FRI-1.417-2-MEMBT-01

INFLUENCE OF THE PHASE TRANSFORMATION RATE OF NICKEL-SULFIDE INCLUSIONS ON THE STRESS CONCENTRATION IN TEMPERED GLASS

Assoc. Prof. Veselin Iliev, PhD
Department of Applied Mechanics,
University of Chemical Technology and Metallurgy
Phone: 02-8361 467
E-mail: veso@ustm.edu

Abstract: *The presence of nickel sulfide inclusions in tempered glass usually results in a sudden rupture caused by the sharp volume increase of the inclusion during its phase transformation. Preventions of such defects at the flat glass production process is impossible for now. They often cause micro cracks and breakage of the glass.*

This work presents a study of the stress-strain state around the inclusion with phase transformation inhomogeneity, the conditions for the cracks formation and the stress concentration around them. The study is implemented by numerical simulations using the analogy between temperature and phase expansion. The crack propagation is evaluated by the stress intensity. The volume change during allotropic transformation is modeled using different coefficients of temperature expansion for alpha and beta phases.

Keywords: *Nickel-Sulfide inclusion, temperature expansion, stress-strain analisis, numerical analysis.*

INTRODUCTION

The phenomenon of spontaneous breakage of tempered glass caused by nickel-sulfide inclusions (NiS) was originally investigated by Ballantyne (Ballantyne, E., 1961). In his work, the various types of inclusions have been identified and it has been found that the position of the inclusion in the glass pane is important in terms of the likelihood of cracking. Subsequently, other authors provide additional evidence to support these findings, and it has been found that NiS-containing with a composition of approximately 65 weight % of Ni and 34 weight % of S are generally primarily responsible for the spontaneous breakage of the tempered glass.

These inclusions undergo a phase transformation from high temperature hexagonal form in a low-temperature rhombic form (R-phase) at a temperature of about 380 ° C (the exact phase change temperature depends strongly on the phase transformation stoichiometry). It has been found that only one phase of the inclusion is left in the glass during the fast-cooling process. However, after subsequent heating, the inclusion may be converted into the R-phase at conversion time being a sensitive function of the temperature. A study of the process of forming microcracks around phase transformed inclusion and comparison of the results, obtained with a traditional analysis performed by the fracture mechanics is presented in (Swain, M., 1981). A generalized mechanical analysis of crack formation from such inclusions was developed in this work with the values, set out in Table 1.

Table 1. Thermo-mechanical properties of materials

Property	Glass	NiS inclusion	
		alfa phase	beta phase
Module of elasticity E, Nm^{-2}	7.0×10^{10}	8.0×10^{10}	7.0×10^{10}
Poisson ratio ν, –	0.23	0.27	0.20
Density ρ, Kg/m^{-3}	2.51×10^{3}	5.46×10^{3}	5.25×10^{3}
Thermal expansion α, K^{-1}	88×10^{-7}	163×10^{-7}	145×10^{-7}

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These relatively old studies largely reveal the theoretical foundations of the phenomenon do not answer the question: how to prevent its negative effects. Activities undertaken in this direction are rather imposed by practice (Lawn, B.R. & E. R. Fuller, 1975) (Wagne, R., 1977) (Lawn, B.R. & A.G. Evans,1977) (Gromowski, K., 2010) and open new areas of research. The existing theoretical dependencies and recent studies in (Barry, J., & Ford, S., 2001) and (Balan, B., & Achintha, M., 2015) are taken into account in this paper. The stress-strain fields around inclusion with non-homogeneity of phase transformation, crack formation conditions and stress concentration are investigated. The study is implemented by numerical simulation using the analogy between temperature and phase expansion. The crack propagation is estimated by the maximum value of the principal stresses. The change in volume during allotropic transformation is modeled using coefficients of temperature expansion, different for the alpha and beta phases.

