LANL Accelerator and Material Science Activities for C-band

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LANL Accelerator and Material Science Activities for C-band

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• LANL Accelerator Projects
  – Overview
• LANL Mission Needs
  – Gradient, pulse length, burst mode
• Multi-disciplinary Program Plan
• FY19 Accomplishments
  – RF Technology
  – Material Science Tools
  – Dielectric Insertions
• Summary and Outlook
LANL Accelerator Efforts – An Overview

New efforts in accelerator physics starting at LANL since 2018

• SCORPIUS, a multi-pulse induction linac for hydrodynamic experiments

• DMMSC (Dynamic Mesoscale Materials Science Capability) with a trajectory leading to a MaRIE type XFEL

• Accelerator in Space (AIS) in support of the NASA CONNEX mission. The goal is to study magnetospheric processes and their role for different types of auroral and ionospheric activities

• Compact accelerators for national defense missions, e.g transportable accelerator driven ICS sources

• Build-up of an Accelerator Development and Engineering Facility (ADEF), a local electron beam test facility for technology development

• Modernization & upgrade of the LANSCE proton accelerator
LANL Mission Needs

DMMSC (if accelerator chosen as source)
- Cryo-cooled (non-SRF) high gradient tech will reduce cost by ~ $200M
- Accelerator will fit at TA-53 for higher beam energies
- Avoids cost and complexity of superconducting RF
- High frequency enables temporal resolution of burst mode
  - L-band - S-band - **C-band** - X-band

LANSCE (reduced $\beta$ structures, > 0.4)
- Modernization of 0.8 GeV linac in place with old accelerator (larger customer base)
- Upgrade (~ 20 GeV) would fit into existing tunnel

Accelerator Development and Engineering Facility (ADEF)
- Multi-physics accelerator facility
- Induction linac and RF linac technology
- C-band: 50 MW RF power, cavity testing (FY20), e-beam (FY22+)
Multi-disciplinary Program Plan

Design, prototyping & operation of a ultra-high gradient, high-efficiency RF-structure as product of a tool & engineering capability development

- Thrust areas that contribute to solving the technology challenges
  - **Material Science (T):** Understanding physics of breakdown and development of strategies for breakdown suppression, design tools for materials in extreme fields
  - **RF technology (AOT/E):** Resonator design for high gradient and long pulse operation (cryo-cooled), and build-up of a permanent testing capability
  - **Advanced manufacturing (SIGMA):** Fabrication processes and joining techniques that create and preserve surface and bulk properties of metal alloys for breakdown suppression
FY19 Accomplishments (RF)

• Systematic evaluation of RF-structures for
  – Efficiency (power, cost, longer pulse length)
  – Wakefields (beam quality)
  – Spacing in bunch trains (dynamic experimentation)
  – Energy spectrum controls (effort for good FEL operation)

• Comparison for S-band (3 GHz), C-band (6 GHz) and X-band (12 GHz)
  – demonstrated the superiority of C-band for the relevant performance criteria

• Capital funds for 50 MW $P_{peak}$ C-band source ($1.3M$)

• RF-source development for higher power and pulsed power technology for MaRIE- and advanced pRAD-type pulse formats
Why C-band?

- Identical RF shape scaled to S, C & X
- Calculated performance RF metrics
- Calculated beam-structure interaction
- Calculated temporal bunch train characteristics
- Compared with SRF

<table>
<thead>
<tr>
<th>Parameter</th>
<th>L-band</th>
<th>S-band</th>
<th>C-band</th>
<th>X-band</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shunt impedance [MΩ/m]</td>
<td>9.8E+6</td>
<td>85</td>
<td>120</td>
<td>170</td>
</tr>
<tr>
<td>Wakes longitudinal [V/μC]</td>
<td>10.2</td>
<td>26.4</td>
<td>36.4</td>
<td>50.4</td>
</tr>
<tr>
<td>Energy change @ 1 GeV</td>
<td>0.3%</td>
<td>2.5%</td>
<td>3.5%</td>
<td>8.0%</td>
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<tr>
<td>Wakes transverse [V/μC/m]</td>
<td>15.1</td>
<td>155</td>
<td>835</td>
<td>4420</td>
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<tr>
<td>Deflection @ 1μm [kV]</td>
<td>0.0</td>
<td>1.5</td>
<td>8.0</td>
<td>67.4</td>
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<tr>
<td>Gradient [MV/m]</td>
<td>30</td>
<td>50</td>
<td>100</td>
<td>150</td>
</tr>
<tr>
<td>Dechirper length @ 1 GeV</td>
<td>N/A</td>
<td>2.9</td>
<td>1</td>
<td>0.8</td>
</tr>
<tr>
<td>Fabrication tolerances</td>
<td>good</td>
<td>good</td>
<td>good</td>
<td>hard</td>
</tr>
<tr>
<td>Long range wakes for burst</td>
<td>bad</td>
<td>bad</td>
<td>good</td>
<td>good</td>
</tr>
</tbody>
</table>
Technologies Considered

