Detailed Photoemission Modeling Using The 3D Finite-Element PIC Code MICHELLE*

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June 26, 2007

* Work supported by the Office of Naval Research and the Joint Technology Office.
Outline

- Photoemission Modeling Issues
- Overview of the MICHELLE Code
- Photoemission Modeling Examples
  » Full RF Gun
  » Surface Roughness
  » Surface Grains
Photoinjectors & Photocathodes

- Bulk & Surface of Complex Materials
  Produced by Empirical Techniques; Short Lifetime, Complex Replacement Process.
- Cathode Selection Influences Drive Laser Chosen (e.g., wavelength, spot bandwidth, laser energy, QE, etc.)

- Drive-laser Reliability <=> System Reliability:
  UV Unsuitable for Hi-duty
- Non-linear Crystals Decrease $\lambda$ by 2-4;
  Efficiency Very Low for UV
- Conversion by 2 From IR to Green ok:
  Seek High QE Photocathode in Visible

![Diagram of Photoinjectors & Photocathodes]
Photocathode Density Modulated RF Gun

- **Disparate spatial scales**
  - 1 mm beam radius in a 4 cm radius cavity (40:1).
  - 6 mm long beam bunch in a 120 mm long device (20:1).
  - The beam bunch must be resolved spatially.

- **Disparate time scales**
  - The laser has a time scales on the order of 4-8 ps.
    - Smaller if laser ripple is included.
  - The RF has a time scale of 350 ps (~ 45:1 - 90:1).
  - There may be finer time scale oscillations as a function of the photoemission process that may need to be modeled to accurately predict the emittance.

- **Realistic representation of geometry**
  - Waveguides, ports & tuning stubs may have a significant effect on the beam dynamics.

Taking into account these features allows us to accurately predict beam formation & optimize gun designs.
MICHELLE Capabilities

- Advanced design tool for electron guns & collectors
  - Electron Guns
    - Modulation control and shadow grids
    - Electron surface emission models
    - Multi-beam and sheet beam devices
  - Multistage Depressed Collectors
    - Anisotropic collectors
    - Improved secondary emission models

- With the ability to support...
  - Tolerance analysis – alignment and clocking errors
  - Fine structure representation
  - Multiple species

BOOTH 402
2nd Gen: Experiment vs. Theory

- Analyze copper photoemission and compare to data from Rosenzweig, et al.

- 1st Gen theory had to be divided by a factor of 6.6 to give a "match" to the experimental data.

- The newer code has made major modifications in areas including…
  - The scattering operator
  - The implementation of the moments-based QE estimate
    - Rather than the previous Modified Fowler-Dubridge method.

- Using the default copper parameters and no fudge multiplier gave the agreement shown.

TUPMS091
“A Theoretical Photocathode Emittance Model Including Temperature and Field Effects”
Kevin Jensen, et al.
RF Gun Optics Modeling Using MICHELLE

**STEP 1**
Solve for Eigenmode cavity fields and frequency. Using a Finite-Element Frequency-Domain code. GENOME or ANALYST.

**STEP 2**
Import cavity E & B fields into MICHELLE. MICHELLE clocks these field in time.

**STEP 3**

**STEP 4**
MICHELLE calculates ES image & self fields. These are superimposed with the RF drive fields. MICHELLE calculates self-consistent particle trajectories. Final beamlet data can be exported.

- Simulation Products
  - Beamlet properties.
    - Particle phase space data.
    - Particle current.
    - Calculated quantities – emittance, etc.
  - Temporal beam data provided to the next simulation along the beamline.

Courtesy of Mark Cattelino, CPI
Example: BNL 1 ½ Cell RF Gun

- Peak Field: 120 MV/m
- Frequency: 2.859 GHz
- Laser Energy: 20 microJoules
- Laser Spot Size: 1 mm
- Laser Pulse: 8 ps FWHM
- Beamlet Charge: 1-2 nC

Courtesy of Vitaly Yakimenko, BNL
Example: Detailed Effect of Laser Ripple

- Consider emission into a Pillbox.
  - 15 mm long x 10 mm radius
- Use 1st Gen Jensen photoemission model
- Hybrid structured/unstructured mesh
  - Structured mesh in the beam region
  - 750,000 elements
- BNL parameters from previous slide are used
Photoemission: Modeling Surface Roughness Effects

- Research modeling of photoemission with surface roughness.
  - What effect does surface roughness have on beam emittance? (idea by Kevin Jensen)
  - How do we model it?
- Start off with a 1-cell periodic model.
  - 6 micron hemisphere hexagonally packed.
  - 12 micron center to center spacing.
  - 45 micron length.

Sintered tungsten

45 micron length

6 micron diameter

12 micron width

Courtesy Nathan Moody, UMD

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Photoemission: Modeling Surface Roughness Effects

- Copper
- Applied Field: 5 MV/m
- Laser Intensity: 160 MW/cm²

- A significant portion of the beam current emits from the tip of the hemisphere.
  - This picture only shows those particles emitting from the tip to illustrate the transverse particle motion.
  - They emit everywhere on the flat region as well, with much less current.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fermi Level</td>
<td>7.00000 eV</td>
</tr>
<tr>
<td>Work function</td>
<td>4.60000 eV</td>
</tr>
<tr>
<td>Atomic Weight</td>
<td>63.5460 grams/mole</td>
</tr>
<tr>
<td>Mass Density</td>
<td>8.96000 grams/cm³</td>
</tr>
<tr>
<td>Bulk Temp</td>
<td>300.000 Kelvin</td>
</tr>
<tr>
<td>Gamma (Ce/T)</td>
<td>96.9800 Joule/(K² meter³)</td>
</tr>
<tr>
<td>Field enhance</td>
<td>5.00000 –</td>
</tr>
<tr>
<td>Wavelength</td>
<td>2660.00 Ångstroms</td>
</tr>
<tr>
<td>Gauss time</td>
<td>6000.00 femtoseconds</td>
</tr>
<tr>
<td>Skin depth</td>
<td>126.000 Ångstroms</td>
</tr>
<tr>
<td>Field(force)</td>
<td>0.500000E-03 eV/Ångstroms</td>
</tr>
<tr>
<td>Laser Intens</td>
<td>160.000 MW/cm²</td>
</tr>
</tbody>
</table>
Photoemission: Modeling Surface Roughness Effects

