LANL Accelerator and Material Science Activities for C-band

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Frank Krawczyk

AOT - Accelerators and Electrodynamics

LANL

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Contributions from:

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LANL Accelerator and Material Science Activities for C-band

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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)

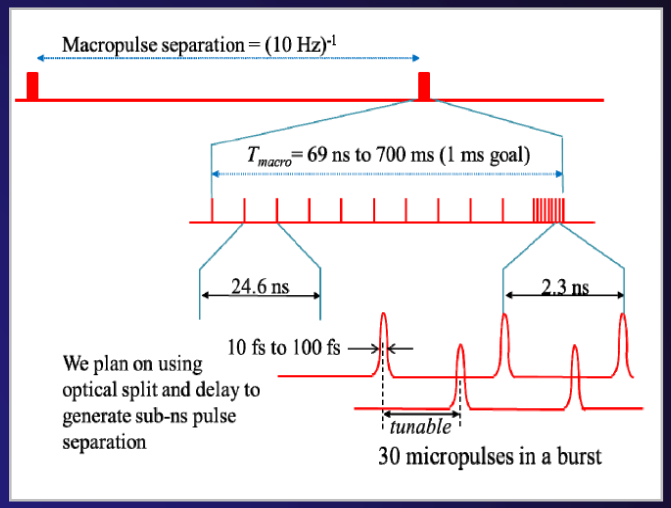
- Cryo-cooled (non-SRF) high gradient tech will reduce cost by ~ $200M
- Accelerator will fit at TA-53 for higher beam energies
- Avoids cost and complexity of superconducting RF
- High frequency enables temporal resolution of burst mode
  - L-band - S-band - **C-band** - X-band

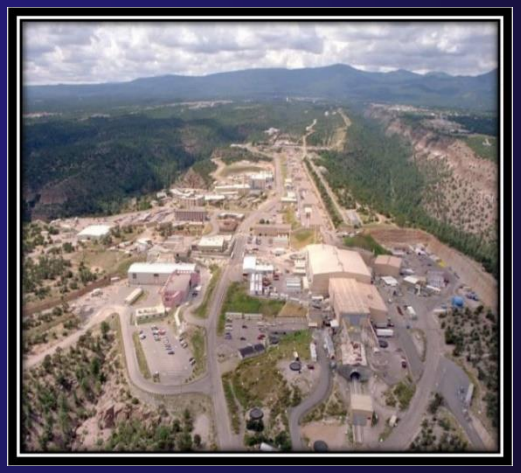
LANSCE (reduced β structures, > 0.4)

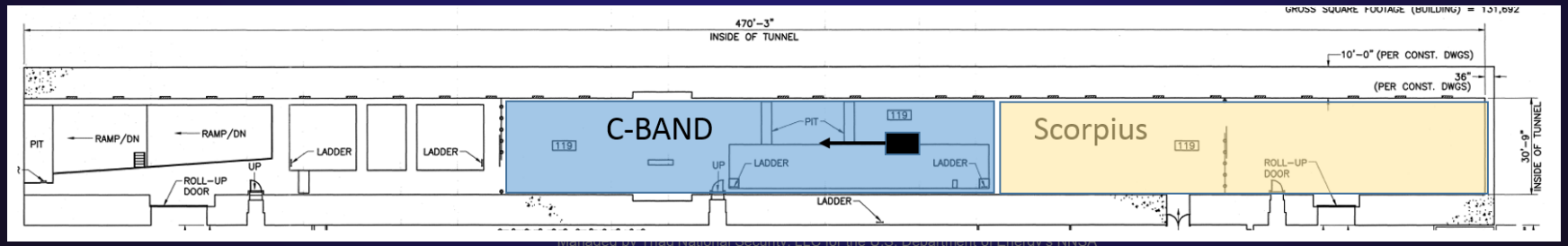
- Modernization of 0.8 GeV linac in place with old accelerator (larger customer base)
- Upgrade (~ 20 GeV) would fit into existing tunnel

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+)

