

## Regular article

## Fracture surface energy and toughness of inorganic glasses



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## ABSTRACT

A simple model is proposed to predict the fracture surface energy ( $\gamma$ ) and the fracture toughness ( $K_{Ic}$ ) of glasses from their nominal compositions. The theoretical values are compared with the experimental ones, as obtained by means of self-consistent methods such as the Single Edge Pre-crack Beam (SEPB) and Chevron Notch (CN) ones, when available. A remarkable agreement is observed for ionocovalent glasses. This corroborates previous investigations showing that crack tip is nearly atomically sharp. In the case of metallic glasses, the theoretical values are much smaller than the experimental ones, which support the occurrence of crack tip plasticity and shielding effect.

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$K_{Ic}$  defines the resistance of a material to the extension of a pre-existing flaw (crack) in the opening mode, by far the most critical for brittle materials. Values smaller than  $2 \text{ MPa} \cdot \sqrt{\text{m}}$ , which are indicative of brittleness, are common for ionocovalent glasses while values above  $20 \text{ MPa} \cdot \sqrt{\text{m}}$  were reported for metallic ones (Fig. 1) [1–14]. Environmental effects (especially humidity) on fracture toughness are extensively documented in the literature. Therefore, neither these effects, nor the domain of surface treatments (thermal and chemical tempering, grinding and polishing, coatings), are considered in this short article.  $K_{Ic}$  can be deduced from  $\gamma$  associated with a stable fracture (tearing) process, Young's modulus ( $E$ ) and Poisson's ratio ( $\nu$ ). When plane strain conditions are supposed to prevail,

$$K_{Ic} = \sqrt{\frac{2\gamma E}{1-\nu^2}} \quad (1)$$

It is noteworthy that the possible mechanisms affecting the crack tip geometry as well as the surrounding process zone where the intensity of the stress field is large enough to promote dramatic events might be responsible for the crack extension regime toughness (deduced from Eq. (1)) being significantly different from  $K_{Ic}$  as obtained from the onset of crack extension by means of standard fracture toughness tests.

A relatively simple approach to predict  $\gamma$  and  $K_{Ic}$  in a quantitative manner consists in assuming that a propagating crack extends following a path disrupting the weakest links of the energy landscape, and to estimate the surface energy from the bond strength and the bond concentration along this fracture surface. The intrinsic (or theoretical)

fracture surface energy is obtained from the surface density of representative structural units and from the relevant bond strength. Let  $\rho$  and  $M_o$  be the glass density (specific mass) and the molar mass of a representative unit (gram-atom of glass), then the volume concentration of the gram-atom is expressed as:

$$\rho_v = \frac{\rho}{M_o} \mathcal{N} \quad (2)$$

where  $\mathcal{N}$  is Avogadro number.

The surface concentration is then

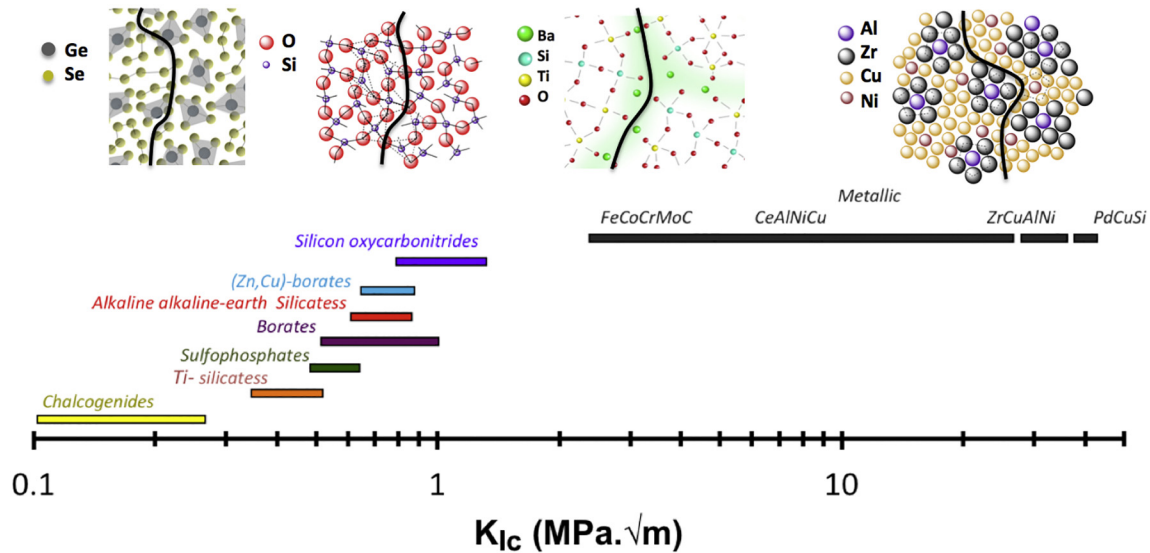
$$\rho_s = \left( \frac{\rho}{M_o} \mathcal{N} \right)^{2/3} \quad (3)$$

