \rho/\rho_0 \times (v/v_0)^2 \cong 1 - \lambda\,S \qquad (2.4)$$

with λ=10.6. It has to be noted that this value holds for isotropic damage since the natural OH-content doesn't show any preference for a special direction.
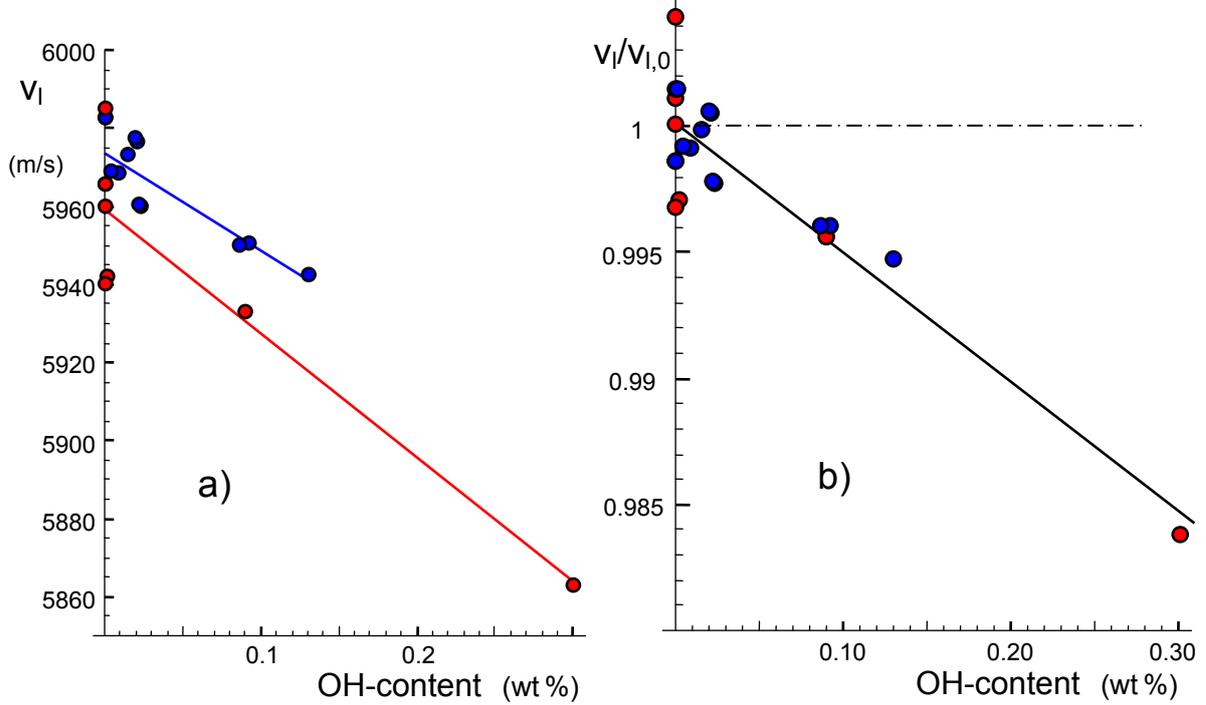
Fig. 1 a) Longitudinal sound velocity in silica with different OH-content (blue circles: results by Fraser [5], red circles: results by LeParc et al. [6]), b) normalized representation of the two data sets.

It is self-evident that eq.(2.4) can describe the modulus decrease only for small hydroxyl contents. For $S \geq 1/\lambda$ a negative E-module would result. This would be without physical sense. A comparable effect on E holds for porosity in ceramics. Figure 2a shows results for hot-pressed silicon nitride (HPSN) with MgO and CeO_2 as was reported by Phani and Niyogi [8], (see e.g. [9]). The solid curve introduced in Fig. 2a describes the modulus as a function of porosity P by

$$\frac{E}{E_0} \cong 1 - 2.56P + 4.53P^4 \tag{2.5}$$

with the consequence that material would be disintegrated at about P=0.52.

