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## EXPERIMENTAL CHARACTERISATION AND NUMERICAL MODELLING OF DIRECT BONDED INTERFACE

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### ABSTRACT

In this paper, the fused silica glass direct bonding is studied to understand its mechanical behaviour. A phenomenological law, using Cohesive Zone Model (CZM), is described to model direct bonding. This model is based on several experiments which allow determining the fracture energy  $G$  (wedge test) and the fracture initiation load  $F$  (cleavage test).

**Keywords:** direct bonding, cohesive zone model, wedge test, fracture initiation.

### INTRODUCTION

The fused silica glass direct bonding is based on the contact of two surfaces without glue or any other material (Tong, 1994 and Kendall, 2001). The bonding phenomenon is due to hydrogen bonds formation between the surfaces. The direct bonding requires a low surface roughness (in the order of a few nanometre), not polluted and flat surfaces. The surfaces are polished (Tang, 2008 and Johnson, 1995 and Galanoy, 2011 and Liao, 2011) and treated chemically. This step is not described here because it is a confidential process of Winlight Optics (the direct bonded assemblies' manufacturer). After this step the surfaces are adhered together at room temperature. Finally a thermal treatment can be applied (Kissinger, 1993 and Stengl, 1989) which allows to change the nature of bonds responsible for the adhesion. In this way, stronger bonds like covalent Si-O-Si bonds can be obtained (Stengl, 1989).

Today, this technology is used in terrestrial optics; optical slicers or interferometers, assemblies manufactured using the direct bonding process, are used in telescopes. For example, Fig.1 **Erreur ! Source du renvoi introuvable.**show 1152 blades bonded together to form the larger slicer ever used for the MUSE project (Laurent, 2008).

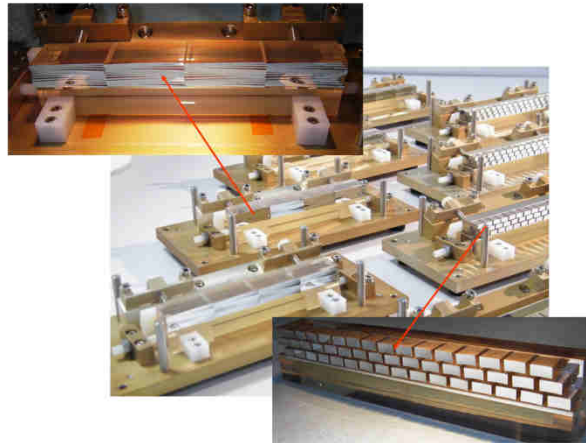


Fig.1 Slicer made with direct bonding method developed for the Multi Unit Spectroscopic Explorer (MUSE) in the Very Large Telescope (VLT) (Laurent, 2008)

The final aim will be to integrate these assemblies in spatial optics systems. A more detailed characterization of the process and an improvement of the adhered interfaces mechanical strength are necessary to validate the European Spatial Agency ESA standards. Indeed, constraints in space are very different from those of the earth. In space thermal fatigue, accelerations, vibrations, shocks are applied to the assemblies especially during launching.

To meet the ESA requirements, mechanical experiments, double shear tests, cleavage tests and wedge tests, were performed in a previous paper (Cocheteau, 2014). They allowed to study the influence of some process parameters, such as annealing time and temperature, roughness on the mechanical strength. Some tests were made to find the optimal parameters, and get the best mechanical strength (Cocheteau, 2014).

This paper, proposed to model the fused silica direct bonding in a finite element software. Developments are performed on samples without any thermal treatment. The interface is composed mainly by hydrogen bonds.

In the first step, a description of wedge test and cleavage test is proposed. The results performed are necessary to obtain data for models based on cohesive zone model (CZM). In second step, three models are presented to simulate by finite element the cleavage test. The first one is a macroscopic model which makes an analogy between mechanical model and physical and chemical properties of the interfaces (Cocheteau et al., 2014). The second one is a multiscale model based on molecular dynamic simulation proposed by Kubair (Kubair, 2009). And the last one is a classical phenomenological cohesive zone model identified by inverse method.

