Visualization of Perovskite Octahedral Tilts in Augmented Reality

NAYMAN LEUNG
MENTOR - WILLIAM RATCLIFF
Background

- Perovskites
  - Crystals with $ABX_3$ structure
    - X - anion
    - A - cation
    - B - cation

Perovskite Unit Cell (Courtesy of Fu and Itoh)
Crystal Distortions

- Distortions
  - Jahn-Teller Distortion
  - Cation Displacements
  - Octahedral Tilts
- Causes
  - Size of A and B ions
  - State Variables

Courtesy of Dr. Gorman
Cation Size

- Goldschmidt’s tolerance factor ($t$) - ratio of A and B ionic radii that describe stability
  \[ t = \frac{r_A + r_0}{\sqrt{2}(r_b + r_0)} \]

  - $t > 1$ = A ion too big or B ion too small = hexagonal
  - $0.9 - 1$ = A and B ions are ideal = cubic
  - $0.71 - 0.9$ = A ion too small = Orthorhombic/Rhombohedral

Courtesy of Mark Levy

CaTiO$_3$ Courtesy of Nick Greeves
Glazer Notation

- **Describe octahedral distortion**
  - Sequence of symbols - axes
    - a, a, a - x, y, z
  - Identical characters - relative magnitude
    - a, a, c
  - Superscript - phase of tilt for layers
    - 0 = no
    - + = in phase
    - - = anti phase

Courtesy of Rondinelli and Fennie
Project Goal

- Improve visualization of Perovskite distortions by working in Augmented Reality
- 3D modeling programs
  - VESTA
  - SPuDS
  - Diamond

Courtesy of SPuDS
Unity3D

- Game engine for developing video games
- Language - Javascript/UnityScript, C#, Boo
- Deployment to VR/AR
  - Gear VR (phones)
  - HTC Vive
  - Oculus Rift
  - Windows Hololens

Courtesy of Guido Henkel

Courtesy of Wired

Courtesy of Microsoft
Microsoft Hololens

- Augmented Reality
- Spatial mapping, gesture/speech/gaze recognition

Courtesy of Forbes
Pin Demo
<table>
<thead>
<tr>
<th>Glazer Stereophotographs</th>
<th>Notation</th>
<th>Unity App Viewed in Hololens</th>
</tr>
</thead>
<tbody>
<tr>
<td>THREE TILTS</td>
<td>$a^+, b^+, c^-$</td>
<td><img src="image1.png" alt="Image" /></td>
</tr>
<tr>
<td>TWO TILTS</td>
<td>$a^0, b^+, c^-$</td>
<td><img src="image2.png" alt="Image" /></td>
</tr>
<tr>
<td>ONE TILT</td>
<td>$a^0, b^0, c^-$</td>
<td><img src="image3.png" alt="Image" /></td>
</tr>
<tr>
<td>NO TILTS</td>
<td>$a^0, b^0, c^0$</td>
<td><img src="image4.png" alt="Image" /></td>
</tr>
</tbody>
</table>
Results

- Visualize and manipulate a crystal
- Detect when crystal is being selected (audio)
Future Goals

- Toolbar – rotation, movement, initiating “octahedral tilt”
- Voice and Spatial Recognition
- Implementation of data
Practical Applications

- Solar Cells
  - organic-inorganic semiconductors for efficient photovoltaics
- Microelectronics and Telecommunications
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