Karlsruher Institut für Technologie

Swelling stresses ahead of slender notches

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Gabriele Rizzi, G. Schell, Theo Fett

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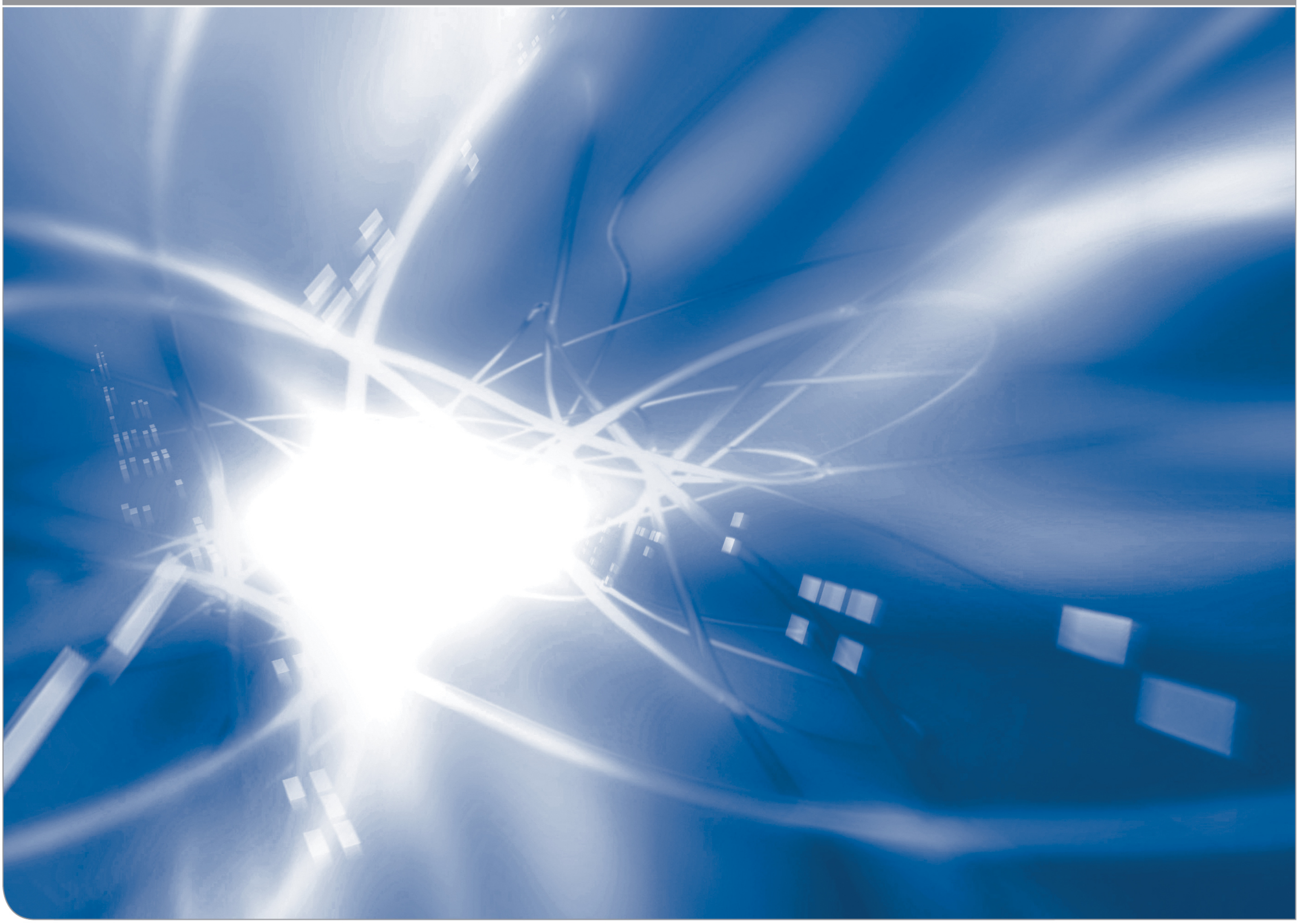

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Abstract

The prediction of hydroxyl concentration in the near-tip region of surface cracks in silica needs knowledge of swelling stresses caused by the silica/water reaction in the surface region. They are available for mathematically sharp cracks as are necessary for the continuum mechanics theory of Linear-Elastic Fracture Mechanics. In a micro-structurally motivated approach, the crack tip region is considered as a slender notch with root radius ρ in the order of the average radius of the SiO_2 rings.