## MECHANICAL EXPERIMENTS

In this section, cleavage tests are shortly presented followed by the wedge tests set up and results. These two tests are performed to obtain an experimental characterization of direct bonded interface. This characterization is useful to develop modelling to simulate the direct bonded interface behaviour. The first test is a qualification test of the Winlight Optics society. The second one is a classical test to characterize the bonding fracture energy.

The cleavage test gives the value of the load at crack initiation and the wedge test gives access to the critical rate of energy  $G$ . These parameters are essential for the modelling based on

CZM, presented in the next section. These results correspond to the Winlight Optics process for samples bonded without any thermal treatment.

### Cleavage tests

Samples are constituted by two blades of 12.5 mm of thickness, 40 mm of width and 40 mm of length, bonded together. On these fused silica glass samples, two aluminium rigid handles are bonded with a classical flexible epoxy glue (Fig.2). A displacement is applied on these handles to characterize the crack initiation on one edge of the specimen.

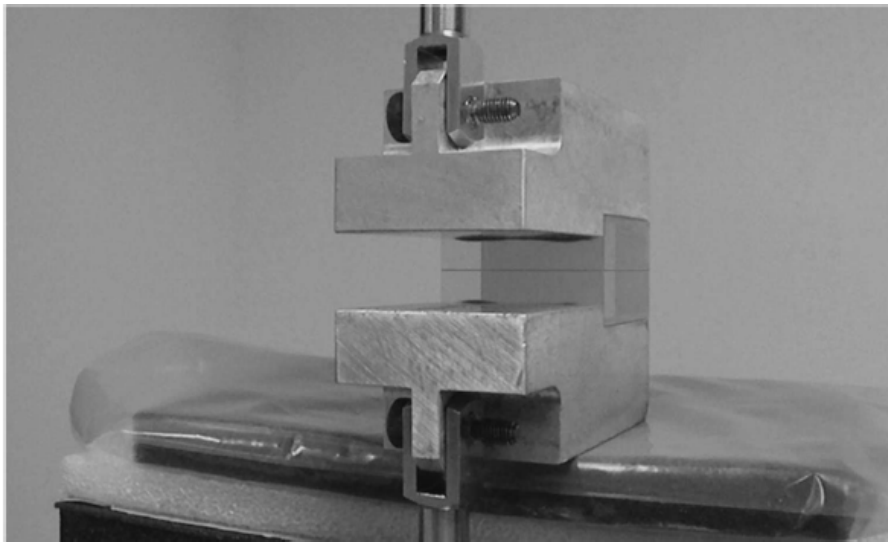


Fig.2 Cleavage test sample and experimental device

A test campaign is lead on to obtain (an average of) the load at crack initiation. Five tests are performed at room temperature and constant humidity. The load ( $F_{\text{fracture}}$ ) is measured and the stress ( $\sigma$ ) is calculated numerically by Winlight Optics with a point stress criteria. Results and test conditions are related in Table 1. A main value of these results is calculated and used in next section for modelling.

Test number	Temperature (°C)	Hr (%)	F <sub>fracture</sub> (N)	$\sigma$ (MPa)
1	20,2	52	371	4,6
2	20	55	310	3,8
3	20,3	57	266	3,3
4	20,5	55	250	3,1
5	20,2	54	355	4,4
Average test			310,4	3,84