RF-structure
- Tantawi Style (clamp shell, distributed coupling, SW, C-band)
- LANL Design focus: better materials, focus on XFEL wake reduction, plus reduced $\beta$ variants (S- or C-band)

RF sources
- Joint effort with SLAC on either maximizing peak power (100+ MW) or use many small sources for individual structure feed (C-band)
- Development of faster modulators

Beam source
- Joint effort with UCLA on TOPGUN derivative (C-band)
- LANL focus on symmetrized RF-feed and XFEL optimized bunch parameters
FY19 Accomplishments (Material Science)

• Developed a classical charge equilibration model
• Classical model parameterized and validated against DFT energies (quantum approach)
• Showed excellent agreement, <10% error even for defective surfaces
• Reproduced coupling of charges to microstructure
• Dynamics shows spontaneous breakdown at very high fields
• Demonstrated that Lorentz forces alone cannot induce plastic deformation
  • Leads to a key role of thermal fatigue in creating precursors to breakdown
Quantum Approach – Density Function Theory (DFT)

• Quantum description:
  – Explicit description of the electron gas
  – Variational approach: find the electronic density that minimizes quantum Hamiltonian

• Strengths:
  – Very accurate (~100 meV/atom)
  – First principles (few parameters, transferable)

• Weakness:
  – Very expensive (scales as $N_{\text{electrons}}^3$)
    • Small systems (~few 100 atoms): cannot capture microstructure effects
    • Static or short dynamic simulations (~ps): cannot explicitly simulate surface evolution

Example from VASP
• Determines equilibrium charge distribution
• Change in work-function to release charges

Why are we doing this?
Fit classical model on DFT data – is well established process for copper
Classical Approach – Molecular Dynamics (MD)

• Classical description:
  – Molecular dynamics (integration of classical EOM)
  – Charge-equilibration formalism (qEq) to capture effect of induced charges

• Strengths:
  – Reasonably accurate empirical description of Cu
  – Relatively fast
    • “Large” systems (~10^6 atoms): can capture some microstructural effects
    • “Long” simulations (milliseconds): can capture surface evolution

• Weakness:
  – Scales are still very limited compared to engineering scales
MD Verification and Path Forward

The model captures the key physics of metal surfaces under fields.

- Informed proposed modeling strategy:
  - Trust 1: use large-scale MD to study deformation under thermal stresses vs microstructure, composition.
  - Trust 2: use Accelerated MD to characterize breakdown propensity of surface structure under high fields.

- This will allow for a science-based optimization of materials solutions.
• High dielectric constant and large bandgap (low losses) are desirable
• Most materials have one or the other
• Can new materials be designs (like Ti-doped alumina)?
• Do compromise materials have good vacuum and/or breakdown properties?
Summary and Outlook

• LANL is in the first year of a 4 year program for an integrated UHG resonator development that includes
  – material simulations to understand and improve breakdown behavior
  – Establish RF-structure designs (SW) for long-pulse operation at C-band
  – Use LANL advanced manufacturing capabilities for “gentle” manufacturing
  – Electron beam testing capability (ADEF) - to be extended by other programmatic needs. Test bed for diagnostics, RF-structures, and cathodes
    – collaborative effort with UCLA/SLAC
  – Establish dielectric for performance improvement at moderate gradients

• The developed technologies are expected to
  – Establish custom material designs for high performance RF resonators
  – Provide the foundation for improved LANL-XFEL and LANSCE designs
  – Provide technologies for compact FEL designs
  – Establish a path to transportable SNM detection devices using ICS gammas