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Wafer bonding across surface steps in the nanometer range

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Abstract

AbstractThe present paper reports on measurements of the extension of unbonded areas, caused by surface steps in the nanometer range at the interface of bonded silicon wafers. For the experiments, wafers with surface steps between 9 and 400 nm in height were used. The unbonded areas at the interface were identified by scanning acoustic microscopy (SAM) and transmission electron microscopy (TEM). The experimental results are compared with theoretical models. In silicon wafers of a thickness of 525 μm the bonding across steps < 55 nm is comparable to the elastomechanical behavior of an edge dislocation. For steps > 55 nm the unbonded area can be calculated based on thin plate theory. © 1999 Elsevier Science S.A. All rights reserved.

Keywords: Wafer bonding; Elastomechanical instability; Surface steps

1. Introduction and theoretical background

Mechanical parameters like waviness and surface microroughness play an important role in estimating the bondability of two wafers. If waviness and microroughness are too large, the wafers will not bond, or unbonded areas will appear [1,2]. The existence of particles and raised artificial surface structures such as microelectronical and micromechanical structures can also prevent perfect bonding. Tong and Gösele [3] described the bonding behavior across particles. They distinguish two sizes of particles. If the height h (or $2\times$ radius) of the particle is much smaller than the wafer thickness d, and if the radius R of the resulting unbonded area is much larger than d, the extension of the unbonded area can be estimated using the theory of small elastic deflections of a thin plate,

$$R = \left(1.2\,Ed^3/\gamma\right)^{1/4} h^{1/2} \tag{1}$$

where E is Young's modulus and γ the specific interface energy of the bonded wafers. However, for the case that the particle size causes an unbonded area $R < 2d$, based on Eq. (1), Tong and Gösele suggested an elastomechanical instability to occur. In this case the unbonded area essentially decreases to the smaller value of

$$R \approx kh \tag{2}$$

where k is a dimensionless constant in the order of 1. Up to now there has been no experimental evidence of such an elastomechanical instability involving very small structures.

Studies involving the bonding behavior across elevated step structures are important since they directly relate to the applicability of wafer bonding technology to wafers with raised surface structures such as conducting metal lines. Another interesting aspect of such studies is the question whether there exists an elastomechanical instability at steps of very small step heights ($h < 100$ nm) analogously to what had been predicted by Tong and Gösele [3] for small particles.

Hiller [4] investigated the bonding behavior across step structures of down to 300 nm in height, concluding that the extension of the unbonded area L can be estimated by