STATEMENT OF THE STUDY

Volumetric deformation at phase transformation of NiS

Allotropic transformations of NiS inclusions in glass at their phase changes from high temperature alpha phase to low temperature beta phase cause about 4% change in volume. That can be described by the following expression (Swain, M., 1981):

$$\frac{\Delta V}{V} = \frac{\rho_\alpha}{\rho_\beta} - 1 , \qquad (1)$$

where ρ_α is the density of the α-phase and ρ_β is the density of the β-phase. Taking a spherical shape for the inclusion, as it's shown in fig. 1, the stress, caused by the bulk expansion is given by the expression:

$$\sigma_r = -2\sigma_t = -P_O \left(\frac{R}{r}\right)^3 \; ; r \ \geq R , \qquad (2)$$

where σ_r and σ_t are the radial and circular stresses, R is the radius of the inclusion, r is the distance from the center of the inclusion, and P_O is the hydrostatic pressure.

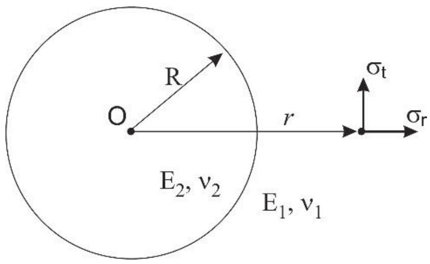

Fig.1 Spherical inclusion parameters

Another expression, given in the same source, is about the radial deformation $\frac{\Delta R}{R}$:

$$\frac{\Delta R}{R} = P_O \left(\frac{1+\nu_1}{2E_1} + \frac{1-2\nu_2}{E_2}\right) = \frac{\Delta V}{3V} , \qquad (3)$$

where ν_1, E_1 and ν_2, E_2 are the Poisson ratio and the modulus of elasticity respectively for the base material and the inclusion. By replacing $\frac{\Delta V}{V}$ from (1) in (3) the resulting pressure is:

$$P_O = -\left(\frac{\rho_\alpha}{\rho_\beta} - 1\right) /3 \left(\frac{1+\nu_1}{2E_1} + \frac{1-2\nu_2}{E_2}\right) , \qquad (4)$$

A value of 834 MPa is obtained from eq. (4) with the values of Table 1.

In addition, the stress caused by the volumetric expansion can be obtained by the stress (σ)–strain (ε) ratio under the law of Hook: σ = E ε.

For a spherical inclusion of diameter D, the deformation can be obtained as the ratio of the lengthened circumference S =$\pi D^4/4$ and the initial circumference S_{in} of the inclusion ($\varepsilon = \frac{S-S_{in}}{S}$, Fig.2). For inclusion with diameter D = 100μm and glass elastic modulus E = 70 GPa the volume expansion is 4% ang the resulting normal stress is approximately 920 MPa.

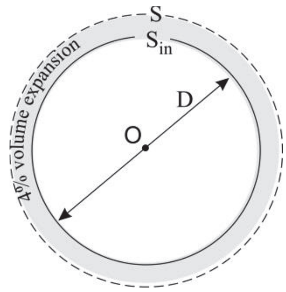

Fig.2 Cross section of spherical inclusion

These two techniques allow to determine stresses caused by a spherical isotropic inclusion and complete phase transformation by a relatively simple way. The computational procedure for the ellipsoidal or lentic form of inclusion and incomplete transformation is considerably more complicated. In this case, it is necessary to use more powerful computing tools and numerical simulation. The ANSYS Workbench platform is used in the current work for numerical simulation of these processes. NiS particles in flat tempered glass with different sizes and stages of phase transformation are studied. Nominal stresses and stress intensity coefficients are computed for variations of nominal diameters from 50μm to 400μm. The obtained results give opprtunity to estimate the initiation and propagation of the cracks and the reliability of the product.

Model

A three-dimensional spherical inclusion pattern in a 4 mm thick glass plate is created for the purposes of the present investigation. The geometry of the object is modeled in the Ansys Design Modeler environment. The study is performed with respect to the three principle planes at 1/8 of the volume around the particle because of the existing of symmetry (Fig.3).

