X-RAY DIFFRACTION IMAGING FOR PREDICTIVE METROLOGY OF CRACK PROPAGATION IN 450MM DIAMETER SILICON WAFERS

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ABSTRACT
Apparatus for X-ray Diffraction Imaging of 450mm wafers now in place at the ANKA synchrotron radiation source in Karlsruhe is described in the context of the drive to inspect such wafers for plastic deformation or mechanical damage. It is shown that full wafer maps at high resolution can be expected to take a few hours to record. However, we show from experiments on 200, 300 and 450mm wafers that a perimeter-scan on a 450mm wafer, to pick up edge damage and edge-originated slip sources, can be achieved in just over 10 minutes. Experiments at the Diamond Light Source, on wafers still in their cassettes, suggest that clean room conditions may not be necessary for such characterisation. We conclude that scaling up of the 300mm format Jordan Valley tools, together with the existing facility at ANKA, provides satisfactory capability for future X-ray diffraction imaging analysis of 450mm wafers.

I. INTRODUCTION
For a number of years, the International SEMATECH Manufacturing Initiative (ISMI) has been coordinating development activities (Abell, 2008) aimed at building infrastructure to allow pilot scale introduction of device fabrication on 450mm silicon wafers by 2012. Despite comments from senior industry executives at Semicon West in 2009 that the move to 450mm diameter wafers is “just a distraction”, in December 2010, Intel announced that it has plans to migrate production at its Oregon-based DX1 plant (Intel, 2010) to 450mm format. Its intention is to open the 22nm node plant in 2013. Increase in wafer diameter will reduce manufacturing costs (Jones, 2009; Chien et al., 2007) and increase output volume. However, there are significant materials issues remaining and initially yield may fall on introduction of 450mm wafer production.

Materials issues associated with use of 1mm thick, 450mm diameter, wafers include planar chemical mechanical polishing at this diameter, (Borucki, Philipossian and Goldstein, 2009) plastic deformation associated with gravitational sag and the increase in process and cooling times required. Additionally, the increased weight poses an increased risk of mechanical damage at the edge of the wafer. As part of the European Union funded SIDAM project, cracks
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introduced mechanically by misaligned handling tools have been identified as being responsible for fracture of 300mm diameter wafers during high temperature processing. We have used X-ray Diffraction Imaging (Topography) (Bowen and Tanner, 2006) in both the laboratory and at the ANKA (Germany) and Diamond (UK) synchrotron radiation sources to record the images of cracks, similar to those produced by repeated collision of misaligned tools, generated by indentation at the bevel edge of 200mm (8 inch) wafers. Using a semi-kinematical model of image formation, we have been able to identify those cracks which are likely to propagate and we define a single critical parameter $\kappa_c$ for their identification which can be directly determined from the X-ray images (Tanner et al., 2012). The predictions from the measured $\kappa$ values have been shown to agree very well with experimental measurements of the probability of breakage of these wafers during rapid thermal annealing, using finite element modelling to determine the high temperature thermal stresses.

Heavier wafers and larger handling tools are likely to result in a higher risk of fracture than on the existing fabrication lines. As the scale increases, the cost of halting the line to diagnose and remedy the faulty tool also increases. It is thus important that there exists a facility to study wafer damage and plastic deformation in 450mm wafers. Extension of the capability of X-ray Diffraction Imaging (XRDI) (Fig 1) to the inspection of 450mm wafers has been one of the objectives of the SIDAM programme. Facilities are now in place at the ANKA synchrotron radiation source.

![Diagram](image)

**Fig. 1:** Principle of large area transmission topography at a synchrotron radiation source
II. SYNCHROTRON RADIATION XRDI

II.1 450 MM APPARATUS
Facilities for inspection of 300mm silicon wafers by white radiation XRDI have been in place at the Topo-Tomo beamline (Simon and Danilewsky, 2003) of the ANKA synchrotron radiation source in Karlsruhe, Germany for some time (Danilewsky et al., 2008a). The energy of the electrons inside the ANKA storage ring is 2.5 GeV which results in the characteristic wavelength of 2 Å. This is perfect for topography of inorganic materials and with a beam current of 200 – 100 mA, real time imaging is possible using a CCD camera lens coupled to a thin phosphor screen (Rack et al., 2008; Danilewsky et al., 2008b). A special feature of the beamline is that there are no optical components between the source point from bending magnet and the experiment, except one 0.5mm thick, highly polished, Be-window directly in front of the experiment. The 30 m long beamline and the small source result in the high resolution of the topographs of about 1 µm.