In the present report we compile Finite Element results on swelling stress components ahead of the root of slender edge notches as functions on the notch root distance and the height of the swelling zone.

Contents

1. Crack-tip models

Two crack-tip models are commonly used in fracture mechanics for the description of stresses ahead of a crack. Whereas continuum mechanics assumes the existence of a mathematically sharp crack, in a micro-structurally motivated approach the slender notch with a finite radius at the crack end is considered.

Stresses at a sharp crack tip are described by the crack-tip stress intensity factor K_{tip}. They become singular if the tip is approached, $\sigma \rightarrow \infty$ for $r \rightarrow 0$. However, the *K*-description via continuum mechanics must fail for very short distances, when the tip distance competes with the microstructure of the material. In the micro-structurally motivated approach, the crack tip region, Fig. 1a, can be considered as a slender notch with root radius ρ in the order of the average radius of the SiO_2 rings, Figure 1b. Wiederhorn et al. [1] suggest a crack-tip radius ρ = 0.5 nm for the silica network.

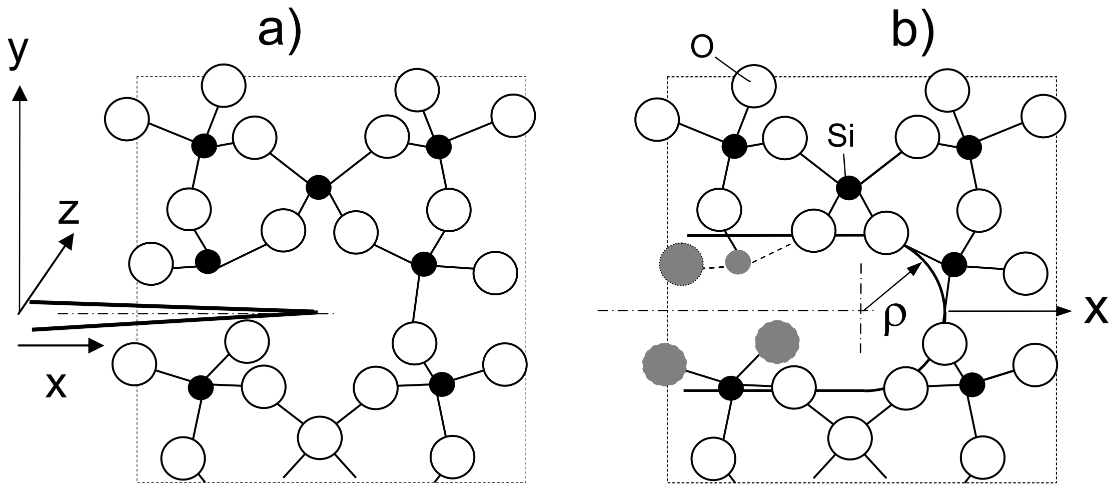

Fig. 1 a) Crack in silica terminating in a nano-pore, b) equivalent slender notch with a finite notch root radius ρ, grey molecules are mechanically inactive.

Whereas shielding stress intensity factors are well known for sharp cracks [2,3], there is a lack in multiaxiality behaviour of swelling stresses for the slender notch model. The individual swelling stress components and also the hydrostatic stress terms are necessary for computations on stress-enhanced equilibrium of the silica/water reaction. In contrast to *internal swelling*, the stress components by *externally applied* loading are known from Creager and Paris [4].

In the present note we carry out Finite Element computations in order to determine swelling stresses for the slender notch model as a function of the distance from the notch root and differently high swelling zones.

