MECHANICAL STRENGTH OF MC-SILICON WAFERS CONSIDERING MICROSTRUCTURAL DEFECTS

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Outline

- Motivation
- Modeling Multicrystalline Silicon Wafers
  - Theoretical Approach
- Strength of Grain Boundaries
  - Experimental Approach
- Summary
Motivation
Market Share of Multicrystalline Silicon Wafers

- mc-Si-wafers still dominating the market with >60%
- prediction to hold significant share around 40% of crystalline market
- cost requirements: high yield, no breakage
  ⇒ mechanism of breakage well understood?

(source: ITRPV 2015)
Monocrystalline silicon wafers have higher strength than multicrystalline wafers (though, same defect distribution)\(^1\)

<table>
<thead>
<tr>
<th>Test Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>BR mono</td>
<td>ball-on-ring test</td>
</tr>
<tr>
<td>BR multi</td>
<td></td>
</tr>
<tr>
<td>4PB mono</td>
<td>4-point-bending test</td>
</tr>
<tr>
<td>4PB multi</td>
<td></td>
</tr>
</tbody>
</table>

hypothesis: grain structure influences fracture stress

⇒ theoretical approach
⇒ experimental approach

\(^1\) Bohne et al., 23rd EU PVSEC, 2008, Valencia, Spain
Motivation
Defects in Multicrystalline Silicon Wafers

- Mechanical strength of silicon is given by
  - Anisotropic elastic material parameters
  - Fracture mechanical material properties

- Defects in the material:
  - Micro cracks
  - Residual stresses
  - Inclusions
  - Grain structure
  - Dislocations
  - Grain boundaries

Strength
Fracture Probability
Yield
Modeling Multicrystalline Wafers

Objective and Approach

Objective

- theoretical investigations of the influence of grain structure on the strength of silicon wafers

Approach

- creating a Finite-Element model including grain structure
- obtaining stress distributions caused by grain structure and anisotropic elastic properties
- statistical evaluation and calculation of failure probabilities for wafers

⇒ comparison of failure probabilities between monocristalline and multicrystalline wafers
Modeling Multicrystalline Wafers
Setup of Finite-Element-Model – Grain Geometry

Samples (image analysis of real wafers)

Wafer 1 (small grains)
Wafer 2 (medium grains)
Wafer 3 (big grains)
Modeling Multicrystalline Wafers
Setup of Finite-Element-Model – Grain Orientation

- experimental analysis of grain orientation on wafer scale is difficult
  - EBSD, XRD, optical methods

Alternative:
- random assignment of grain orientations (Monte-Carlo-Method)
  - definition of orientation by Euler angles (anisotropic material parameters)

![Diagram showing initial grain orientation, random rotation about Euler angles, and random orientation for each grain.](image)
Modeling Multicrystalline Wafers
Setup of Finite-Element-Model – Grain Orientation

- selection of three probability distributions for defining grain orientations

- uniform distribution

- normal distribution
  \[ \mu(\phi_1, \Phi, \phi_2) = (0°, 0°, 0°) \]
  \[ SD = 4° \]

- normal distribution
  \[ \mu(\phi_1, \Phi, \phi_2) = (0°, 0°, 0°) \]
  \[ SD = 40° \]
Modeling Multicrystalline Wafers

Simulation Parameters

Simulation Parameters:

- uniaxial tensile load (1 MPa)
  ⇒ stress distribution (principal stresses)

Cases:

- 3 probability distributions each
- 3 grain size distributions each
- 800 grain orientation distributions for each case (necessary for convergence of Monte-Carlo-Method)

⇒ approx. 7200 FE simulations

Failure Probability:

- calculation of failure probabilities P from stress fields by using Weibull distribution considering the size effect of strength
Modeling Multicrystalline Wafers
Results: Stress Distributions

- homogenous stress field in monocrystalline wafer
- grain structure causes inhomogeneous stress field
- local stress concentrations at grain boundaries
Modeling mc-Wafers
Results: Fracture Probability

Fracture probability $P_{\text{mono}}$ is always smaller than $P_{\text{multi}}$ (assuming equal defect distributions!)

- small deviations of grain orientation result in smaller $P_{\text{multi}}$
  - adjacent grains with strong difference in elasticity increase $P_{\text{multi}}$
- grain shape and size influence strength, cf. wafer geometries (1,2,3)

![Graph showing failure probability](image)
Strength of Grain Boundaries

Introduction

- theoretical analysis showed possible influence of size effect due to inhomogeneous stress fields
  - but: influence is small and requires
    - identical defect distributions
    - perfect grain boundaries

⇒ Strength of grain boundaries?
⇒ Are they weak compared to the crystal?