The sample goniometer is mounted on linear slides and conversion from the 300mm format (Danilewsky et al., 2008a) to 450mm capacity was straightforward. As there is plenty of space surrounding the goniometer, the additional capability, (Fig 2), has been achieved simply by replacing the slides with ones capable of 500mm travel in the X and Y directions, normal to the X-ray beam direction (Z). Strain-free mounting of 200 and 300mm diameter wafers has been successfully achieved by use of a grooved specimen holder with an adjustable clamp at one corner. The 450mm sample holder is again just a scaled up version of the 300mm wafer holder (Fig 3). Under conditions of strict commercial confidentiality, we have successfully run 450mm wafers using the translation stage and holder. There are no new experimental issues above those encountered in the inspection of 300mm wafers and the data collection strategy described below proves satisfactory for 450mm wafer inspection.

Fig 2: 300 mm wafer mounted in the goniometer and 500mm translation stage
II.II DATA COLLECTION STRATEGY
A single shot inspection of large diameter silicon wafers at high resolution is clearly impossible and scanning of the sample is obviously a necessity. Further, for rapid inspection, long integration times are unacceptable. An initial rapid survey is thus necessary, balancing resolution (and hence detection capability) with speed, followed by detailed inspection of identified defects (Danilwesky et al., 2011). All instruments use charge coupled device (CCD) detectors coupled optically to a thin phosphor screen, enabling a variety of magnification strategies, either based on interchangeable lenses or fibre-optics, to be employed.

The design of the CCD detector at ANKA is based on the concepts of Hartmann et al. (1975) as well as Bonse and Busch (1996): the luminescence image of a scintillator screen is coupled via diffraction limited visible light optics to a camera (CCD or CMOS). For our experiments, the macroscope was equipped with a Rodenstock TV-Heliflex objective (f = 50 mm, max. NA = 0.45), a Nikkor 180/2.8 ED (f = 180 mm) objective as tube lens, a pco.4000 CCD camera (4008 × 2672 pixels, 9 μm in size) and a 25 mm × 25 mm CdWO₄ (CWO) or Ce-doped Lu₃Al₅O₁₂ (LuAG) both polished scintillator single crystals, 300-μm-thick (3.6x magnification, 2.5 μm effective pixel size, spatial resolution R > 5 μm, 10.0 mm × 6.7 mm field of view (Nagornaya et al., 2005; Rack et al., 2009)). The high stopping power of the CWO crystal in combination with the light collection efficiency of the Rodenstock objective permits live imaging as already
demonstrated for cineradiography with up to 250 images/s of living insects at Topo-Tomo (Betz et al., 2008). Here, the pco.4000 camera with a Kodak KAI-11000 interline transfer chip gives access to frame rates of up to 5 images/s in full-frame mode (depending on the dynamic range). Higher frame rates up to 40 frames per second are accessible when working with a region of interest.

The small size of the scintillating crystals compared to the 13 x 18 cm² limits the field of view to one single topograph and e.g. the 022 reflection in the case of Si, has to be chosen. Improved resolution and sensitivity allows continuous imaging at frequencies of between 1-10 Hz whilst maintaining adequate topographic resolution. This increase in speed of the camera integration time allows us now to achieve a nearly real time metrology of large wafers with high speed scanning of the wafer.

Fig. 4 shows a topograph from a perimeter scan of a 200 mm wafer, performed at the ANKA Topo-Tomo beamline. The originally dislocation free wafer shows, after a 60 seconds plateau anneal, a high number of extended defects, originating mainly at the wafer edge similar to the wafer shown in fig. 5. After image processing and dark correction a frame rate of 40 frames per second results in effective integration of 8 frames. The clarity of the laser label in fig. 4 is a sign of the high resolution which is achieved with the 0.2 s exposure time. Dense slip bands originate directly from the notch and we note that single 60°-dislocations can be resolved in the lower single slip band which is located some distance from the edge.