$$L = \sqrt[4]{\frac{3Ed^3h^2}{8\gamma}} \tag{3}$$

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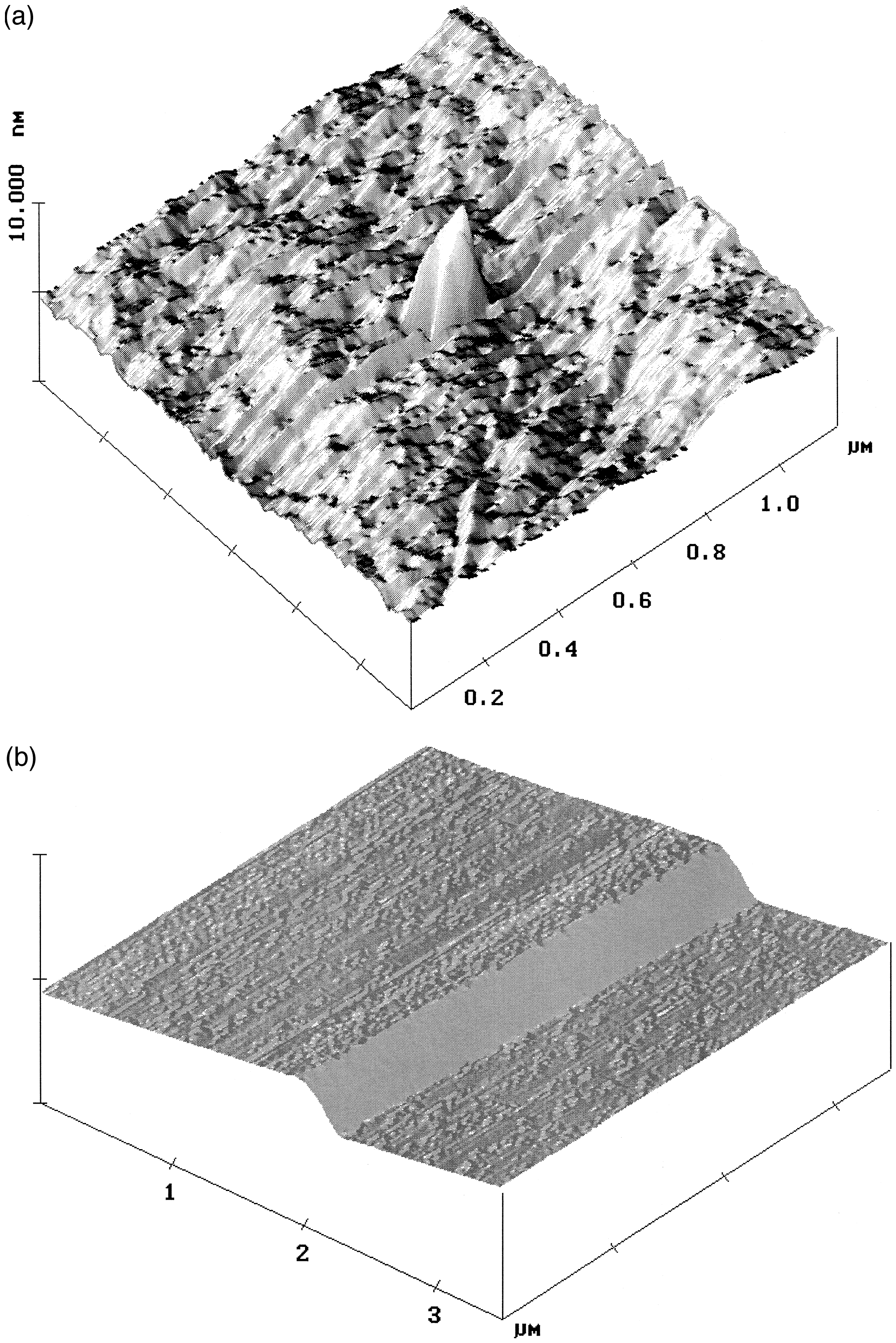

Fig. 1. AFM image of a sample with (a) a particle generated by field enhanced oxidation and (b) a surface step 32 nm high.

Eq. (3) results from the assumption that the bonding across surface steps can be calculated from thin plate theory.

Up to now the literature does not cite any experimental investigation of the bonding behavior across step structures of very small step heights. Very small, here means that the extension of the unbonded area, calculated by Eq. (3) is smaller than $2d$.

One way of calculating the extension of unbonded areas in small steps $(L < 2d)$ is to employ the mechanical continuum theory of dislocations, which is suitable as it does not differentiate between monoatomic steps and higher ones. The extension L of the unbonded area at the interface of bonded wafers with steps can be estimated by minimizing the total energy. The total energy of the bonded system is approximately given by

$$E_{\text{total}} = E_{\text{surface}} + E_{\text{elastic}} \tag{4}$$

where E_{surface} is the surface energy required to open up the bonded materials and E_{elastic} represents the elastic energy around the step structure.

The surface energy per unit length of the steps is given by

$$E_{\text{interface}} = 2\gamma L \tag{5}$$

The elastic energy per unit length is approximately given in Ref. [5], yielding

$$E_{\text{elastic}} = \frac{Eh^2}{4\pi(1-\nu)^2}\ln\left(\frac{d}{L}\right) \tag{6}$$

with d being the wafer thickness, h the step height, E Young's modulus, and ν Poisson's ratio.