## Wedge tests

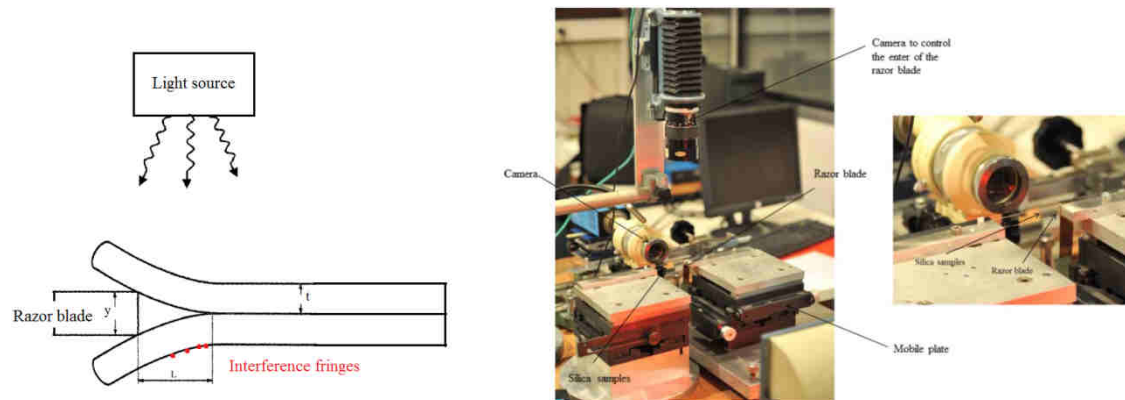


Fig.3 Wedge test principle and experimental device pictures

The bonding energy  $W$  is classically used to characterize adhesion (Maszara, 1988). The bonding energy can be connected to the critical strain energy release rate (Plöbl, 1999). The crack propagation method, or wedge test; is the most popular method to measure the bonding energy.

As related in Fig.3 a razor blade is inserted at the interface between two blades bonded together. Then a crack appears along the bonded interface until the establishment of the equilibrium between the elasticity of blades and the chemical bonds responsible for the adhesions (hydrogen bonds in this case). The length of the crack  $L$  is measured with a camera using interference fringe due to the small thickness of air trapped at the open interface.

At the equilibrium, the critical strain energy release rate is equal to  $W$  (Cognard, 1986) and relating to the crack length using linear elastic fracture mechanics. When both surfaces are identical, we can write:

$$G = W = 2\gamma \quad (1)$$

With  $\gamma$  the surface energy. Moreover critical strain energy release rate – thus the bonding energy  $W$  - can be approximately related to the length  $L$  using the following equation 2:

$$W = G = \frac{3Et^3 y^2}{16L^4} \quad (2)$$

Where  $E$  is the Young modulus of blades,  $t$  the blade thickness,  $y$  the razor blade thickness and  $L$  the length of the crack.

The wedge tests samples are constituted with two blades of fused silica glass with 500  $\mu\text{m}$  of thickness ( $t$ ), 10 mm of width and 80 mm of length bonded together. The razor blade (100  $\mu\text{m}$  ( $y$ ) of thickness) is always inserted by the same length using a mobile plate and the insertion is controlled by a camera above the blades as shown on Fig.3. The procedure and the different parameters of this test are described more precisely in (Cocheteau, 2014).

Table 2 relates the results of this test.

Table 2 – Results of experimental wedge tests

$L$ (mm)	$G$ (J/mm <sup>2</sup> )
28.591	0.0255

## MODELING OF FUSED SILICA DIRECT BONDING WITH CZM

In this section, three numerical models, based on CZM, are exposed. The first one is a macroscopic model which makes an analogy between mechanical model and physical and chemical properties of the interfaces (Cocheteau et al., 2014). The second one is a multiscale model based on molecular dynamic simulation proposed by Kubair (Kubair, 2009). And the last one is a classical phenomenological cohesive zone model identified by inverse method.

Values  $F_{fracture}$  and  $G$  are essential for those modelling and are given by the cleavage test and wedge test results.

These three models are implemented in Abaqus to simulate the cleavage test and the wedge test. The simulations are carried out in 2D to limit the computation time. Samples are modelled with plane strain elements and the interface is modelled by cohesive elements without thickness (type of element COH2D4 in Abaqus). For each model tested, a sensitivity analysis to the mesh is performed. The mesh of the cleavage test is related in Fig.4, it is the larger mesh used where the cohesive element length  $L_e$  is 0.1mm. The numerical simulation results depend strongly to the cohesive element size. This size can be linked to the value of  $G$ . Turon et al. give two equations, (3) and (4), to calculate the cohesive element size  $L_e$  (Turon, 2007).

$$L_{cz} = M \frac{EG}{\sigma_{max}^2} \quad (3)$$

$$L_e = \frac{L_{cz}}{N} \quad (4)$$

Where  $L_{cz}$  is the cohesive zone length,  $E$  the Young modulus,  $L_e$  the cohesive element size,  $M$  and  $N$  are chose to respect  $0.21 < M < 1$  and  $3 < N < 10$ .

