Silicate glass, hydration, chemistry and defects

Author: Russell J Hand and Damir R Tadjiev Department of Engineering Materials, University of Sheffield, Sir Robert Hadfield Building, Mappin Street, Sheffield, S1 3JD, UK

Abstract:

What constitutes a strength controlling defect in silicate glasses? In most situations this question remains unanswered so that we are not able to identify *a-priori* those feature that will control the strength of glass. What seems clear is that ultimately such defects must bear some relationship to the underlying structure of the glass as well as being affected by interactions with mobile atmospheric species such as water. If there is a linkage with the underlying glass structure then it is reasonable that there are relationships between mechanical properties and composition. However because bulk production of silicate glasses is based around a narrow range of soda-lime-silica compositions any variation in mechanical properties with composition is normally considered to be of little interest and thus has been relatively little studied. It might also be said that mechanical contact during manufacture is the dominant factor in determining defect formation, yet it seems reasonable to suggest that defects are still formed preferentially at specific sites within the glass surface.

Furthermore those studies of the variation of mechanical properties of glasses with composition that have been made over the last 50 years or so have demonstrated some intriguing variations of properties such as toughness, brittleness and, more controversially, strength with composition. Although far from conclusive, such studies have led to suggestions that the equilibrium crystalline structures corresponding to a particular glass composition or alternatively that non-annealable composition dependent residual stresses have a bearing on the observed mechanical properties of the glass. Also from consideration of the wider literature it is clear that interactions of glass surfaces with species such as atmospheric water are composition dependent.

To try to address some aspects of the above we have been studying the effects on the near surface mechanical properties of a range of alkali-mixed alkaline earthsilicate glasses. The range of glasses has been studied using nanoindentation to assess the reduced modulus and hardness before and after immersion in water and using micro-hardness indentation to study the toughness, hardness and brittleness of the glasses. As well as looking at some of the wider questions mentioned above this presentation will review the results we have obtained to date and will attempt to draw out some wider conclusions concerning the compositional dependences of the mechanical properties of silicate glasses.

Questions to be answered:

1.) What will be a topic stating an exceptional success to be published in a well known high ranking Research Journal in 2025 concerning your presented R&D field of work? Please think in headlines.

Dream headline: Scientists find a way of preventing defects in glass!

More realistic headlines:

Identification of structural sites in glass where strength controlling defects preferentially form.

A-priori identification of strength controlling defects in glass objects.

2.) Please name up to 10 future key challenges (till 2025) regarding your presented field of expertise and indicate please the specific year when you expect the topic to become a real bottleneck for the future developments. The bottlenecks already exist.

One key challenge is actually understanding the linkage between the (nano)structure of glasses and the macroscopic mechanical properties. We could probably argue that until our structural models can deal with suitably large arrays of atoms (many times larger than we do currently) that any real developments in this area will be very limited. In the meantime experimental measurements may lead to useful empirical correlations and possibly breakthroughs in understanding.

Another key challenge is resolving defects with sub-micron widths on macroscopic objects in a non-destructive fashion.

3.) Concerning the topics, what would be

a) the key breakthrough and when is it likely to occur

b) what must happen concerning the research field if this topic will never be successful

Key breakthroughs

Direct a-priori observation of strength controlling defects (other than extremely large controlled damage)

Predictive, albeit probably empirically based, models for mechanical properties as a function of composition

Atomistic modelling of glass structures and surfaces with the number of atoms being of the order of Avogadro's number!