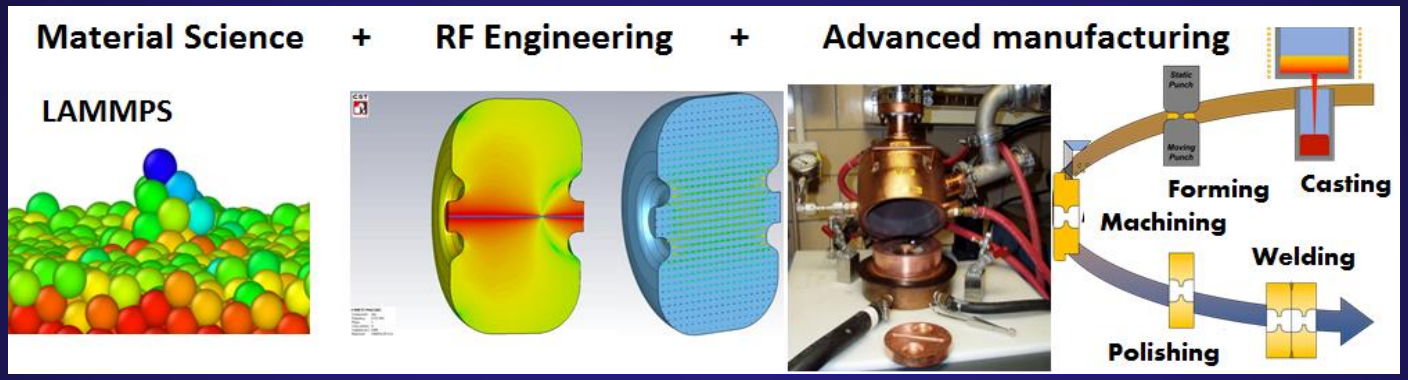






Multi-disciplinary Program Plan

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

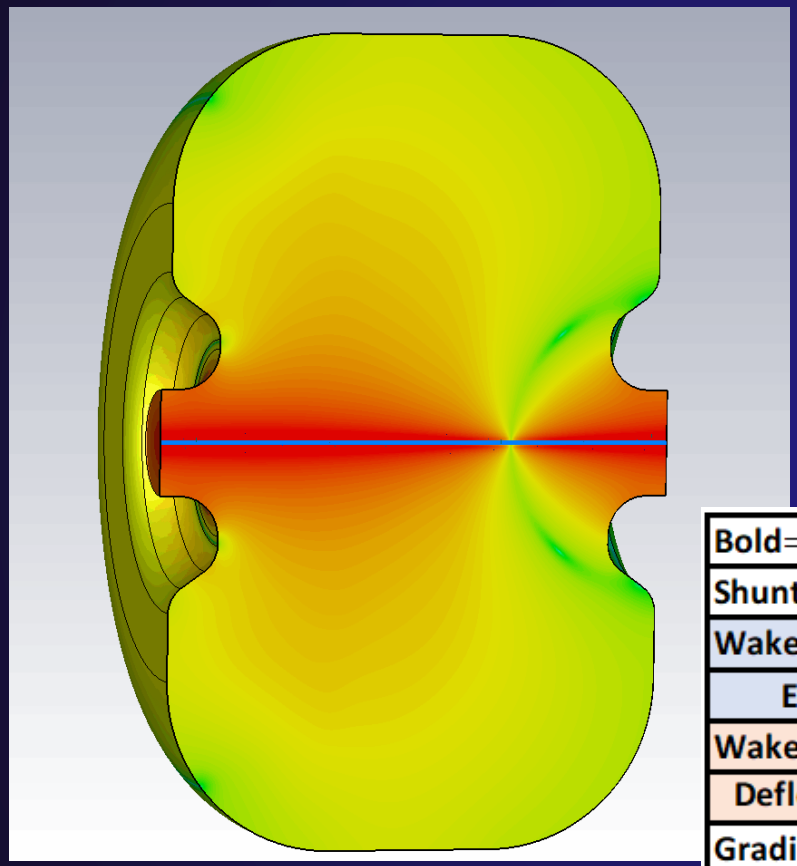


- Thrust areas that contribute to solving the technology challenges
  - Material Science (T): Understanding physics of breakdown and development of strategies for breakdown suppression, design tools for materials in extreme fields
  - RF technology (AOT/E): Resonator design for high gradient and long 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