A plausible value for  $\gamma$  is obtained by considering the number and the type of bonds involved in the fracture process as the crack proceeds through the considered structural unit. Let  $x_i$  be the stoichiometric fraction of the species involved in the  $i$ th bonding energy  $U_{oi}$  (in  $\text{J} \cdot \text{mol}^{-1}$ ), between the  $i$ th cation ( $A_i$ ) and a first neighbor oxygen anion in the case of an oxide glass, and let  $n_i$  be the number of such bonds supposed to be broken as the crack front propagates to the next unit, then  $\gamma$  is expressed as

$$\gamma = \frac{1}{2} \left( \frac{\rho}{M_o} \right)^{2/3} \mathcal{N}^{-1/3} \sum_i x_i n_i U_{oi} \quad (4)$$

where the  $1/2$  prefactor on the right hand side member accounts for the fact that the bond disruption process leads to the formation of two complementary surfaces.

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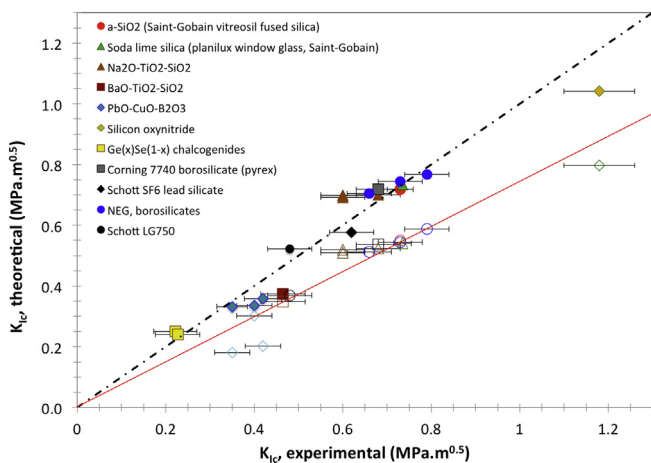
**Fig. 1.** The apparent fracture toughness of glasses, as obtained by means of various experimental methods [1–14]. The schematic drawings depict the expected crack path, tending to follow the weakest links of the atomic network (for example the Ba–O bonds in the BaO(30)–TiO<sub>2</sub>(30)–SiO<sub>2</sub>(40) glass).

It is noteworthy that the A<sub>i</sub>–O bond dissociation energy in a glass network is usually not known accurately. U<sub>oi</sub> was taken either as the dissociation enthalpy of the A<sub>i</sub>xO<sub>y</sub> compound (D°(A<sub>i</sub>xO<sub>y</sub>)) divided by x and by the coordination number of A<sub>i</sub> to oxygen (empty marks in Fig. 2), following the approach suggested by Sun [15], or as the A<sub>i</sub>–O bond dissociation enthalpy (D°(A<sub>i</sub>–B)) or fission enthalpy (solid marks in Fig. 2), where the thermochemical characteristics were taken from ref. [16]. It turns out that a better correlation between experimental and theoretical K<sub>Ic</sub> values is obtained with D°(A<sub>i</sub>–B), although this latter parameter significantly overestimates the bond strength in the network.