2. Finite element model

A single crack embedded in a swelling zone of height *h* and constant volume swelling is shown in Fig. 2. The crack length, *a*, is small compared to the specimen dimensions, realizing the edge-cracked semi-infinite body. On the other hand, the crack length is at least a factor of 10 larger than the notch radius ρ so that a "slender" notch is sufficiently guaranteed.

Zones of different heights were modelled in a finite element (FE) study. Solid continuum elements (8-node bi-quadratic) were chosen and the computations were carried out with ABAQUS Version 6.8. The volume strain was replaced by the equivalent thermal problem by heating the swelling zone by ΔT keeping T=0 in the rest of the structure.

This results in the strain

$$\varepsilon_v = 3\alpha\Delta T \tag{1}$$

(α=thermal expansion coefficient) with isotropic expansion in *x*-, *y*-, and *z*-directions

$$\varepsilon_v = \varepsilon_x + \varepsilon_y + \varepsilon_z \tag{2}$$

Requirements for the coordinate were chosen as "plane strain" as is fulfilled at crack tips.

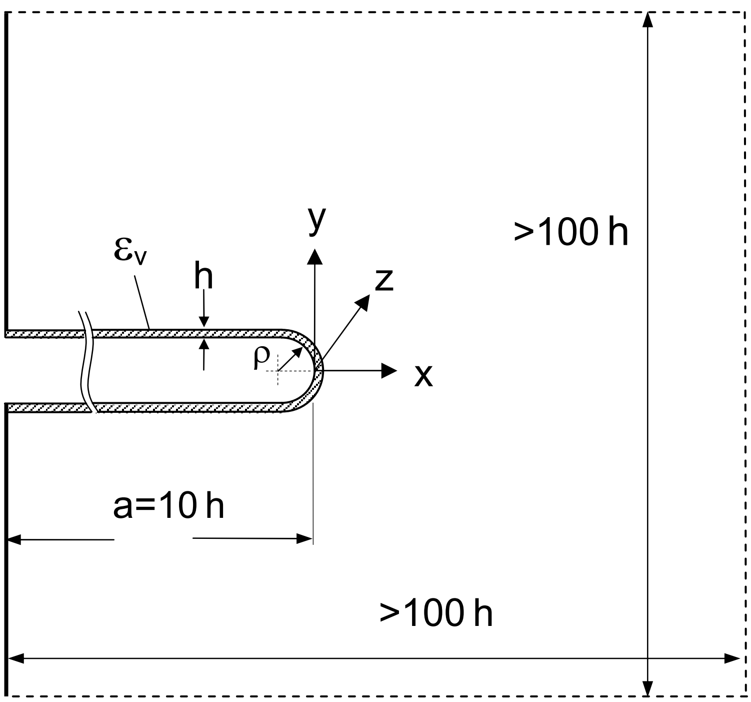

Fig. 2 Slender notch at a surface with swelling zone of thickness *h*.

3. Results

Swelling stresses in *x*-, *y*-, and *z*-directions are plotted in Fig. 3 for zone heights of h/ρ=0.2, 0.5 and 1.0. The black data represent the hydrostatic stress, defined by