As the scan time for a perimeter scan of a 200mm wafer was approximately 5 minutes, it was immediately projected that the time for a similar scan of a 450 mm wafer would be approximately 11 minutes, as was found in practice. The greater weight of a 450mm wafer results in greater bowing of these wafers in comparison to 300mm wafers. This stronger bending results in a larger (continuous) deviation of the position of the 022 diffracted beam during the map which must now be corrected by moving the camera during the scan in a direction parallel to the wafer. To enable this to be done automatically, we performed a calibration at four positions, rotated by 90°, close to the wafer edge at the beginning of the experiment and from which the camera position correction was then calculated for every frame.

The ANKA facility therefore provides an acceptable European facility for characterisation of 450mm wafers by X-ray Diffraction Imaging. At present, this cannot be achieved under clean-room conditions and significant investment would be required if this were to be set up. However, we have shown that for 200mm wafers, high quality and high resolution XRDI can be performed on wafers in their cassettes (fig 5). The critical energy of sources such as ANKA, Diamond and the ESRF are such that transmission experiments on 1 mm thick wafers in cassettes is quite realistic. The exposure time penalty would be typically 20%.
Fig 4: Metrology of 200 mm Si wafer ex situ at room temperature after 60 seconds plateau annealing at 1000 °C. Slip bands originate from the notch and laser written number.

Fig 5: 200mm wafer in its cassette mounted for white radiation XRDI at the Diamond Light Source. Note the radiation damage to the cassette as indicated by the red circle.
III LABORATORY-BASED INSPECTION

The Jordan Valley BedeScan™ tool (Bowen, Wormington and Feichtinger, 2003) was operated initially in survey mode and subsequently in a high resolution setting. In survey mode, a CCD detector of pixel size 23.5 µm and the adjacent three pixels were binned, giving an effective resolution of 70.5 µm. The step size between each successive section topograph in the scan was six times the pixel size (141 µm), giving a reasonable compromise between resolution and scan time. In high resolution mode, over a limited wafer area, a different CCD camera was used with an expanding fibre-optic faceplate, resulting in a pixel size of 5 µm. There was no binning of pixels and the scan step was set at 20 µm (four pixels). MoKα (wavelength 0.708 Å) radiation in the 022 reflection was used for the BedeScan™ images.

Examination of the full wafer map, taken with the BedeScan™ tool, of a 200mm wafer which has been subjected to Rapid Thermal Annealing (RTA) (fig. 6) reveals that after the heat treatment the originally dislocation free wafer shows a high number of dislocations and dense slip bands which arise from the wafer edge. From the notch (circled) it can be concluded that all the slip bands run parallel to <110>, as is expected for the diamond structure type. The analysis of a number of wafer maps with different heating profiles shows that the length of a slip band is a function of the time the temperature stays above the brittle-ductile transition of Si at about 850 – 900 ºC (Tanner et al., 2011). The asymmetry associated with the slip band density, which is not predicted from the four-fold symmetry of the (001) wafer, has been shown to result from thermal anisotropy in the RTA furnace (Garagorri et al., 2012). From the fast laboratory map it is difficult to identify the origin of the slip bands; this could be done in high resolution scans which were performed at the Topo-Tomo beamline of the ANKA synchrotron. However, we see from fig. 6 that slip is usually initiated at the wafer edge and we have very few examples of slip starting in the middle of the wafer. Further, we have also determined that critical cracks resulting in wafer fracture originate at the wafer edge. Thus, an acceptable metrology is to undertake a perimeter scan, which can be done much more rapidly and in which the data collection time scales with wafer diameter, not area.

