Fractal Geometry Applied To Fracture (Part 3)

J. J. Mecholsky, Jr.
Materials Science & Engineering Department
University of Florida
Gainesville, FL 32611-6400

jmech@mse.ufl.edu

Glass Tutorial Series: prepared for and produced by the International Material Institute for New Functionality in Glass
An NSF sponsored program – material herein not for sale
Available at www.lehigh.edu/imi
Technical Approach

• Molecular Orbital (MO) Modeling of Fracture - determines $a_0$.

• Molecular Dynamics (MD) Modeling of Fracture - determines $D^*$ (e.g. in Si)

• Experimental determination and comparison of parameters obtained in MO and MD Modeling, i.e., $a_0$ and $D^*$
Bell & Dean Model Used for MO Calculations

cf. Varsheneyya, Fundamentals of Inorganic Glasses
(After Bell and Dean, Nature 212, 1354 [1966])
cf. Varsheney, Fundamentals of Inorganic Glasses
(after T. F. Soules, Glass Sci & Tech 4A, 318)
cf. Varsheneyya, Fundamentals of Inorganic Glasses
MO Simulates Bond Breaking At The Crack Tip

Simulated SiO$_2$  $\Delta$ displ. = 1 Å
Strain Can Be Measured In Model

\[ a_0 = \frac{a}{\varepsilon} = \frac{c \ a}{c' - c} \]

J. Non-Crystalline Solids
Modeling and Experimental Results Agree

\[ a_0 = \frac{2\gamma}{(ED^*)} \]

<table>
<thead>
<tr>
<th>Material Class</th>
<th>$a_0$ (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single Crystals</td>
<td>1-10</td>
</tr>
<tr>
<td>Glasses</td>
<td>10-20</td>
</tr>
<tr>
<td>Glass Ceramics</td>
<td>20-80</td>
</tr>
<tr>
<td>Polycrystalline Ceramics</td>
<td>3-10</td>
</tr>
<tr>
<td>Polymers</td>
<td>2700-14000</td>
</tr>
</tbody>
</table>

$a_0$ is related to structure.
FSA Can Be Applied To Single Crystals

Single Crystal Silicon
Simulated Fracture Can Form Fracture Surface
Simulated Fracture Can Form Fracture Surface
Simulated Fracture Can Form Fracture Surface
Simulated Fracture Can Form Fracture Surface
Surface Can Be Created From MD Simulation
Slit Island Contour Can Be Made From 3-D Map
FRACTAL DIMENSION IS MEASURED ALONG CONTOUR

Log Length (A-B)

A-B = Slit Island Contour

Slope = -D*

Log (Ruler Length)
<table>
<thead>
<tr>
<th>Material</th>
<th>Fracture Plane/Surface</th>
<th>$K_{IC}$ (MPam$^{1/2}$)</th>
<th>Fractal Dimension (Experimental)</th>
<th>Fractal Dimension (MD Simulation)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si {100}/{110}</td>
<td>1.26 ± 0.06</td>
<td>2.16 ± 0.04</td>
<td>2.16 ± 0.06</td>
<td></td>
</tr>
<tr>
<td>Si {110}/{100}</td>
<td>1.23 ± 0.08</td>
<td>2.10 ± 0.04</td>
<td>2.11 ± 0.05</td>
<td></td>
</tr>
<tr>
<td>Si {111}/{110}</td>
<td>1.17 ± 0.08</td>
<td>2.06 ± 0.02</td>
<td>2.09 ± 0.04</td>
<td></td>
</tr>
<tr>
<td>Silica (amorphous)</td>
<td>0.75</td>
<td>2.11 ± 0.02</td>
<td>2.1</td>
<td></td>
</tr>
</tbody>
</table>

CRACK SIZE (c) to MIRROR-MIST (r_1) RATIO: \( D^* = \frac{c}{r_1} \)

where \( D^* \) = FRactal Dimensional Increment

(a)

MD SIMULATION OF FRactal FRACTURE SURFACE

\[ \gamma_c = \frac{a_0 D^* E}{2} \]

(b)

RING DIAMETER TO STRAIN FRACTION RATIO: \( a_0 = \frac{a}{\varepsilon} \)

(c)
Fracture Is A Fractal Process

• Fracture transcends many length scales; Self-similar (or self-affine), scale invariant & characterized by $D^*$.  

• Hypothesis: $2\gamma = [a_0 \ E \ D^*]$  

• Observations seem to support the hypothesis. 

\[
c/r = D^* \ ; \ \gamma \propto ED^* \\
(D^* \text{ is a geometric & energy scaling factor.}) \\
(a_0 \text{ is a fracture surface structural element})
\]

• MD & MO modeling provide framework for understanding macroscopic observations
Many Tools Are Needed for Unified Fracture Theory

<table>
<thead>
<tr>
<th>Model</th>
<th>Scale</th>
<th>Experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>MO</td>
<td>sub-atomic</td>
<td>fractoemission</td>
</tr>
<tr>
<td>Ab initio</td>
<td>atomic</td>
<td>AFM</td>
</tr>
<tr>
<td>Quantum Mechanics</td>
<td>nano</td>
<td>STM</td>
</tr>
<tr>
<td>MD</td>
<td>micro</td>
<td>Raman</td>
</tr>
<tr>
<td>Monte Carlo</td>
<td>Meso</td>
<td>Fractography</td>
</tr>
<tr>
<td>Finite diff.</td>
<td>Macro</td>
<td>fracture mechanics</td>
</tr>
</tbody>
</table>

Fracture Process

Fractal Geometry
Summary

• At the atomic level, quantum mechanics describes the fracture process as a ring contraction process dictated by minimum energy and availability of free volume.

• On the molecular scale, MD modeling describes creation of the fracture surface.

• On the macroscopic scale, mirror, mist & hackle form & $c/r = D^*$

• At all length scales, $2\gamma = [a_0 E D^*]$
Critical Questions Need To Be Asked

- What are the energetic & geometric steps to fracture?
- Is a flat fracture (of primary bonds) possible above absolute zero? What is bond rupture?
- Is roughness a meaningful parameter in fracture?
- How does energy scale?
- How does a crack propagate at all length scales?
CONCLUSIONS

• Fractal fracture implies that the same fracture process should be able to be observed at all length scales.

• Experimental data & analytical modeling have to be interactive to be successful.

• All models should be compared to (real) experimental data.

• Analytical models have to explain fractal nature of fracture, mirror, mist & hackle and crack branching.
Bond Breaking Leads to Characteristic Features

\[ \log K = \log (Y\sigma c^{1/2}) \]
University of Florida, Gainesville