The actual volume occupied by the gram-atom of glass is larger than the sum of the volumes of the individual atoms constituting this unit, as estimated from the ionic radii,  $\sum_i 4/3\pi r_i^3$ . This is where the atomic packing density (C<sub>g</sub>) comes into play

$$C_g = \frac{\sum_i 4/3\pi r_i^3}{V_o} \quad (5)$$

where V<sub>o</sub> (= M<sub>o</sub>/ρ) is the molar volume (gram-atom).



**Fig. 2.** Theoretical K<sub>Ic</sub> values (from γ, Eqs. 1 and 4) as a function of experimental values obtained by means of self-consistent methods, using either the diatomic fission enthalpy (solid marks) or the compound dissociation enthalpy (empty marks) for the calculation of U<sub>oi</sub> in Eq. 4. The red line corresponds to K<sub>Ic,theo</sub> ≈ 0.7 K<sub>Ic,exp</sub>.

Let's further write  $\langle U_o \rangle$  the mean bond strength considered in the fracture process,  $\langle U_o \rangle = \sum_i x_i n_i U_{oi}$ , then γ can be written

$$\gamma = \frac{1}{2} \left( \sum_i 4/3\pi x_i r_i^3 \right)^{-2/3} \mathcal{N}^{-1/3} C_g^{2/3} \langle U_o \rangle \quad (6)$$

Eqs. (4) to (6) were applied to 23 glasses with known elasticity and fracture toughness characteristics (Table 1) (Fig. 2), including 7 commercial glasses from different glass making companies [1–14].

### 1.1. Amorphous silica

a-SiO<sub>2</sub> is characterized by a low atomic packing density preventing from reaching high elastic moduli and toughness in spite a relatively strong interatomic bonding. Indentation cracking methods (IF) sounds inappropriate for the estimation of K<sub>Ic</sub> of a-SiO<sub>2</sub> and SiO<sub>2</sub>-rich glasses since densification in those glasses (due to a significant free volume content) impedes the formation of the radial/median crack system. In these latter cases, the absence of surface radial cracks extending from the indentation corner cannot be related to a dramatic improvement of K<sub>Ic</sub>. The gram-atom writes Si<sub>1/3</sub>O<sub>2/3</sub> and weighs 20 g/mol. With a specific mass of 2.2 g·cm<sup>-3</sup> for a-SiO<sub>2</sub>, this gives a molar volume of 9.1 cm<sup>3</sup> (V<sub>o</sub> = M<sub>o</sub>/ρ). A surface concentration of the gram-atom unit of 1.64 10<sup>19</sup> m<sup>-2</sup> is further obtained by means of Eq. (3). The fracture surface energy is then calculated using Eq. (4) considering that one Si–O bond is broken per Si–O<sub>4/2</sub> tetrahedron (n<sub>i</sub> = 1 in Eq. (4)) since the crack front travels to the next unit once a Si–O–Si bridge between two tetrahedra is broken. With a diatomic bond energy of 799 kJ·mol<sup>-1</sup> for the Si–O bond, this gives a value of 3.62 J·m<sup>-2</sup> for γ. A theoretical prediction for K<sub>Ic</sub> is then achieved by means of Eq. (1), taking (E,ν) = (70 GPa, 0.15). A value of 0.718 MPa·√m is finally reached, which is in excellent agreement with the experimental values (0.73) as measured using the DCC method, in inert environment to prevent against moisture effects [1]. The agreement between the theoretical and experimental values without accounting for any reconstruction process and possible relaxation mechanism at the crack tip, suggests that the fracture surface energy is strongly correlated to the Si–O bond dissociation reaction, and to the surface concentration of such bonds. Note that the Si–O bond strength (~465 kJ·mol<sup>-1</sup>) ~ as deduced from the SiO<sub>2</sub> dissociation enthalpy results in a significantly smaller K<sub>Ic</sub> value (0.549 MPa·√m).

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