Fig. 7 shows a full BedeScan™ image of a 200mm diameter wafer that had been indented with a 50N load on a Vickers tip at three points at 90, 180 and 270º with respect to the orientation notch, at the bottom of the image. When the indent was placed within about 70µm of the bevel edge, long cracks were generated running towards the wafer centre. These appear with strong contrast in both BedeScan™ and synchrotron radiation topographs. In particular, the smaller crack, encircled in Fig 7, is not visible under an optical microscope, although it does appear in polarised infrared images. Such cracks, which result in catastrophic wafer fracture when heated to above 850ºC in an RTA furnace, are imaged in both transmission and reflection diffraction conditions, though the strongest contrast comes in the transmission geometry.
Fig 6: BedeScan™ transmission XRD Image of 200 mm plateau annealed Si wafer at 1000 °C for 30 s showing slip bands developing from the edge. Scan time 0.3 hours.

Fig 7: BedeScan™ transmission XRD Image of 200 mm (001) Si wafer which had been indented at 90, 180 and 270° with respect to the notch at the bottom of the image, (see arrow). The small crack circled on the right side is not visible optically.
IV. DATA COLLECTION TIMES

Table 1 indicates the times needed for complete maps of wafers with different diameters at the ANKA Topo-Tomo beamline, compared with the laboratory BedeScan™, QCRT™ and QCTT™ tools running in a configuration optimized for speed. The ANKA data were taken using the digital camera system and the $0\overline{2}2$ reflection at 1 mm overlap between sequential images.

**Table 1:** Process time for complete wafer mapping at Topo-Tomo beamline, ANKA, $0\overline{2}2$ reflection, transmission mode and in the laboratory on Jordan Valley BedeScan™, QCRT™ and QCTT™ instruments.

<table>
<thead>
<tr>
<th>Diameter:</th>
<th>200 mm</th>
<th>300 mm</th>
<th>450 mm</th>
<th>450 mm*</th>
</tr>
</thead>
<tbody>
<tr>
<td>ANKA beam size [mm²]</td>
<td>5 x 5</td>
<td>4.5 x 7.5</td>
<td>5 x 8*</td>
<td></td>
</tr>
<tr>
<td>Number of images</td>
<td>4700</td>
<td>7372</td>
<td>4000*</td>
<td></td>
</tr>
<tr>
<td>Integration time [sec]</td>
<td>0.5</td>
<td>0.5</td>
<td>0.1</td>
<td></td>
</tr>
<tr>
<td>Motor + Camera movement [sec]</td>
<td>1.9</td>
<td>1.9</td>
<td>1.9</td>
<td></td>
</tr>
<tr>
<td>Total time [hours]</td>
<td>3.1</td>
<td>5.0</td>
<td>2.2*</td>
<td></td>
</tr>
<tr>
<td>BedeScan™ [hours]</td>
<td>0.3</td>
<td>0.5</td>
<td>-</td>
<td>(1.1)*</td>
</tr>
<tr>
<td>QCRT™/QCTT™ [hours]</td>
<td>0.16</td>
<td>0.25</td>
<td>-</td>
<td>(0.6)*</td>
</tr>
</tbody>
</table>

* Optimum performance, estimated from the actual experimental data in the previous columns. Minimum image overlap and integration time. Translation stage programmed to scan just the wafer area, eliminating blank frames.
+ 450 mm wafer capacity currently not available and time is estimated from experimental data in previous columns.

It is evident from Table 1 that full area maps of 300 and 450mm wafers both at low resolution (BedeScan™/QCRT™/QCTT™) and at high resolution (ANKA) can be taken in a matter of hours.

CONCLUSIONS

Full high resolution X-ray diffraction imaging of 450mm wafers has been performed in a few hours at the TOPO-TOMO beamline on the ANKA storage ring. Experiments, using
conventional source equipment on 200 and 300 mm wafers, indicate that full-wafer images of 450 mm wafers can be obtained in-fab, at low resolution, in less than an hour. Despite the significant size change imminent in the industry standard, X-ray diffraction imaging of these very large wafers therefore remains possible both at synchrotron radiation sources and in the fab, though the latter does require apparently straightforward scaling up of present 300mm tools. Facilities are thus in place to accommodate the extension of our studies of 200mm and 300mm wafer fracture to the 450mm format when it becomes readily available. The application of our methodology for predicting the probability of catastrophic wafer breakage (Tanner et al., 2012) during high temperature processing will be appropriate for this new step in silicon wafer technology.

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