With

$$\frac{\partial E_{\text{total}}}{\partial L} = 2\gamma_0 - \frac{Eh^2}{4\pi(1-\nu)^2 L} = 0 \tag{7}$$

we can estimate the extension L of the unbonded area, viz.

$$L = \frac{Eh^2}{8\pi\gamma_0(1-\nu)^2}. \tag{8}$$

2. Experimental and results

Two different structures with heights in the nanometer range have been investigated. The first structure involved artificially generated particles consisting of locally oxidized areas and the second one artificial step structures. For all experiments (100)-silicon wafers with a thickness of 525 μm were used.

In order to produce the nanometer scale particles in a scanning force microscope (AFM) the field-enhanced oxidation (FEO) method, as proposed by Day and Allee [6], was used. A dc voltage of 7–12 V was applied between the silicon wafer and the tip of the AFM for about a minute. This treatment caused local oxidation. The lateral extension of the localized oxidized spots was about 100 nm and their maximum height 5 nm. In Fig. 1a, such a FEO-produced structure is shown. Subsequently, analysis of the samples after bonding did not display any particles or any unbonded area caused by particles during bonding. There may be two different reasons for this result: (i) If there is an elastomechanical instability an unbonded area will arise having a radius of several nanometers. The only method to detect such small structures (extension of unbonded area less than 20 μm) in the interface of two bonded wafers is transmission electron microscopy. Obviously, it is unlikely that the cross-section sample prepared

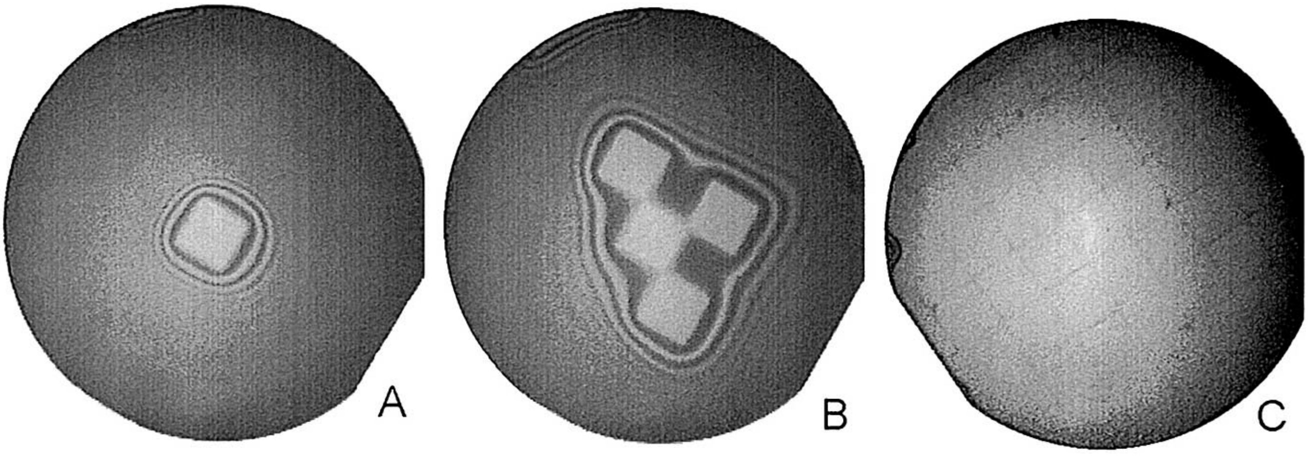

Fig. 2. Infrared pictures of spontaneous lateral spreading of the bonded area across 55 nm high steps after 1 s (A), 20 s (B) and 60 s (C). The diameter of the wafers is 100 mm.