We suggest for large S a description similar to the effect of porosity on E in ceramics. Therefore, we assume that nano-pores in SiO_2, caused by hydroxyl generation, might behave like normal pores. Unfortunately, there is actually no information at which hydroxyl concentration disintegration of the silica ring structure occurs with $E/E_0 \to 0$. Including this assumption in eq.(2.4) gives

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$$\frac{E}{E_0} = 1 - 10.6\,S + \mu S^4 \tag{2.6}$$

The coefficient μ is not yet known. Consequently, the behaviour at smaller values of E/E_0 remains unknown. Besides of elasticity measurements at high S-concentrations or molecular pore modelling of the glass structure may give more information in this region. For a modelling by hole-like pores see e.g. Tsukrov and Kachanov [10]. Crack-like defects were modelled in [11].
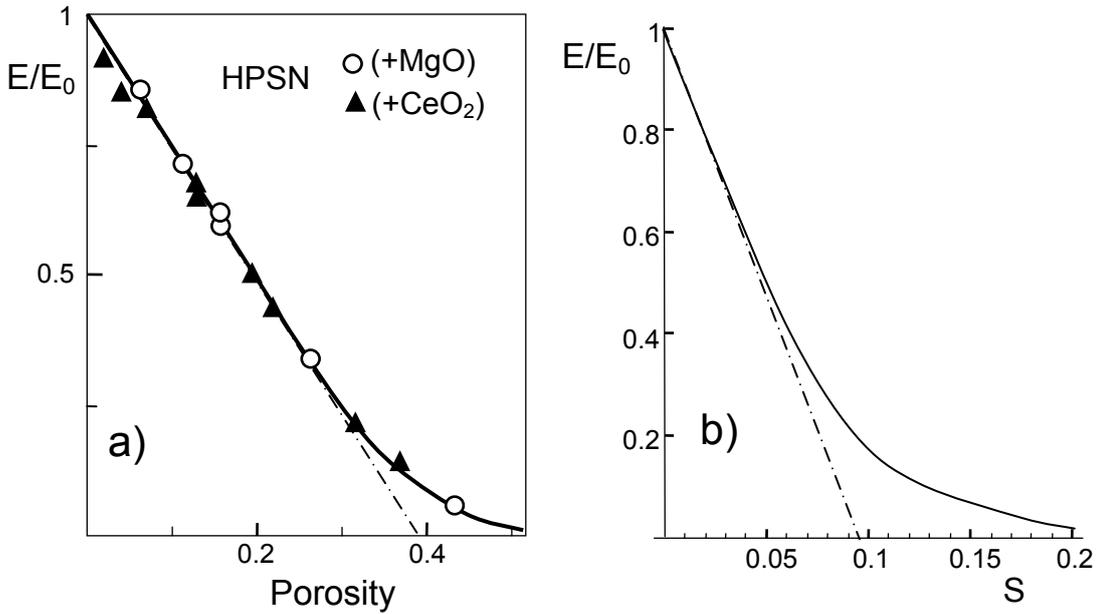
Fig. 2 a) Effect of pores on Young's modulus of HPSN-ceramics, b) behaviour for silica; expected behaviour tentatively introduced by the curve (dash-dotted lines: extrapolation of initially linear variation).

3 Effect of damage

3.1 Global stress

Hydroxyl formation in silica damages the initial ring structure. The mechanical cohesion is weakened. Such "defects" in the glass structure can be treated by using the "rule of mixture" with the encircled regions of broken bonds (Fig. 3) with modulus $E \cong 0$ and the intact regions having the modulus E_0 of virgin glass. The damage variable D is the volume share of the "voids" with $E=0$.

As a consequence, the effective elastic modulus, E, decreases with increasing damage

$$E = E_0(1 - D) \tag{3.1}$$

Due to the condition that plane cross-sections must remain plane under load, the strain in the surface layer $\varepsilon = \sigma/E$ must equal the strain $\varepsilon = \sigma_0/E_0$ in the bulk.

The stress in the damaged surface is therefore

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$$\sigma = \sigma_0(1 - D) \tag{3.2}$$

(σ_0= stress in the bulk). The damage in the material affects also the load-bearing capacity of any area element since it reduces its net cross section and, consequenly, the strength σ_f. If $\sigma_{f,0}$ denotes the strength in the absence of damage, the strength of the damaged material is

$$\sigma_f = \sigma_{f,0}(1 - D) \tag{3.3}$$

The strength of water-damaged silica fibres is strain-controlled. This means that

$$\varepsilon_c = \frac{\sigma_f}{E} = \frac{\sigma_{f,0}(1 - D)}{E_0(1 - D)} = \frac{\sigma_{f,0}}{E_0} \tag{3.4}$$