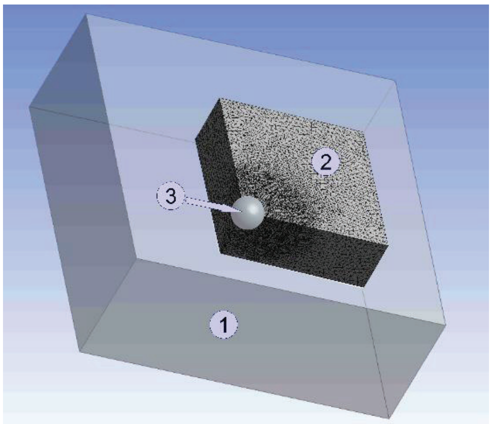

Fig. 3 Geometric model
1 – glass domain; 2 - calculational volume; 3 - spherical inclusion.

Finite element analisys of the stress-strain field is obtained by a mech with 116420 nodes and 74000 Solid187 elements from the ANSYS library. The volumetric strain ε_v is derived from the volumetric-axial strains relationship:

$$\varepsilon_v = \varepsilon_x + \varepsilon_y + \varepsilon_z = 3\varepsilon^{el} \quad (5)$$

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The volume expansion is modeled as a temperature expansion at a temperature difference of 100°C and a coefficient of thermal expansion for NiS of $1.33.10^{-4}$, which corresponds to 4% volume strain, forming the temperature deformation vector $\{\varepsilon^t\}$. The vector of elastic deformation is obtained by eq. (5) and the full deformation vector $\{\varepsilon\}$:

$$\{\varepsilon\} = \{\varepsilon^{el}\} + \{\varepsilon^t\}. \tag{6}$$

The vector of full deformation takes part in the formation of the virtual energy of the deformation at applying the principle of virtual work:

$$\delta V = \delta U_1 = \int_{Vol} \{\delta\varepsilon\}\{\sigma\} d(Vol)^T, \tag{7}$$

where U_1 is the deformation energy (work of internal forces), V = work of the external forces, δ = operator, $\{\sigma\}$ = stress vector, Vol = investigated volume.

The stresses in the computational volume (the components σ_x ,σ_y, σ_z, σ_{xy},σ_{xz}, σ_{yz} of the stress-vector $\{\sigma\}$) can be determined by minimizing functional (7). Since the glass is a brittle material, the fracture criterion is derived from the maximum principal stress σ_1, obtained from the cubic equation:

$$\begin{vmatrix} \sigma_x - \sigma_1 & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_y - \sigma_1 & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_z - \sigma_1 \end{vmatrix} = 0 \tag{8}$$

The inclusion is in the center of the investigated volume and at the point of intersection of the three planes of symmetry. Three of the boundaries of the computational volume are planes of symmetry and others are free surfaces - these determine the boundary conditions (Fig. 4 and Table 2).

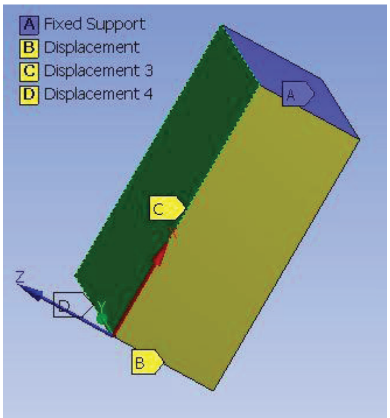

Fig. 4 Boundary conditions (coordinates starts at the center of the Inclusion)

Table2. Boundary conditions according to Fig.4

Boundary	Fixed Support	Displacement	Displacement 3	Displacement 4
X displacement	zero	free	free	zero
Y displacement	zero	zero	free	free
Z displacement	zero	free	zero	free