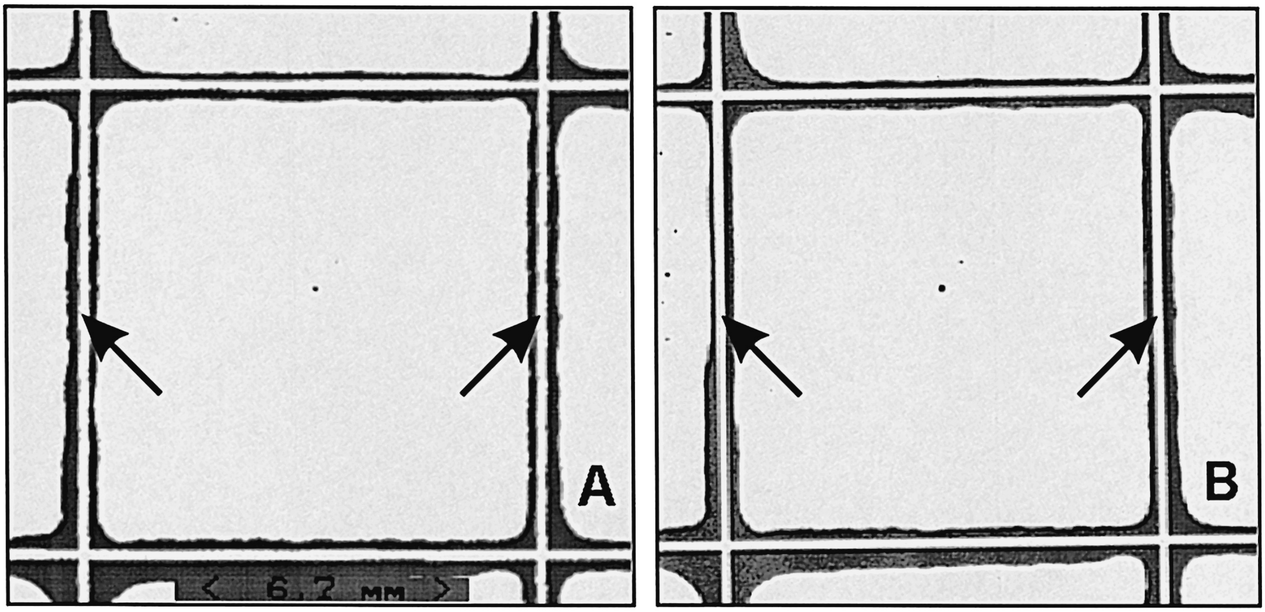

Fig. 3. SAM images of a bonded 55 nm high structure after annealing (A) at 400°C for 1 h, and (B) at 800°C for 1 h. The location of the ridges (corresponding to a double step) is indicated by arrows.

for TEM contains one of the few particles formed. (ii) The elastomechanical instability does not exist but the features could nevertheless not be detected by TEM because of their low density. Consequently, this experiment does not exclude nor confirm the existence of an elastomechanical instability for small particles.

The samples with step structures were prepared in a typical lithographic silicon structuring procedure as a