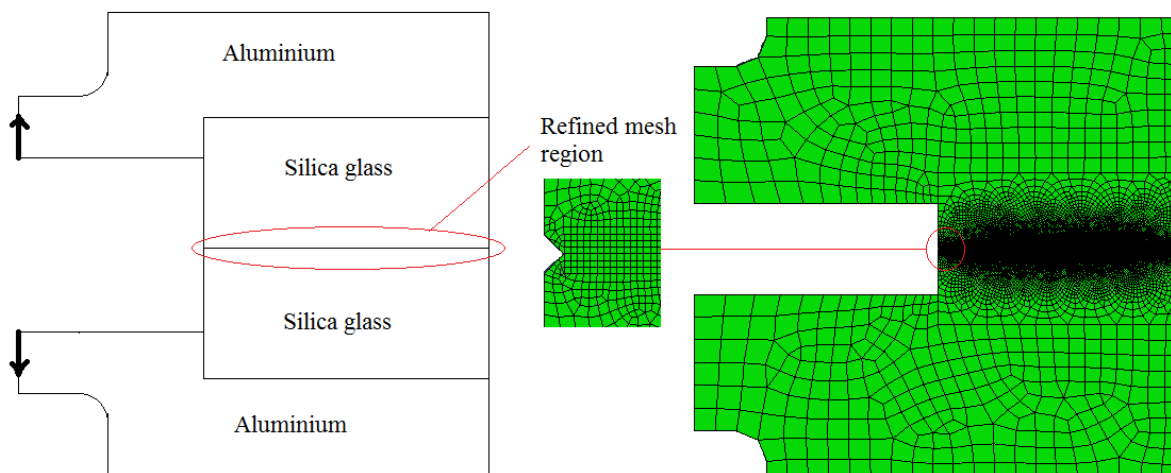


Fig.4 Mesh for cleavage test numerical simulation

### Macroscopic interface modelling

In order to model the direct bonded interface behaviour, an adhesive law has been developed (Cocheteau, 2014). The originality of this law is to couple unilateral contact, adhesion and a description of the bonding energy. In numerical simulation, this model is a particular case of traction-separation model. Indeed, a brittle elastic law is imposed with  $\delta_0 \approx \delta_f \approx 0.12nm$ . This value corresponds to the characteristic distance of hydrogen bond.

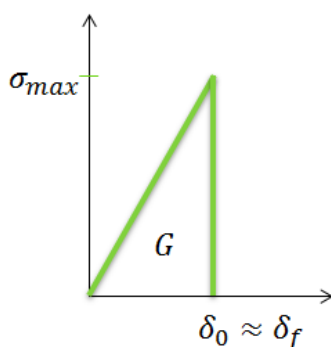


Fig.5 Contact mechanics analogy macroscopic model (Cocheteau, 2014)

The numerical model results are presented in Table 3.

Table 3 - Results of the simulation cleavage test with macroscopic model

<b>G</b> (J/m <sup>2</sup> )	<b>L<sub>e</sub></b> (mm)	<b>δ<sub>0</sub></b> (nm)	<b>δ<sub>f</sub></b> (nm)	<b>σ<sub>max</sub></b> (MPa)	<b>K</b> (MPa/mm)	<b>F<sub>num</sub></b> (N)	<b>F<sub>exp</sub></b> (N)
0.0255	0.1	0.12	0.13	425	3.54.10 <sup>9</sup>	41323.2	310.4
0.0255	0.05	0.12	0.13	425	3.54.10 <sup>9</sup>	23837,6	310.4

This model is not well adapted to simulate the fused silica direct bonding. Indeed, the numerical load obtained is totally different from the load obtained experimentally. The relative difference is close to 7580%.

## Kubair model

Kubair et al. studied the direct silicon wafer bonding (Kubair, 2009). They described molecular dynamics simulation as a set of bonds (describing the direct bonding, Fig.6) and proposed a cohesive zone model with a traction separation law identified at nanoscale with their numerical results. This multiscale approach has the potential to model directly the effects of surface roughness, nanotopography and small-scale patterning on the efficacy of direct wafer bonding.