In the case of a crack the stresses in the crack front are computed by the linear fracture mechanics theory: $\sigma_{ij} = \frac{K}{\sqrt{\rho}} f_{ij}(\theta)$, where K is the stress intensity factor for the respective deformation, ρ is the distance from the tip and θ is the angle to the plane of the crack. For example, for the first mode of fracture (opening) the stresses are (Ansys Documentation, 2015, Fig. 1):

$$\sigma_r = \frac{KI}{\sqrt{2\pi\rho}} cos\left(\frac{\theta}{2}\right)\left[1 - sin\left(\frac{\theta}{2}\right) sin\left(\frac{3\theta}{2}\right)\right],$$
$$\sigma_t = \frac{KI}{\sqrt{2\pi\rho}} cos\left(\frac{\theta}{2}\right)\left[1 + sin\left(\frac{\theta}{2}\right) sin\left(\frac{3\theta}{2}\right)\right],$$
$$\sigma_{rt} = \frac{KI}{\sqrt{2\pi\rho}} cos\left(\frac{\theta}{2}\right) sin\left(\frac{\theta}{2}\right) sin\left(\frac{3\theta}{2}\right).$$

EXPERIMENTS AND RESULTS

For the purposes of this study numerical experiments are initially performed to determine the influence of the diameter of the inclusion on the maximum value of the principal stresses at full phase transformation. Calculations are performed at variations of the initial diameter of 50 μm to 400 μm.

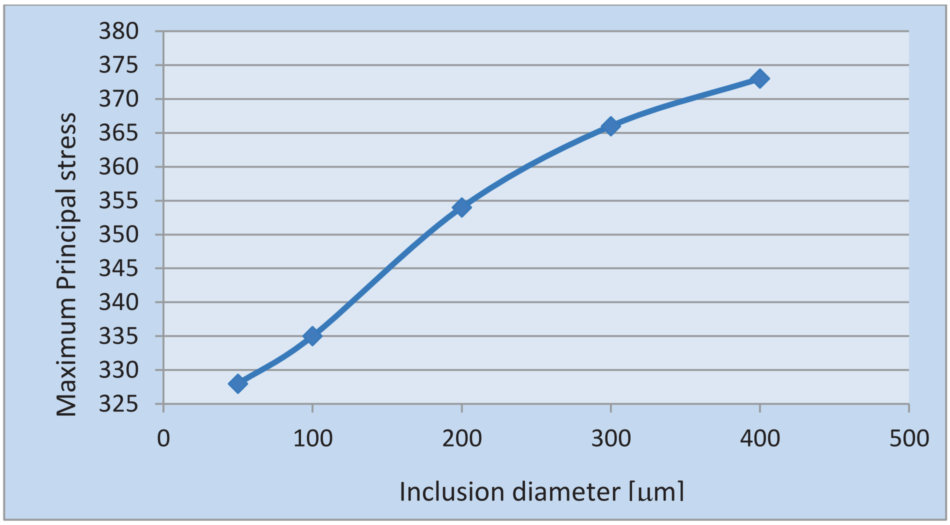

Fig. 5 Normal stress during full phase transformation

The results show that at these diameters the maximum stress far exceeds the strength of the glass, indicating that even the inclusions with insignificantly sizes would lead to destruction at full phase transformation (Figure 5). At the same time there are sufficient sources (e.g. Oussama Yousfi et al., 2010) showing that in many cases the phase transformation of the inclusion is not homogeneous and complete. Fig. 6 shows the results of an incomplete inclusion transformation study (10 to 100 percent). The results show that fracture of the material in the absence of additional load can be expected with a stage of transformation of 20% and higher.