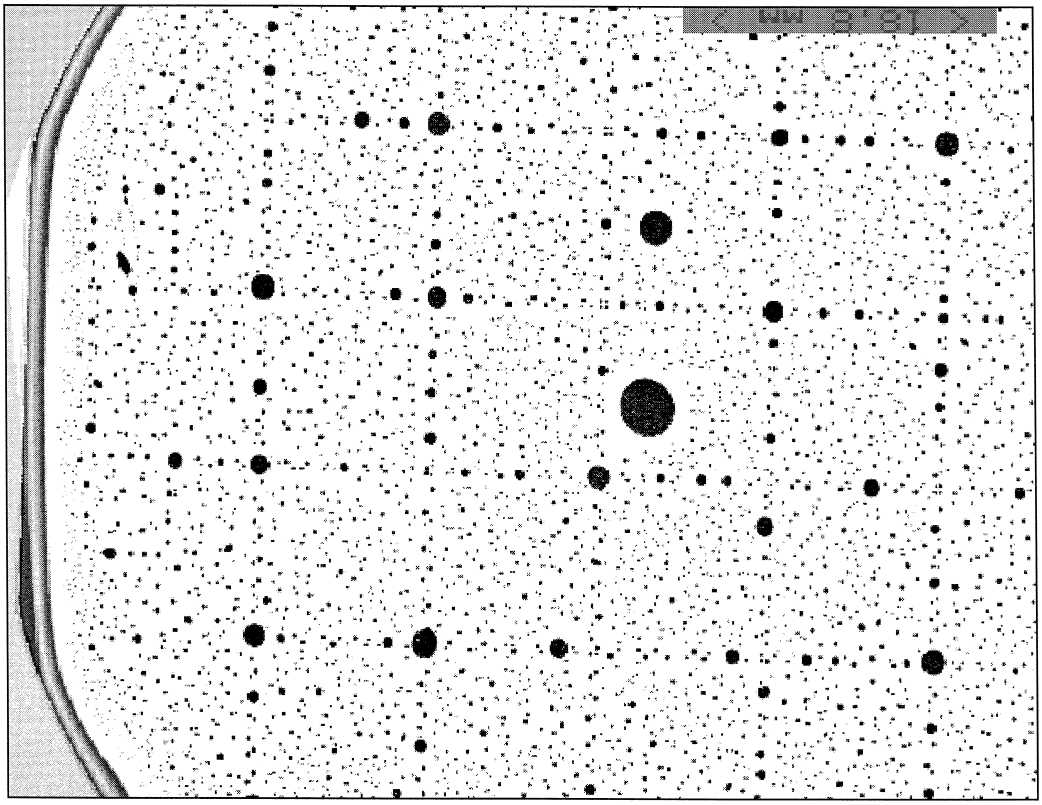

Fig. 4. SAM image of a bonded wafer pair with an 18-nm high structure after annealing at 400°C for 1 h. The unbonded area is not detectable. But the location of the structures can be determined from the distribution of the larger interface bubbles.