Equation (3.4) tells us that the damage problem can be handled simply by using bulk material parameters (E_0, $\sigma_{f,0}$) since the damage by broken bond cancels out in (3.4).
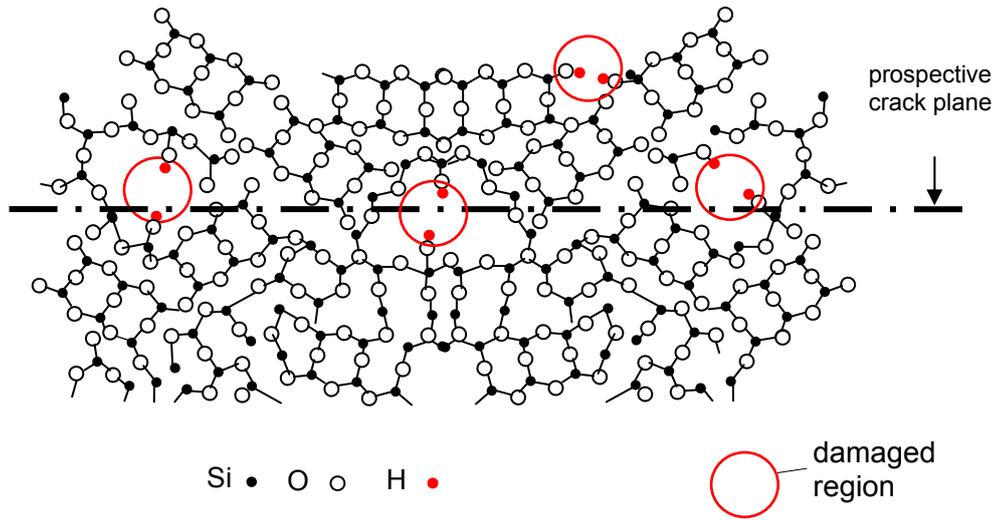
Fig. 3 Volume element of silica showing damage by bond breaking due to water/silica reaction, third dimension ignored.

3.2 Effect on the applied stress intensity factors

In a material with varying Young's modulus, the fracture mechanics J-Integral as the driving force for crack extension remains path-independent, i.e. any path in the near-tip region, J_{tip}, must give the same result as a path far away from the crack, J_{appl}. In the case of linear-elastic fracture mechanics, the J-integral is identical with the energy release rate G. This results in

$$\frac{K_{tip}^2}{E}(1 - v^2) = \frac{K_{appl}^2}{E_0}(1 - v_0^2) \tag{3.5}$$

where K_{tip} is the "true" stress intensity factor acting at the tip and K_{appl} is the externally applied stress intensity factor that can be computed from handbook solutions. Since the Poisson ratio is hardly changed, $\nu \cong \nu_0 = 0.17$, we get from (3.1) and (3.5)

$$K_{tip} = K_{appl} \sqrt{\frac{E}{E_0}} = K_{appl} \sqrt{1-D} \tag{3.6}$$

i.e. the effective load at the tip is reduced, $K_{tip} < K_{appl}$.

3.3 Effect on crack growth resistance

The damage of the initial ring structure of silica, Fig. 3, must also affect the resistance against crack propagation. The dash-dotted line in Fig. 3 may represent the prospective plane for crack extension. The crack growth resistance G_c represents the energy necessary to split all bonds that are broken when the crack passed the considered volume element. Application of the damage variable yields

$$G_{c,tip} = G_{c,\infty}(1-D) \tag{3.7}$$

($G_{c,\infty}$ = crack resistance for the undamaged material) or in terms of stress intensity factors

$$K_{c,tip} = \sqrt{E\,G_{c,tip}} = K_{Ic}(1-D) \tag{3.8}$$

where $K_{c,tip}$ is the crack-tip toughness and K_{Ic} the fracture toughness measured in fracture mechanics tests.

3.4 Applied stress intensity factor for fully embedded cracks

In the special case of a crack *fully embedded* in a material of reduced but constant modulus, the problem simplifies strongly. Then, it holds $E=E_0$ with the consequence of

$$K_{tip} = K_{appl} \tag{3.9}$$

On the other hand the applied stress intensity factor is given by

$$K_{appl} = \sigma F \sqrt{\pi a} \tag{3.10}$$

(F = Fracture mechanics geometric function).
Using the actual stress from eq.(3.2), K_{appl} reads

$$K_{appl} = \underbrace{\sigma_0 F \sqrt{\pi a}}_{K_{appl,0}}(1-D) = K_{appl,0}(1-D) \tag{3.11}$$

where $K_{appl,0}$ stands for the applied stress intensity factor formally computed with stresses σ_0 as present in the bulk material. From (3.8), (3.9) and (3.11) it results equivalently to eq.(3.4)

$$\frac{K_{tip}}{K_{tip,c}} = \frac{K_{appl,0}(1-D)}{K_{Ic}(1-D)} = \frac{K_{appl,0}}{K_{Ic}} \tag{3.12}$$

Also in terms of stress intensity factors, surface cracks fully embedded in the surface layer can be handled simply by using bulk material parameters (K_{appl}, K_{Ic}) instead of the unknown parameters in the layer.

The reduced Young's modulus in the surrounding of a crack must have an effect on crack opening displacements COD.

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