- **Simulation Parameters**
  - Simulation time: 45 fs
  - Time step: 0.15 fs
  - # Elements: 625,000

- **Observations**
  - Increased emittance (x43) compared with smooth surface model.
  - ~3 fs oscillations.
We want to model the effect of surface grains on the beam emitted in the photoemission process.

- How does it effect the beam emittance?

Take Nate Moody’s image of surface, find grains by assuming reflectivity depends on crystal face shown.

1. This is the original picture provided by Nate
2. The Red Box indicates the part under analysis.

Scale: 421 Pixels = 67 \mu m
Grain Work Function Emission Model

1. JPEG from Nate's scan.
2. 421 x 421 Pixel array of scan using 256 "colors" (MATLAB)
3. Plot showing number of pixels of each color. 
   » Extract 3 color bands
5. Recreate image array with similar properties, but without the noise

```
m_1 = (((m_0-m_2)/8)^2 + 1) + m_3/(((m_0-m_4)/8)^2 + 1) + m_5/(((m_0-m_6)/8)^2 + 1)
```
Interpreting pre-processed data…

- It’s a judgment call whether black = <100>, gray = <110> and white = <B> in Gyftopoulos-Levine theory, or some other arrangement.
- This algorithm gives a means of generating the surfaces from which the f-parameter in GL theory is assigned in the Photocurrent code.
Grain Emission Model: MICHELLE Implementation

- Want to study the effects of the crystal face grains on beamlet properties.

- **Model Parameters:**
  - Beam – $r = 2$ mm / 1 nC / 10 ps / 10 MV/m
  - Trial and error led to laser intensity of $1.8$ MW/cm^2
    - This led to a virtual cathode effect
  - Reduced laser intensity to $1$ MW/cm^2 for steady-state behavior.
    - Results in SCLE current emitted

- Choose pillbox that represents a portion of the scanned surface.

![Diagram](image)
Grain Emission Model: MICHELLE Implementation

- Pillbox Model Cases Run...
  1. Single Grain – Grain 0 (Flat)
  2. Single Grain – Grain 1 (Flat)
  3. Single Grain – Grain 2 (Flat)
  4. Mixed Grains - Scanned Grains on a *Flat Surface*
  5. Mixed Grains - Scanned Grains on a *Bumpy Surface*

- Laser Intensity: 1 MW/cm^2
- E = 10 MV/m
- V = 0
- V = 3 kV
Grain Emission Model: MICHELLE Simulations

- Surface Grains - Flat emission surface
  - Particle colors represent Emission Current Density
  - Effect of grain faces captured in photoemission model

![Diagram showing different particle densities and sizes, with color codes for current density and microns dimensions marked as 67 x 67 microns and 30 x 30 microns.]

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Grain Emission Model:
MICHELLE Simulations – Cases 4 & 5

- $|J|$ on emission surface shown as background color contour map
- $|E|$ shown as contour lines
  - Case 4: Flat surface
  - Case 5: Bumpy surface
Grain Emission Model: MICHELLE Simulations – Cases 4 & 5

|J|  |J| & v_perp  | v_perp  
---|---|---|---
Flat | ![Image](image1.png) | ![Image](image2.png) | ![Image](image3.png) |
Bumpy | ![Image](image4.png) | ![Image](image5.png) | ![Image](image6.png) |
Grain Emission Model: MICHELLE Simulations – Case 5

|E| Along Beamline

Full Emission  Bump Emission  Flat Emission
Grain Emission Model:
MICHELLE Simulations – Case 5
Laser Intensity: 1MW/cm^2  
Applied E-field: 10 MV/m

<table>
<thead>
<tr>
<th>Run</th>
<th>Grain</th>
<th>Current (mA)</th>
<th>E-Surface (MV/m)</th>
<th>Emittance Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>1) Face-0</td>
<td>0</td>
<td>1.569</td>
<td>7.48</td>
<td>1 (reference)</td>
</tr>
<tr>
<td>2) Face-1</td>
<td>1</td>
<td>3.881</td>
<td>1.81</td>
<td>5</td>
</tr>
<tr>
<td>3) Face-2</td>
<td>2</td>
<td>&gt; SCLE</td>
<td>“0”</td>
<td>-</td>
</tr>
<tr>
<td>SCLE</td>
<td>uniform</td>
<td>3.939</td>
<td>“0”</td>
<td>6</td>
</tr>
<tr>
<td>4) NoBump</td>
<td>From Scan</td>
<td>2.943</td>
<td>0 - 4.88</td>
<td>64</td>
</tr>
<tr>
<td>5) Bumpy</td>
<td>From Scan</td>
<td>3.319</td>
<td>0 - 12.9</td>
<td>357</td>
</tr>
</tbody>
</table>
Conclusion

- The most recent Jensen Photoemission models are now in the MICHELLE code.

- The MICHELLE code with its ability to resolve very fine features provides a capability for modeling detailed photoemission, which includes…
  - Laser ripple
  - Surface roughness
  - Granularity/Crystals

- Continued validation of these models is an ongoing task.