$$\sigma_h = \tfrac{1}{3}(\sigma_x + \sigma_y + \sigma_z) \quad (3)$$

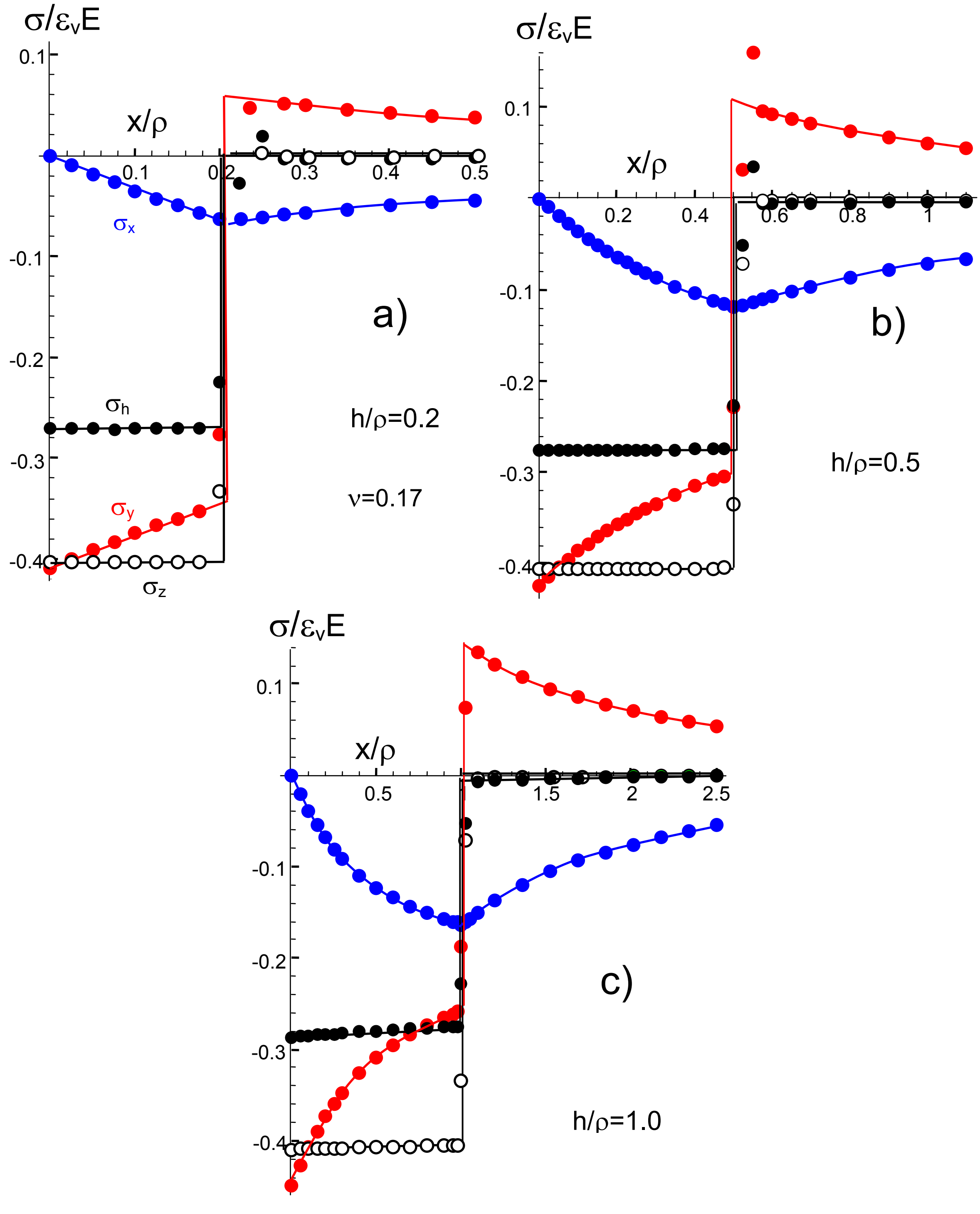

Fig. 3 Swelling stresses, normalized on the volume expansion strain for 3 different zone heights *h*.

Whereas all stresses are compressive within the swelling zone, they roughly disappear outside for the *z*-direction and for the hydrostatic stress. The *x*-component remains in compression and the *y*-component becomes tension as a consequence of the equilibrium condition.

The surface stresses ($x \rightarrow 0$) are represented in Fig. 4 as a function of the relative height h/ρ of the swelling zone. The squares indicate theoretically known values for an infinitely thin surface layer:

At a free surface, the stress state is plane stress and, consequently, also stresses caused by swelling are equi-biaxial (σ_x=0)

$$\sigma_y = \sigma_z = -\frac{\varepsilon_v E}{3(1-\nu)} \tag{4}$$

where E is Young's modulus and ν is Poisson's ratio. For silica it is ν=0.17, consequently: $\sigma/\varepsilon_v E = 0.4016$ for the *y*- and *z*-directions.