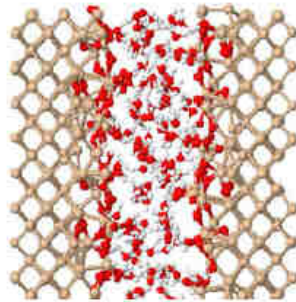


Fig.6 Set of bonds describing the direct bonding

With several molecular dynamics simulations, the authors obtain the cohesive zone model parameters. The model are  $\sigma_{max}=210$  MPa,  $\delta_0=0.2$  nm,  $\delta_f=1$  nm and  $G=0.105$  J/mm<sup>2</sup>, the shape of the curve is related in Fig.7.

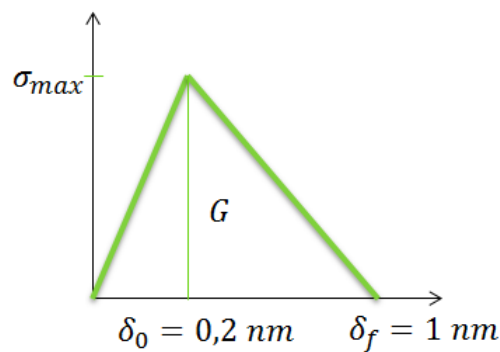


Fig.7 Kubair model

The numerical results of the cleavage test simulation with the Kubair model are presented in Table 4.

Table 4 - Results of the cleavage test with the Kubair model

<b>G</b> (J/m <sup>2</sup> )	<b>L<sub>e</sub></b> (mm)	<b>δ<sub>0</sub></b> (nm)	<b>δ<sub>f</sub></b> (nm)	<b>σ<sub>max</sub></b> (MPa)	<b>K</b> (MPa/mm)	<b>F<sub>num</sub></b> (N)	<b>F<sub>exp</sub></b> (N)
0.0255	0.1	0.2	1	51	2.55.10 <sup>8</sup>	5806.92	310.4
0.0255	0.05	0.2	1	51	2.55.10 <sup>8</sup>	3623.51	310.4
0.0255	0.01	0.2	1	51	2.55.10 <sup>8</sup>	2696.71	310.4

Compared to the results, this model does not allow to simulate the experimental tests. The difference with experimental data is close to 769%.



## Phenomenological model

The models proposed by the literature do not allow to have a precise numerical modelling of direct bonding interface. A phenomenological model will be implemented in order to better describe the behaviour of interface.

The new model is based on the Kubair model. The parameter  $\delta_0$  given by Kubair is defined by the molecular dynamics simulations. This value is assumed to be true so it will be kept. All other CZM parameters are not determined. The value of  $\sigma_{max}$  is identified by inverse method in comparing the numerical and experimental crack initiation load. Finally, we find the law describing the interface mechanical behaviour as related in Fig. 8.

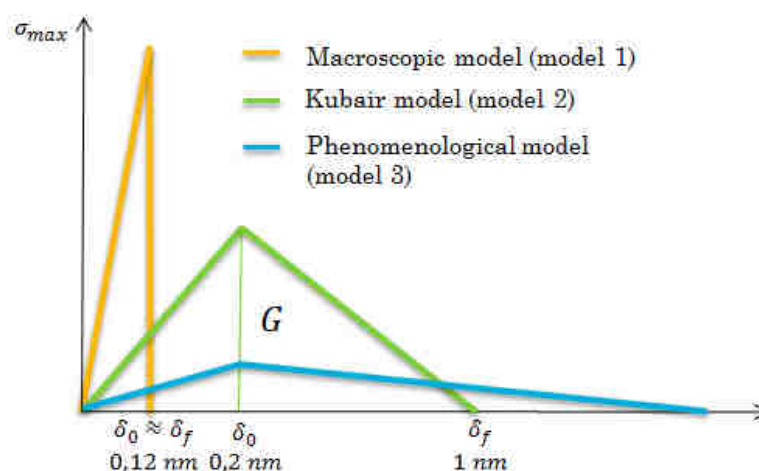


Fig. 8 Adaptation of Kubair model for the phenomenological model

After the identification procedure, a phenomenological law is defined. The value of different parameters is given in Table 5 as the numerical load at crack initiation.