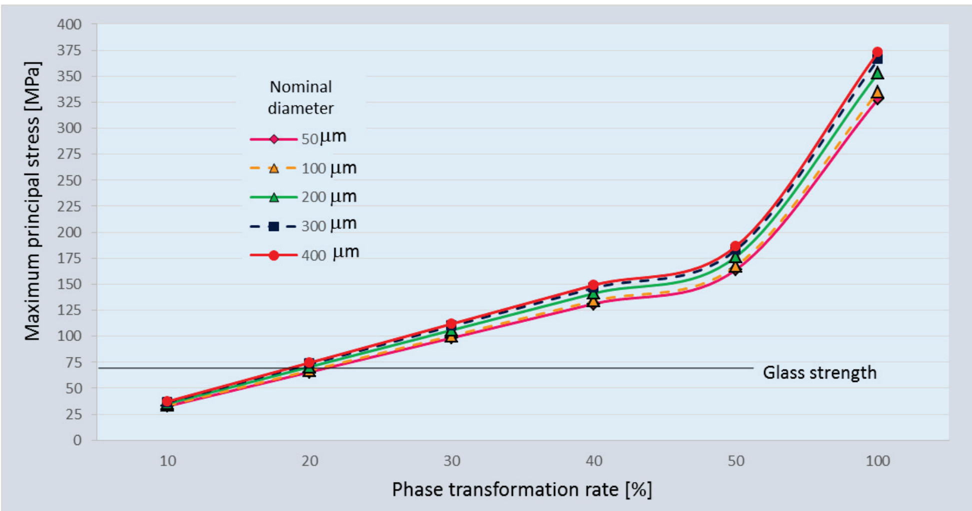

Fig. 6 Normal stresses at incomplete phase transformations

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Cracks with lengths of 50 μm and 200 μm are included in the studied domain in order to determine the impact of possible defects (cracks) on the stresses around the inclusion. Since the direction of the maximal (first) principal stress is in the circular direction (Fig. 7), the plane of the examined cracks is located radially in relation to the inclusion. A Solid185 element with 18 knots and 3 degrees of freedom at the node from the Ansys library is used to model the crack (Fig.8).

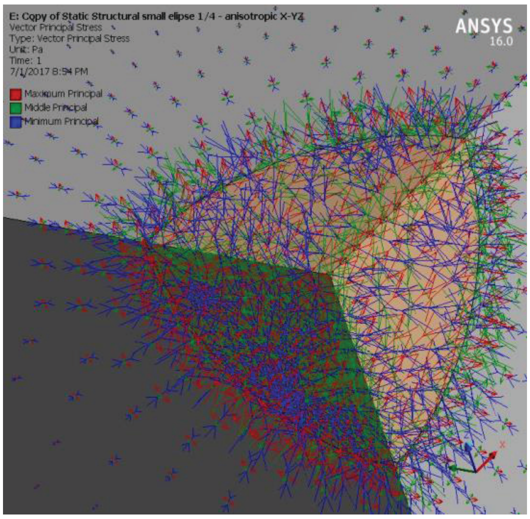

Fig.7 Vector distribution of the principal stresses around the inclusion

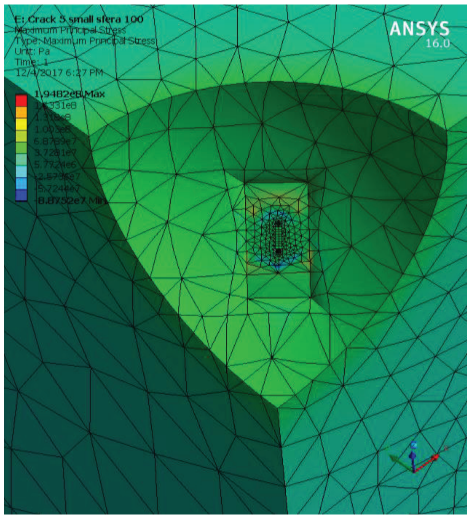

Fig. 8 Mesh of the domain at crack investigation

The results of the numerical experiments show that in the presence of a crack, the tensile normal stresses reaches the material strength at a transformation stage of the inclusion significantly lower than 20%. Fig. 9 shows results for maximum stress at 10% phase transformation, two crack lengths and three inclusion diameters.