The hydrostatic stress reads

$$\sigma_h = \tfrac{1}{3}(\sigma_y + \sigma_z) = -\frac{2\,\varepsilon_v\,E}{9(1-\nu)} \tag{5}$$

i.e. $\sigma_h/(\varepsilon_v E)$=0.2677.

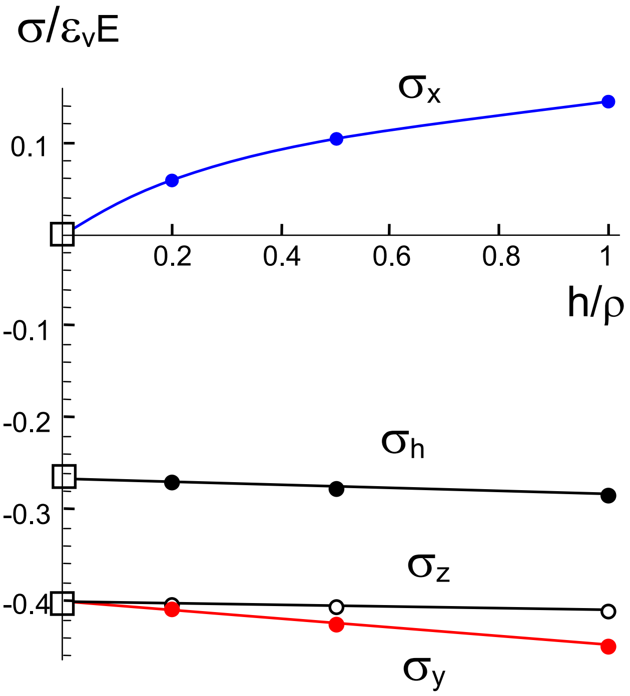

Fig. 4 Effect of zone height *h* on swelling stresses at the notch root, *x*=0.

In order to characterize the "multiaxiality" of the swelling stresses, we plot in Fig. 5a the hydrostatic stress normalized on the *z*-component. This parameter is 2/3≈0.67 for thin swelling layers and decreases slightly for σ_h/σ_y and increases for σ_h/σ_z. The variation over the swelling zones is negligible as can be concluded from Fig. 5b.