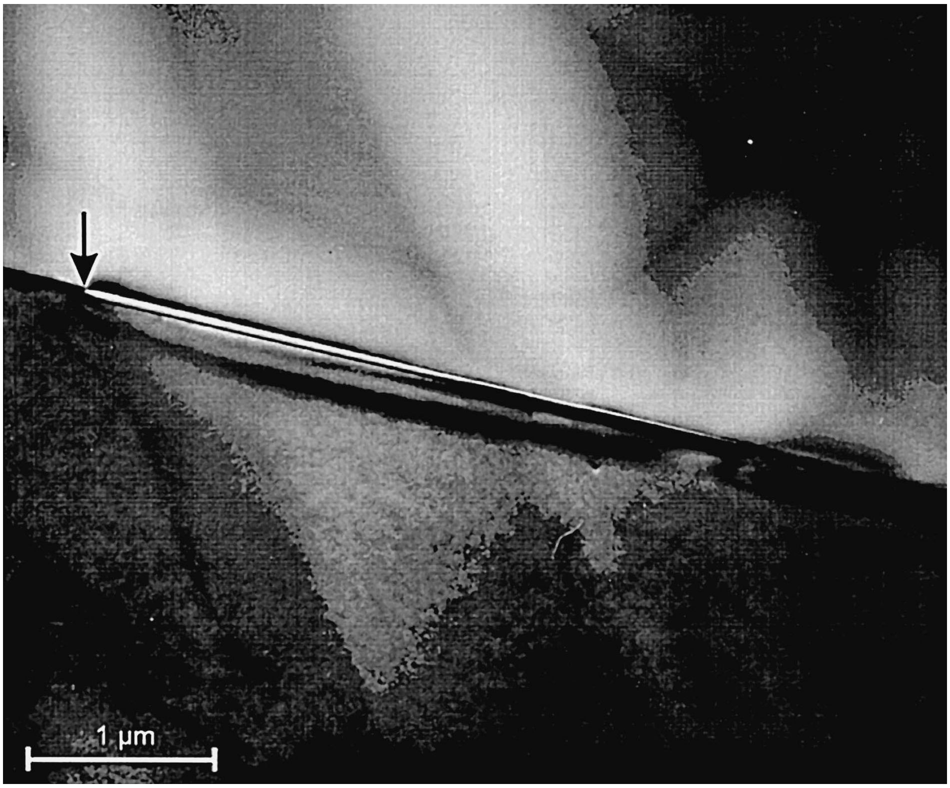

Fig. 5. HVTEM image of the interface with an 18-nm high step. The sample was annealed at 400°C for 1 h. The location of the step is indicated by an arrow.

square pattern. An example of an atomic force microscopy image across such a step is shown in Fig. 1b.

In order to check the influence of air which can be trapped during the bonding process, we designed two different photomasks: (i) one with step structures extending up to the rim of the wafers, and (ii) one with step structures not extending up to the rim. Structured wafers with step heights of 400, 55, 18 and 9 nm were bonded to unstructured silicon wafers in a microcleanroom setup developed by Stengl et al. [7]. Except for the samples with 400 nm high steps, the bonding occurred spontaneously. An example of the lateral spreading of the bonded area across the structured wafer is shown in Fig. 2. For steps higher than 55 nm, we could observe the resulting unbonded area with a scanning acoustic microscope (SAM). In samples with step heights of 18, 9 and 3 nm SAM did not reveal the unbonded areas. These samples were annealed at 400°C for 1 h to increase the bonding strength, which was necessary to prepare cross-section samples for TEM investigations. Then the samples were first investi-

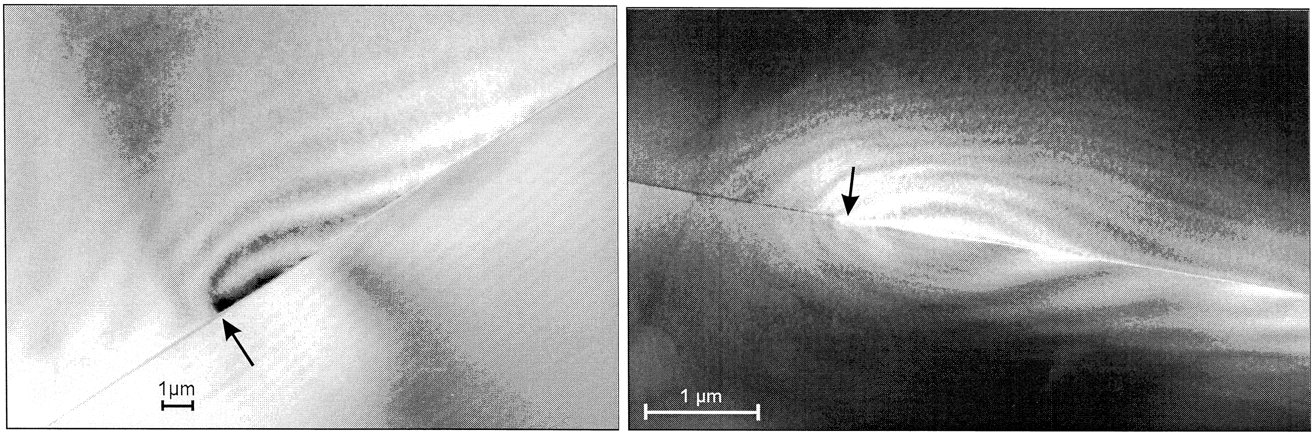

Fig. 6. HVTEM image of the interface with a 9-nm high step (left), and the same step investigated by HRTEM (right). The location of the step is indicated by an arrow.