Bold=good, grey=FYI only		L-band	S-band	C-band	X-band
Shunt impedance	[MΩ/m]	9.E+6	85	**120**	**170**
Wakes longitudinal	[V/pC]	10.2	26.4	36.4	50.4
Energy change	@ 1 GeV	0.3%	**2.5%**	**3.5%**	8.0%
Wakes transverse	[V/pC/m]	15.1	155	835	4420
Deflection @1μm	[kV]	0.0	**1.5**	**8.0**	67.4
Gradient	[MV/m]	30	50	**100**	**150**
Dechirper length	@ 1 GeV	N/A	2.9	**1**	0.8
Fabrication	tolerances	good	**good**	**good**	hard
Long range wakes	for burst	bad	bad	**good**	**good**

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 β 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

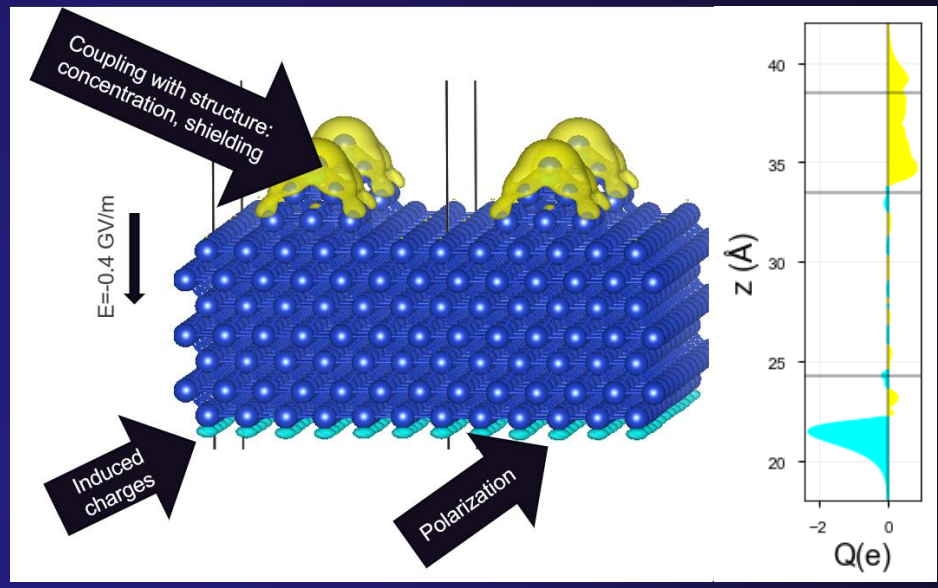
- Joint effort with UCLA on TOPGUN derivative (C-band)
- LANL focus on symmetrized RF-feed and XFEL optimized bunch parameters

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 $N_{electrons}^3$)
    - 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

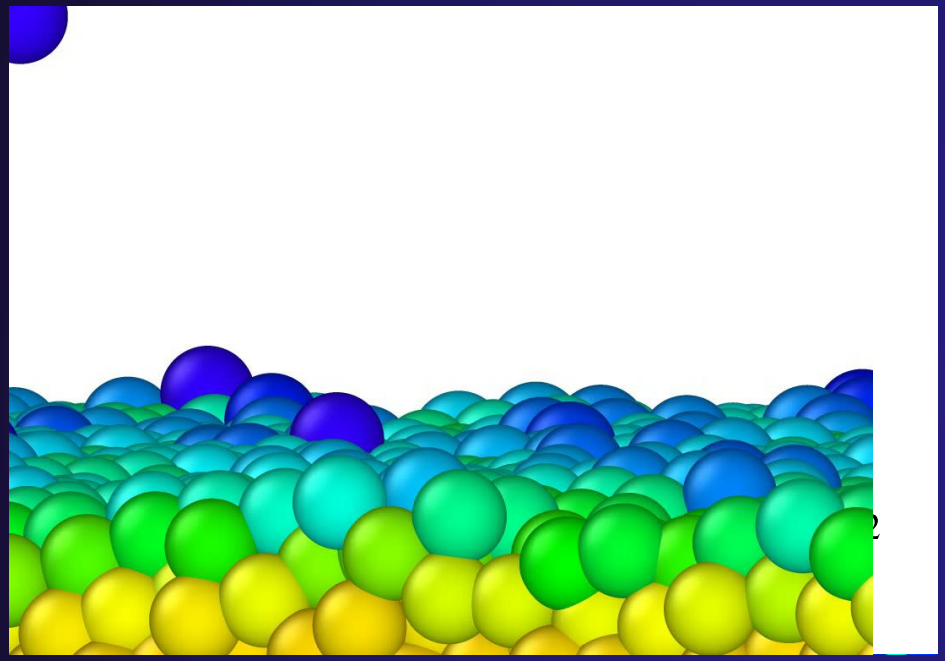
Why are we doing this?