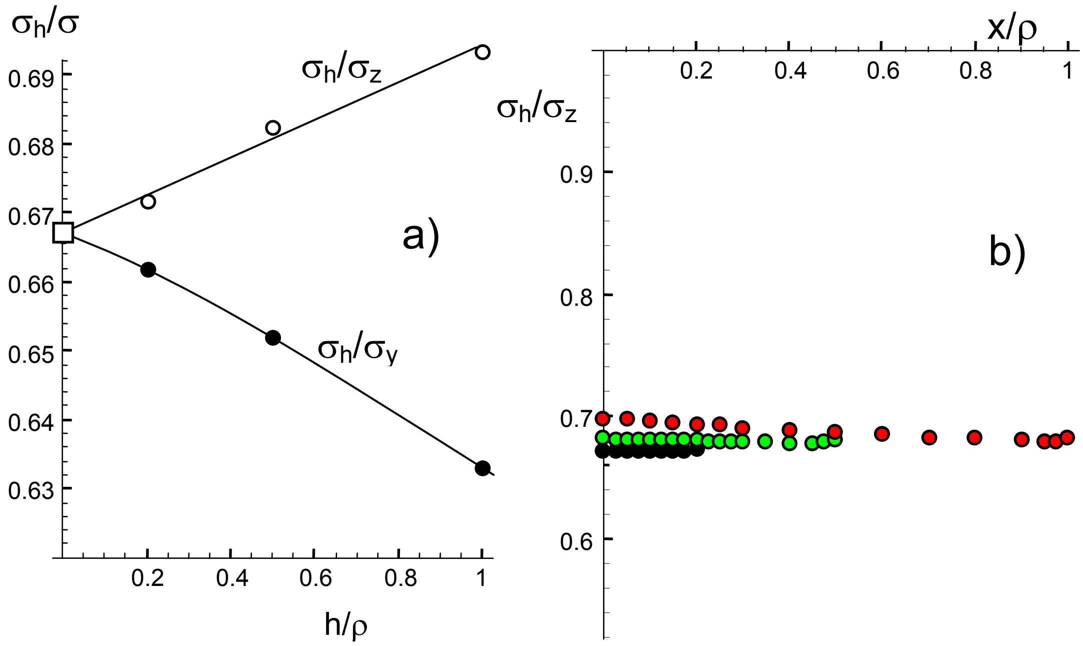

Fig. 5 a) Effect of zone height *h* on multiaxiality at the notch root, *x*=0, b) variation of the multiaxiality ratio σ_h/σ_z over the swelling zones.

4. Effect of finite notch length

From Fig. 3c it is visible that the hydrostatic swelling stress shows a small variation over the swelling zone. For an understanding of this small effect, we increased for $b/\rho=1$ the notch length to $a/\rho=30$. Figure 6a shows the effect for σ_h. In this plot the data for $a/\rho=10$ are represented by the black symbols, those for $a/\rho=30$ by the red ones. It is obvious that the variation over the region $0\le x\le b$ clearly decrease. In Fig. 6b the effect on the normal swelling stress σ_y is shown. Here the variation remains unaffected over the zone size. Only the absolute stress values shift slightly.

5. Including shielding stress intensity factors

Stresses at slender notches were given by Creager and Paris [4]. The stress component normal to the crack plane (the stress σ_y) is in distance *x* from the notch root