Table 5 - Results of the cleavage test with the phenomenological model

$G$ (J/m <sup>2</sup> )	$L_e$ (mm)	$\delta_0$ (nm)	$\delta_f$ (nm)	$\sigma_{max}$ (MPa)	$K$ (MPa/mm)	$F_{num}$ (N)	$F_{exp}$ (N)
0.0255	0.1	0.2	17	3	$1.5 \cdot 10^7$	362.5	310.4
0.0255	0.05	0.2	17	3	$1.5 \cdot 10^7$	287.3	310.4
0.0255	0.01	0.2	17	3	$1.5 \cdot 10^7$	294.2	310.4

In order to validate this phenomenological model, the wedge test is modelled by finite elements method. The goal is to obtain comparable crack lengths with the phenomenological law and with the experiments. The results in Table 6 show that the law allow to find the behaviour of interface. The difference is close to 1.1%. In Fig. 9, the mesh of the wedge test is showed with the smallest size of  $L_e$ , this value is 0,01mm.

Table 6 - Comparison between experimental and numerical results for wedge test

Bonding type	$G_c$ (J/m <sup>2</sup> )	$\delta_0$ (nm)	$\delta_f$ (nm)	$\sigma_{max}$ (MPa)	$K$ (MPa/mm)	$L_{num}$ (mm)	$L_{exp}$ (mm)	Error (%)
Reference	0.0255	0.2	17	3	$1.5 \cdot 10^7$	28.29	28.59	1.1

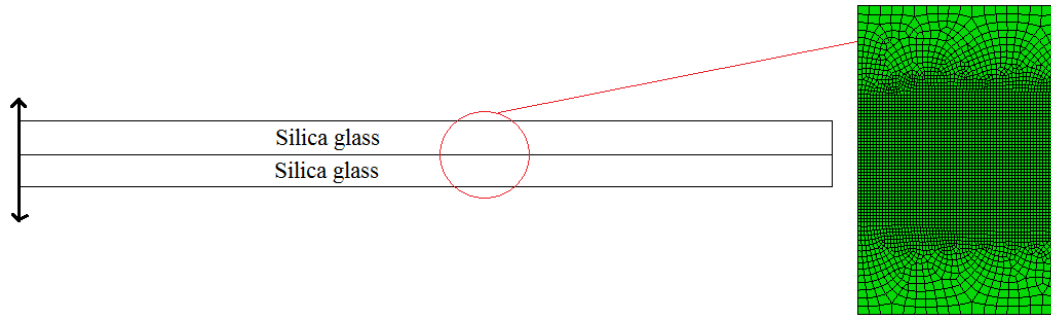


Fig. 9 The mesh of the wedge test numerical simulations

## RESULTS

The macroscopic model (model 1) does not allow to simulate in detail the interface behavior. Indeed, the simulation of the cleavage test gives a load at crack initiation of 41000N instead of 310N. As far as the Kubair model (model 2) does not allow to have the load at crack initiation. The simulated load is 3600N while the experimental load is 310N.

For these two literature models, the cohesive element size  $L_e$ , used in the simulations, can be a reason for the inconsistent results. Indeed, the  $L_e$  size does not respect the Turon equations (Turon, 2007) because it is too small and the computation fails.

The phenomenological model defined and based on the traction-separation law describes well the behaviour of the fused silica glass direct bonding. The parameters of this model are  $\sigma_{\max} = 3$  MPa,  $\delta_0 = 0.2$  nm,  $\delta_f = 17$  nm and  $G = 0.0255$  J/mm<sup>2</sup>. With this model the wedge test is simulated, the numerical and the experimental results are similar.

## CONCLUSION

The aim in the paper consist to understand, to model and to compute mechanical behaviour of fused silica glass direct bonding.

The cleavage test and the wedge test are performed to obtain characteristic experimental values of direct bonding. These parameters are used to model the interface behaviour of fused silica direct bonding. The two models find in the literature, the macroscopic model and the multiscale Kubair model, fail to simulate the direct bonding. A phenomenological model, based on CZM, is identified by inverse method. The mechanical behaviour of the fused silica glass direct bonding is correctly simulated with this model. A numerical simulation of wedge test is performed to validate the phenomenological model.

Applying a thermal treatment on assemblies after adhesion allows improving their mechanical strength (Cocheteau, 2014). In future development, a new model will be proposed to describe the mechanical behaviour of the reinforced direct bonding.

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