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

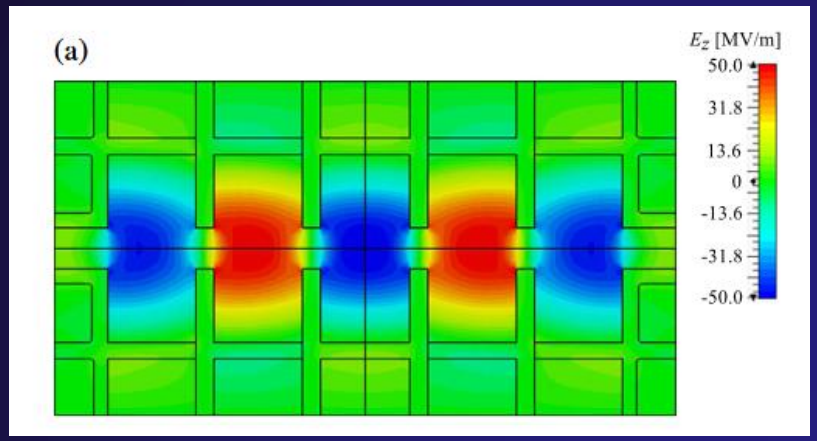
MD Verification and Path Forward

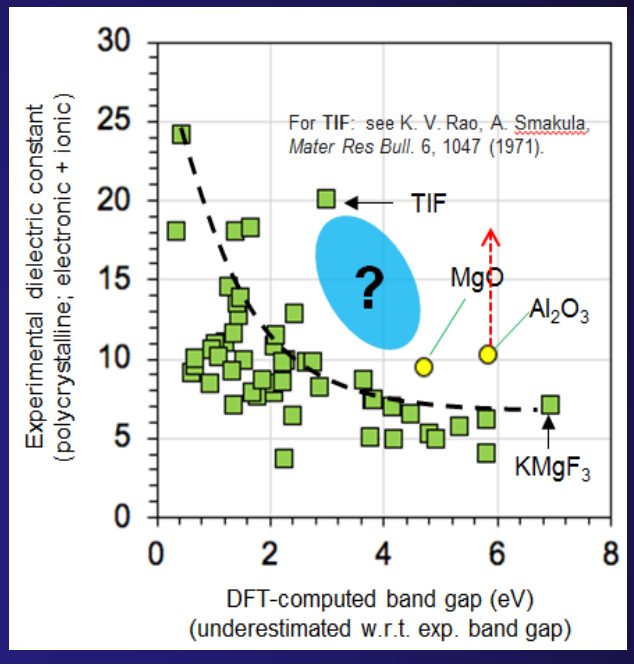


The model captures the key physics of metal surfaces under fields.

- **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.**

FY19 Accomplishments (dielectrics)





- 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?

Dielectric constant versus bandgap (computed within DFT) plot for a set of polycrystalline ceramic materials previously reported in literature. Yellow circles identify materials that have been proposed as promising dielectrics for the hybrid cryogenic copper/ceramic accelerator. The arrow at the alumina dot shows the doping Euclidlabs did for our test dielectric.

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