- strong grain boundaries found by Mansfield et al. in micromechanical tests (microcantilevers)

Mansfield et al. (2010). *Solid State Phenomena, 156-158, 55-60*
Strength of Grain Boundaries

Approach

- using “standard” multicrystalline silicon wafers
- performing Vickers indentation near grain boundaries of different types
  - positions varied in the vicinity of grain boundary
- evaluating the crack length as measure of fracture toughness
- calculate fracture toughness based on fracture mechanical equations

⇒ Analyzing grain boundary strength
Strength of Grain Boundaries: Indentation Positions

Crystallite A

Crystallite B

far away indentation (reference)

500 µm

250 µm

500 µm

250 µm

500 µm

Indentation on the grain boundary

reference crack

Indentation in close vicinity to the grain boundary (near)
Strength of Grain Boundaries
Sample Preparation

- Determination of crystallographic orientation
- Polishing
- Etching I
- Ultra Micro Hardness Testing
- Etching II
- Analysis of crack length

The diagram shows two crystallites, A and B, with their respective CSL classifications and orientations:

<table>
<thead>
<tr>
<th>CSL Classification</th>
<th>Crystallite A (left)</th>
<th>Crystallite B (right)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Sigma 3 )</td>
<td>(111)</td>
<td>(111)</td>
</tr>
<tr>
<td>( \Sigma 21b )</td>
<td>(210)</td>
<td>(323)</td>
</tr>
<tr>
<td>( \Sigma 29b )</td>
<td>(158)</td>
<td>(112)</td>
</tr>
<tr>
<td>( \Sigma 35a )</td>
<td>(110)</td>
<td>(332)</td>
</tr>
</tbody>
</table>

The diagram also includes measurements of 500 µm, 250 µm, and 250 µm for the distances and indentation positions.
Strength of Grain Boundaries

Results

- About **450** Vickers indentations were made
- Approx. 40 with an ideal pattern, 200 with shell fractures in varying degrees (chipping) and 250 with an unacceptable fracture pattern (not evaluable)
- At least 10-15 evaluable cracks per experiment

[Images showing different fracture patterns: unacceptable, acceptable, acceptable.]
Strength of Grain Boundaries
Results: Fracture Toughness (Horizontal Cracks)

- Anstis (HPC)
- Laugier (Palmquist)

Similar fracture toughnesses for all grains
Close to literature values

Ebrahimi et al.\textsuperscript{3}:
\{111\} $K_{IC}$: 0.81-1.03 MPa m\textsuperscript{1/2}
\{110\} $K_{IC}$: 0.83-1.31 MPa m\textsuperscript{1/2}

Anstis et al.\textsuperscript{2}:
Si (Mono): $K_{IC}$: 0.7 MPa m\textsuperscript{1/2}

Mansfield et al.\textsuperscript{4}:
\{110\} $K_{IC}$: 0.7 ± 0.3 MPa m\textsuperscript{1/2}
Strength of Grain Boundaries
Results: Horizontal Cracks

- Cracks far away from GB
- Most cracks towards GB are smaller than opposite cracks
- Crack length influenced by crystal lattice
Strength of Grain Boundaries
Results: Summary Horizontal Cracks

- Comparison of indentation cracks in the grain, near GB and on GB
- No significant crack extension compared to reference!
Strength of Grain Boundaries

Results: Vertical Cracks
Strength of Grain Boundaries
Results: Vertical Cracks

- Vertical cracks on grain boundary do not lead to crack extension.
- No reduced fracture toughness or strength!
Summary

- multicrystalline silicon wafers often show smaller strength compared to monocrystalline wafers
- modeling shows: stress concentrations mainly occur at grain boundaries
- the difference in strength between mono- and multicrystalline wafers depends on load and defect distribution ($\sigma_0$, $m$)
- **due to size effect of strength, grain structure can reduce mechanical strength of silicon wafers**
- cracks indented in crystal lattices show a highly asymmetric crack pattern that results in an anisotropic behavior regarding crack propagation
- statistically, **grain boundaries do not significantly affect** the crack growth caused by Vickers Indenters
  - no significant influence on the critical fracture toughness $K_{lc}$
  - no intergranular fracture behavior => strong GBs
  - **GBs are not the weak point in the wafer** – even in Twin GBs?
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