Numerical Simulation of Ion Transport with Oxide Layer Growth During Anodic Bonding

F. F. Paes[1], M. Fabbri[2]
[1]Laboratory for Computing and Applied Mathematics - LAC
[2]Associate Laboratory of Sensors and Materials
Brazilian National Institute for Space Research - INPE
C. Postal 515 – 12245-970 – São José dos Campos - SP
BRAZIL
E-mail: fabiana.paes@lac.inpe.br, fabbri@las.inpe.br

Keywords: anodic bonding, electrostatic bonding, depletion layer, moving boundary problems.

1. INTRODUCTION

Anodic bonding was introduced by Wallis and Pomeranz in 1969, and is nowadays an important industrial technique for metal or semiconductor glass sealing. The bonding takes place by oxide formation at the metal-glass interface, which is achieved through ionic transport within the glass driven by an external potential. Typically, good quality bonding requires temperatures around 300_oC and electric fields near $3\infty10_5$ V/m.

Numerical modeling of anodic bonding has to deal with the transport of, at least, two distinct ionic species within the glass. For commercial Pyrex, a high sodium containing glass, both Na$_+$ cations and $_{-2}$ O anions counter-migrate within the glass, and an essentially neutral depletion zone is formed near the metal-glass interface, where the arriving oxygen anions build the bonding through metal oxidation. The whole process takes less than a minute.

In a previous work by the Authors (Fabbri and Senna, 2004), a non-uniform movingboundary finite difference scheme was developed to study the electrostatic properties of the depletion layer build-up. Results from the numeric model agree well to the observed electric transient during bonding, and suggest appreciable high-field oxygen mobility within the glass. The external electric current, the depletion layer width and the electric field profile were all accounted for and yield consistent values, when compared to the available experimental data. Those results indicate that anion transport into the glass occurs at very early stages of the bonding process.

The oxygen required for oxide formation at the metal-glass interface are thought to be provided either by the natural humidity near the glass surface prior to bonding (Nitzche et al.,1998) or by oxygen anions coming from the bulk depleted glass (Carlson et al., 1972). In this work we develop a detailed numerical model to account for the oxide growth at a typical silicon-glass bonding process, where all ionic species are originated solely from the depletion process in the glass. The numeric results are then compared with the recent measurements of Helvoort et al. (2004) of the oxide layer thickness and the depletion layer width.

2. IONIC CHARGE TRANSFER WITHIN THE GLASS

The electrostatic and field-drift model for the transport of ionic species was addressed in a previous work (Fabbri and Senna, 2004), and is only briefly outlined here. Denoting by Γ(t) the position of the depletion layer front inside the bulk glass (Fig. 2), and by J$_+$ the charge flux of the sodium cations, the advancement of Γ during the time interval dt, in the absence of carrier diffusion, is

$$d\Gamma = J_+ dt \tag{1}$$

The transport of anions is governed by a continuity equation for the oxygen charge density r_ ,

$$\frac{\partial \overline{\rho}}{\partial t} = \frac{\partial J_-}{\partial x} \tag{2}$$

The electric field build-up in the depletion layer follows Poisson law:

$$\frac{\partial E}{\partial x} = \frac{\rho}{\varepsilon}, \tag{3}$$

where ρ is the local net charge density and ε is the dielectric constant of the depletion layer medium. The total potential drop through the glass thickness L is

$$V_g = \int_0^L E dx \tag{4}$$

The electric field E is uniform in the region Γ < x < L (we assume no anion transport in the glass outside the depletion layer, where the non-bridging oxygen are still tied to sodium cations, and the electric field is relatively small).

Eqs. (1) and (2) are supplemented by adequate constitutive relationships for the fluxes J_+ and J_-. We work with simple ohmic models,

$$J_+ = \mu_+ \rho_+ f(E), \tag{5}$$

$$J_- = \mu_- \rho_- f(E), \tag{6}$$

where μ_+ and μ_- are the cation and anion mobilities.

3. IONIC CHARGE TRANSFER WITHIN THE OXIDE LAYER

We assume that, at the Silicon-Glass (Si-G) interface, the bonding layer of SiO_2 is formed solely by oxygen which is transported from the depleted glass. The physical properties of the bonding layer are thought to be very similar to the bulk SiO_2 glass (except, of course, by the absence of further ionic species). Since the oxide layer is formed in a very high-field region, diffusion of oxygen anions is expected to be negligible in comparison to electric drift transport.

The continuous growth of the insulating oxide layer at the Si-G interface introduces an additional potential drop

$$V_{ox} = \int_{-x_0}^{0} E dx, \tag{7}$$

where x_0 is the oxide thickness at time t and $x_0(0) = 0$. The local values of the electric field must satisfy Eq. (3) in the whole region $-x_0 < x < \Gamma$.

Under a fixed external potential V_0, we impose

$$V_g + V_{ox} = V_0 \tag{8}$$

The dynamics of oxide growth is given by the oxygen flux at the silicon-oxide (Si-O) interface,

$$dx_0 = \frac{dt}{n_{ox}} J_-\left(-x_0, t\right) \tag{9}$$

where n_{ox} is the relative value between the oxygen charge density in the as-grown neutral oxide and the charge density of free (non-bridging) oxygen in the bulk glass.

4. NUMERICAL SCHEME

Eqs. (1) to (9) form a non-linear moving-boundary problem, which we solve numerically by a self-consistent procedure.

5. NUMERICAL RESULTS

Numeric simulations were done for the experimental settings used by Albaugh, 1991 (anodic bonding of silicon to Pyrex glass), which are listed in Table 1 along with estimates of the physical constants that are commonly accepted in the literature.

6. CONCLUSIONS AND COMMENTS

We have shown through numeric simulations that the oxide growth during anodic bonding can be accounted quantitatively by the oxygen available from the depleted region inside the glass.

7. REFERENCES

Albaugh, K.B., 1991. Electrode Phenomena during Anodic Bonding of Silicon to Sodium Borosilicate Glass *J. Electrochem. Soc.* **138**, pp.3089-3094.

Carlson, D.E.; Hang, K.W. and Stockdale, F., 1972. Electrode Polarization in Alkalicontaining Glasses *J. Am. Cer. Soc.* **55**, pp.337-341.

Fabbri, M. and Senna, J.R.S., 2004. *Numerical simulation of ion transport during anodic bonding.* XXV CILAMCE , Recife (CD-ROM).

Helvoort, A.T.J.; Knowles, K.M.; Holmestad, R. and Fernie, J.A., 2004. Anodic Oxidation During Electrostatic Bonding *Phil. Mag.* **84**(6), pp.505-519.

Nitzsche, P.; Lange, K.; Schmidt, B.; Grigull, S. and Kreissig, U., 1998. Ion Drift Processes in Pyrex-type Alkali-borosilicate Glass During Anodic Bonding *J. Eletroch. Soc.* **145**(5), pp.1755-1762.

Ruska, W.S., 1987. Microelectronic Processing. McGraw-Hill.

Schmidt, B.; Nitzsche, P.; Lange, K.; Grigull, S.; Kreissig, U.; Thomas, B. and Herzog, K., 1998. In situ Investigation of Ion Drift Processes in Glass During Anodic Bonding *Sensors and Actuactors* **A**67, pp.191-198.

Wallis, G. and Pomeranz, D.I., 1969. Field Assisted Glass-Metal Sealing *J. Appl. Phys*. **40**(10), pp.3946-3949.

Wallis, G., 1970. Direct-Current Polarization during Field-Assisted Glass-Metal Sealing. *J. Am. Cer. Soc.* **53**, pp.563-567.