$$\sigma_y = \frac{2K}{\sqrt{\pi(\rho+2x)}}\frac{\rho+x}{\rho+2x} \tag{6}$$

The other stress components are

$$\sigma_x = \frac{2K}{\sqrt{\pi(\rho+2x)}}\frac{x}{\rho+2x} \tag{7}$$

$$\sigma_z = \frac{2\nu K}{\sqrt{\pi(\rho + 2x)}} \tag{8}$$

Consequently, the hydrostatic stress term from the applied stresses results as

$$\sigma_{appl,h} = \frac{2(1+\nu)K}{3\sqrt{\pi(\rho + 2x)}} \tag{9}$$

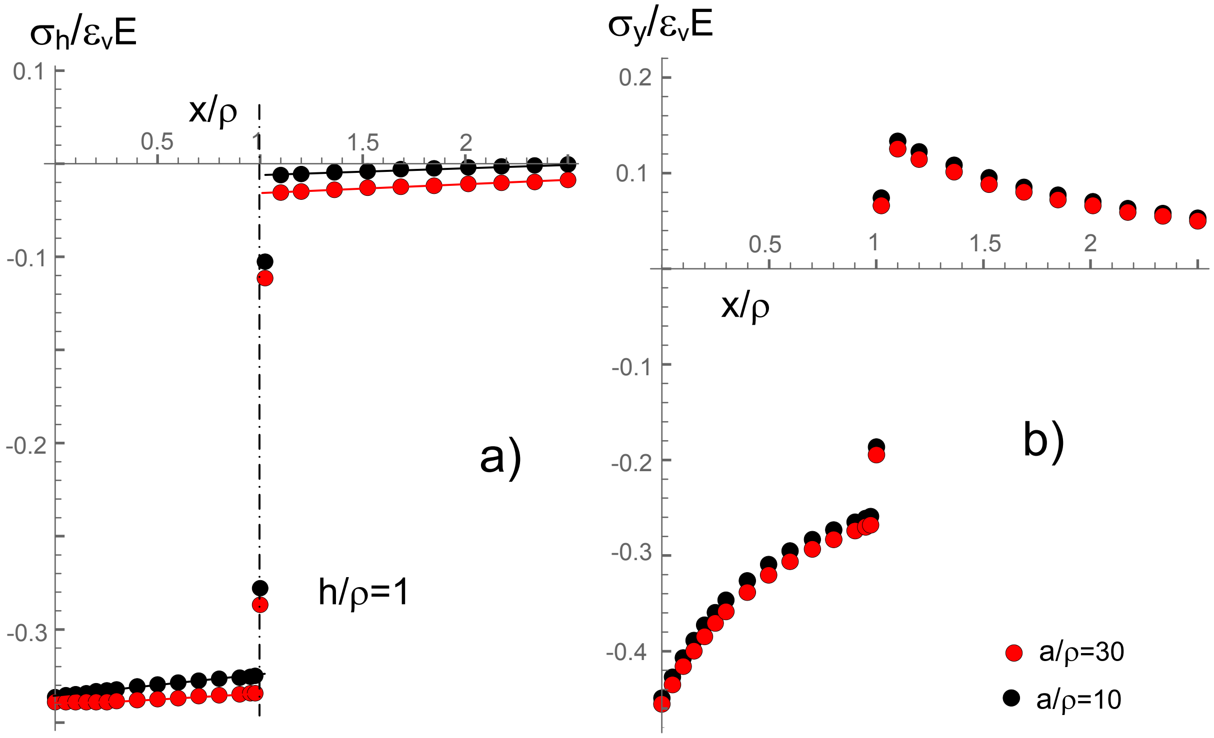

Fig. 6 Effect of the notch length on the hydrostatic and the normal swelling stress.

Equations (6-9) are valid for applied stress intensity factors K_{appl}, shielding stress intensity factors K_{sh}, and total stress intensity factor K_{tip}, which are defined as

$$K_{tip} = K_{appl} + K_h \tag{10}$$

The shielding stress intensity factor for an edge crack of finite length *a*, embedded in a swelling zone of height *b*, was already computed via FE in [5]. Results shown in Fig. 7 by the circles can be expressed by the relation

$$K_{sh}(b/a) \cong K_{sh}(0)\exp\left[-1.18\frac{b}{a}\right] \tag{11}$$

with

$$K_{sh}(0) = -\psi(0)\frac{\varepsilon_v E}{1-\nu}\sqrt{b} \tag{12}$$

and different zone shape [2]

$$\psi(0) = \begin{cases} 0.22 & \text{for heart shape} \\ 0.25 & \text{for semi circle} \end{cases} \tag{13}$$

This solution is shown in Fig. 7.

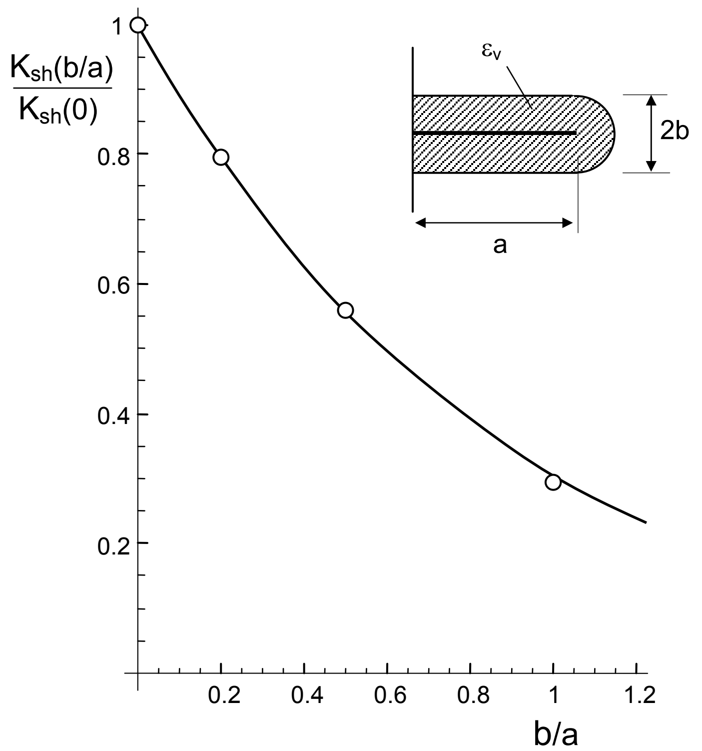

Fig. 7 Shielding stress intensity factor as a function of the relative zone height.