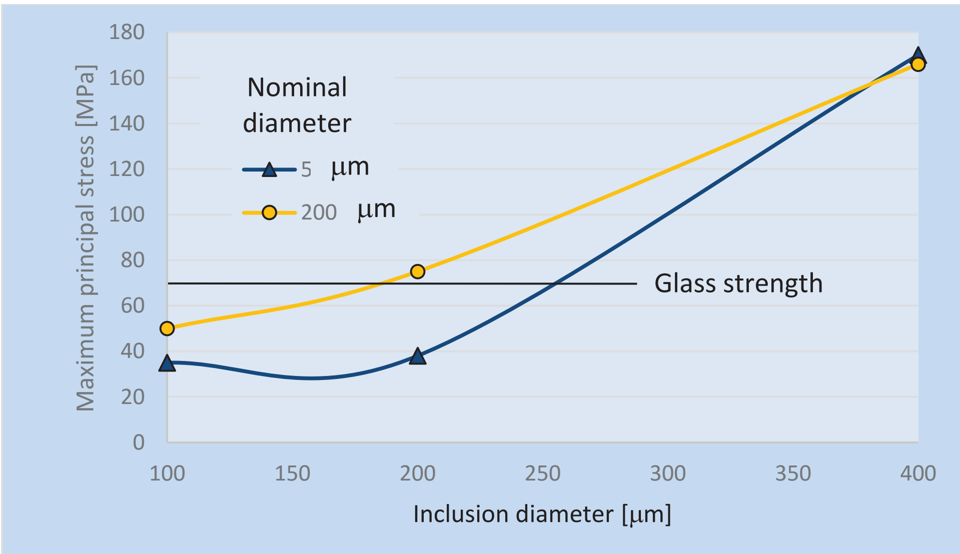

Fig. 9 Maximal stress at 10% inclusion phase transformation

CONCLUSIONS

The nickel-sulphide inclusions in the tempered glass at full phase transformation cause normal stresses higher than the strength of the basic material. The glass strength can be achieved at phase transformation stages between 18% and 22% depending on the diameter of the inclusion.

These values are significantly reduced in the presence of defects in the vicinity of the inclusion and can reach 10% at diameter up to 200μm.

The author is grateful for the financial support of the project DFNI E 02/17 "Parametric analysis for estimation of the efficiency of transparent structures in solar energy utilisating systems" funded by Bulgarian Ministry of education.

REFERENCES

Ansys Documentation (2016). Fracture Mechanical Guide. Release 16.0 - © SAS IP, Inc.

Balan, B. & Achintha, M. (2015). Assessment of Stresses in Float and Tempered Glass Using Eigenstrains. Experimental Mechanics (2015) 55:1301–1315

Ballantyne, E. (1961). Division of Building Research, CSIRO, Melbourne, Australia, Report 061-5 (1961).

Barry, J., & Ford, S. (2001). An electron microscopic study of nickel sulfide inclusions in toughened glass. JOURNAL OF MATERIALS SCIENCE 36 (2001) 3721 – 3730

Davidge, R.W. & J. T. Green, The Strength of Two-Phase Ceramic/. Glass Materials, J. Mater. Sci. 3 (1968) 629.

Evans A.G., The role of inclusions in the fracture of ceramic materials, J. MaterSci. 9 (1974) 1145.

Gromowski, K. , Glass Breakage - Nickel Sulfide Inclusions. BAE/MAE, Penn State, 2010

Hsiao, C.C., Spontaneous Fracture of Tempered Glass, Fracture 1977 Vol.3, pp.985

Lange, F.F. (1974). "Fracture Mechanics of Ceramics" Vol. 2, edited by R. C. Bradt, D. P. Hasselman and F. F. Lange (Plenum Press, New York) p. 599.

Lawn, B.R. & A. G. Evans. (1977). A model for crack initiation in elastic/plastic indentation fields. Journal of Materials Science, 12/2195.

Lawn, B.R. & E. R. Fuller. (2016. Equilibrium penny-like cracks in indentation fracture. Journal of Materials Science, 10 (1975) 2016.

Oussama Yousfi et al. (2010). Phase transformations in nickel sulphide: Microstructuresand mechanisms. Acta Materialia 58 (2010) 3367–3380

Swain, M. (1981). Nickel sulphide inclusions in glass: an example of microcracking induced by a volumetric expanding phase change. JOURNAL OF MATERIALS SCIENCE 16 (1981) 151-158

Wagne, R., Inclusions de sulfure de nickel dans le verre, Glastechn. Ber. 50 (1977) 296.