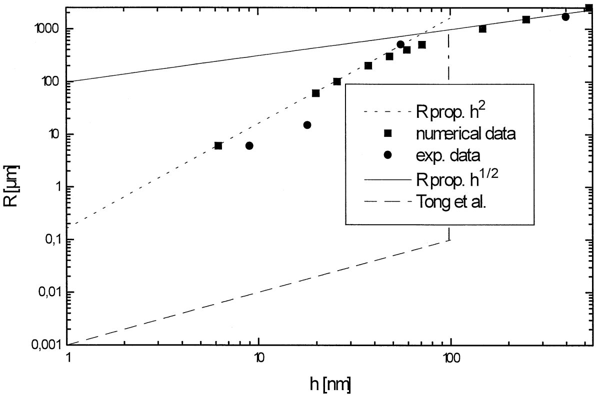

Fig. 7. Theoretically expected and experimentally determined data of the extension of the unbonded area caused by step structures. The boundary element method was used for calculating the numerical data.

gated by High-Voltage-TEM. After a step had been detected in an area investigated, this part of the sample was prepared to be next investigated by High-Resolution-TEM.

First the bonding behavior across step structures of a height of 400 nm was investigated. The resulting unbonded area has an extension of 1800 μm (±100 μm) long, which corresponds well with the value calculated for Hiller's beam bending model, which predicts a length of 1900 μm of the unbonded area, using our experimental setup at a specific surface energy of 0.1 J/m^2.

At 55-nm high steps, the extension of the unbonded area was about 500 μm. The value theoretically expected based on Eq. (8) is 458 μm for a specific surface energy of 0.1 J/m^2. Samples of the same step height were also used to check the influence of trapped gases. At room temperature, there is no difference between the structures extending to the wafer rim and those not extending to the rim. At higher temperatures two different situations may occur. In one case, the extension of the unbonded area is independent of temperature (Fig. 3), within the margin of error. In the other case, interface bubbles are growing along the structures at higher temperatures (Fig. 4) and the unbonded area shrinks partly. These observations have been made for steps with a height of 55 nm and more. In the case of smaller steps we cannot present results after room temperature bonding, since the extension of the unbonded areas was to small for SAM analysis.

Further investigations of samples with even smaller steps (18 nm, 9 nm), using TEM, have shown that the bonding behavior across nanometer high steps ($L < 2d$) can be described by Eq. (8). Fig. 5 shows the interface at an 18-nm high step. The extension of the unbonded area shown is about 3 μm. However, a closer inspection in the high resolution mode (Fig. 6) reveals a disturbed area extending over 15 μm. Even this higher value rather strongly deviates from the theoretically expected one of 49 μm. Two possible reasons responsible for this discrepancy should be considered. One reason could be that the bonding energy γ which we have assumed to be the room temperature value of about 0.1 J/m^2 could have increased to higher values of 0.5–1 J/m during heating. The observation that for larger step height the experimentally observed crack lengths fit very well with the ones calculated based on the room temperature value of 0.1 J/m^2 does not exactly favor this possibility. The other possible reason could be, that in fact for very small step sizes the theory presented might over estimate the crack sizes. Presently this issue remains unresolved.

Fig. 7 compiles the theoretical and numerical data expected for silicon wafers of a thickness of 525 μm and a surface energy of 0.1 J/m^2 and respective experimental data.

3. Conclusions

Studying the bonding behavior across step structures shows that the extension of the unbonded area can be described by the combination of a simple beam bending model and a model which is based on the mechanical continuum theory of dislocations. The applicability of the models depends on the relation between wafer thickness and extension of the unbonded area. The experimental data gave no evidence that the model of an elastomechanical instability as reported by Tong and Gösele [3] for very small point like structures is applicable to step structures in the nanometer range. Unfortunately, because of experimental limitations, we were not able to check the prediction by Tong and Gösele [3] for point-like structures.

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