Now we can use this solution for the computation of the shielding stress intensity factor in eqs.(6-9), resulting in swelling stresses contributed by K_{sh}. The resulting stresses are then subtracted from the results in Fig. 3. The difference is the contribution by local swelling exclusively, i.e. for K_{sh}=0.

Two different procedures are now possible for the computation of swelling stresses:

- Fitting the dependencies of Fig. 8 and adding the swelling stresses caused by the shielding stress intensity factor.
- Use of the data in Fig. 3 directly because these values include already the shielding effect.

Since the resolved data of Fig. 8 vary clearly stronger with the distance x from the notch root it is recommended to use results of Fig. 3.

For the hydrostatic stress term it is suggested for $0<x\leq b$:

$$\sigma_h\left(\frac{x}{\rho},\frac{b}{\rho}\right) = -\frac{2\,\varepsilon_v\,E}{9(1-\nu)}\left(1+0.078\frac{b}{\rho}\right) \tag{14}$$

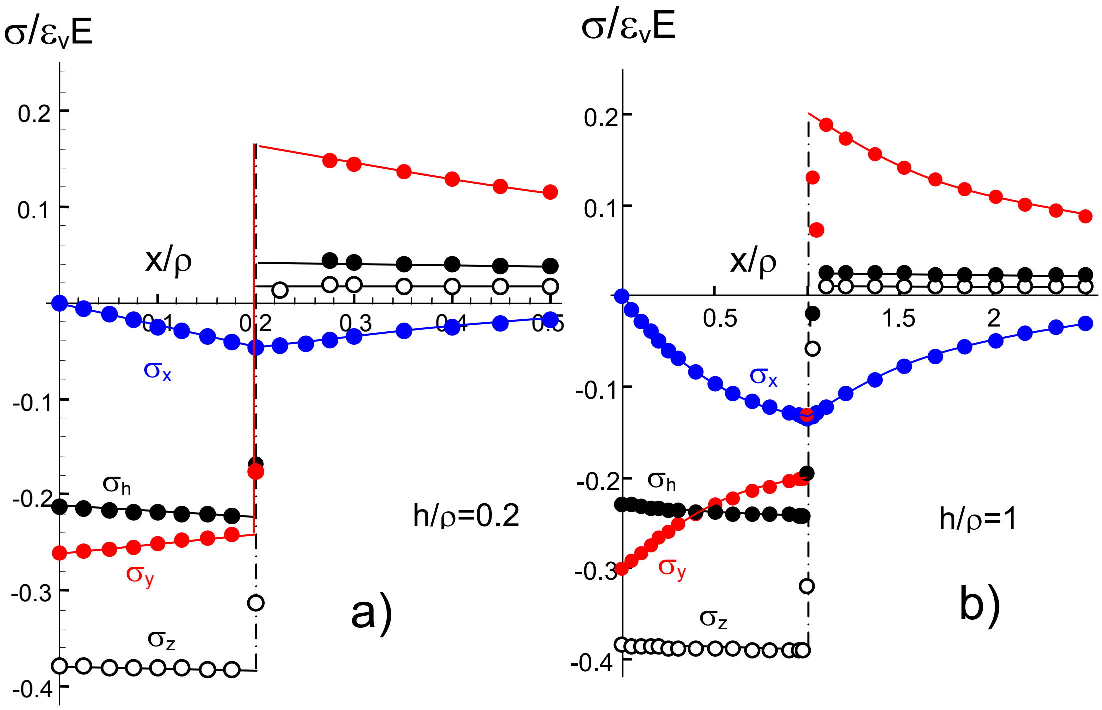

Fig. 8 Swelling stresses for a disappearing shielding stress intensity factor, K_{sh}=0.

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