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HIGH GRADIENT HIGH EFFICIENCY C-BAND ACCELERATOR STRUCTURE RESEARCH AT LANL*

E.I. Simakov†, A.W. Garmon, T.C. Germann, M.F. Kirshner, F.L. Krawczyk, J.W. Lewellen, D. Perez, G. Wang, Los Alamos National Laboratory, Los Alamos, NM, U.S.A.
A. Fukasawa, J.B. Rosenzweig, University of California Los Angeles, Los Angeles, CA, U.S.A.

Abstract

We report on the status of the new high gradient C-band accelerator project at LANL. Modern applications such as X-ray sources require accelerators with optimized cost of construction and operation, naturally calling for high-gradient acceleration. Our goal is to use a multi-disciplinary approach that includes accelerator design, molecular dynamics simulations, and advanced manufacturing to develop high gradient, high efficiency RF structures for both compact and facility-size accelerator systems. We considered common operation frequencies for accelerators and identified C-band as the optimal frequency band for high gradient operations based on achievable gradients and means to control wakefields. We are putting together a high gradient C-band test facility that includes a 50 MW Toshiba klystron and cryo-coolers for operating normal-conducting copper accelerator cavities at long pulse duration. We plan to conduct high gradient testing of the optimized RF structures made of copper and novel copper alloys. We use LANL modelling capabilities to systematically study the formation of breakdown precursors at high fields to develop basic theoretical understanding of the breakdown.

INTRODUCTION

Particle accelerators are established tools for National Security (NNSA, DoD) and basic science missions. Modern day applications such as X-ray sources require accelerator facilities with optimized cost of construction and operation, naturally calling for high-gradient acceleration. Increasing gradients in normal-conducting radio-frequency (NCRF) copper-based accelerator structures requires innovation in two major areas: understanding of the physics mechanisms of radio-frequency (RF) breakdown, and development of novel copper alloys with increased breakdown limits. At Los Alamos National Laboratory (LANL) we initiated a new project with the major goal to use a multi-disciplinary approach that includes accelerator design, molecular dynamics simulations, and advanced manufacturing of metals to develop high-gradient, high-efficiency radio-frequency (RF) structures for both compact and facility-size accelerator systems.

CHOICE OF THE OPERATIONAL FREQUENCY

At the start of the project we conducted the evaluation of the optimal operational frequency for the high gradient RF structure that could be employed for the future X-ray Free Electron Laser (XFEL), such as for example DMMSC at LANL [1]. RF performance versus frequency was evaluated for otherwise identical structures scaled to the three selected frequencies: 2.856 GHz (S-band), 5.712 GHz (C-band), and 11.424 GHz (X-band). One structure was specifically designed for this effort and one was derived from a high gradient high-performance photo-injector designed at University of California Los Angeles (UCLA) [2]. The designs were compared based on achievable gradients, acceleration-efficiency, given by the shunt impedance, the wakefield loss factors, and the expected ease of fabrication. Table 1 summarizes the performance of one of the structures. For comparison, it also shows typical numbers for an L-band superconducting accelerator cavity.

Table 1: Comparison of the accelerator characteristics of representative structures at different accelerator frequencies. The wakes are computed for an electron bunch with a bunch length of 2 ps and the energy of 1 GeV.

	L-band	S-band	C-band	X-band
Gradient, MV/m	30	50	100	150
Shunt impedance, MΩ/m	$9*10^6$	85	120	170
Longitudinal wake, V/pC	10.2	26.5	36.5	50.4
Energy change due to wake	0.3%	2.5%	3.5%	8.0%
Transverse wake, V/pC/m	15.1	155	835	4420
Deflection over 1 μm, kV	0	1.5	8.0	67.4

The gradients quoted in Table 1 are room temperature maximum gradient estimates based on available experimental data. The numbers demonstrate that while the gradient increases with frequency, the strong increase in wakefields restricts operation at frequencies above C-band. The L-band SRF structure has superior efficiency, moderate gradients, and low short range wakes, however the extremely low Ohmic losses result in long-range wakes that are hard to manage. In addition, the bunch separation for a "MaRIE burst mode" [3] at L-band is too slow for good temporal resolution with a bunch proximity that will lead to strong multi-bunch wakes. Evaluation of the energy chirp of a beam for XFEL applications established another advantage for C-band. Beam transport through the RF accelerator introduces a chirp that needs to be removed for

* Work is supported by Los Alamos National Laboratory's LDRD Program.
† smirnova@lanl.gov

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FEL interaction. Systematic analysis shows that dechirping with the C-band structure is accomplished without the need of extra compensation, while S-band dechirping is too weak and X-band is too strong. Therefore, the C-band operational frequency of 5.712 GHz was chosen as an accelerating structure's frequency for the remainder of the project.

SIMULATIONS OF RF BREAKDOWN

So far, although many experiments have confirmed that the RF breakdown in accelerating cavities is a reproducible process, no accurate physical models that predict RF breakdown rate have been developed. Atomistic simulations with molecular dynamics have a long history of contributing novel insights into the nanoscale underpinnings of many phenomena in materials science. However, in spite of the clear technological importance of the problem, applications of these techniques to understanding the fundamentals of RF breakdown remain relatively rare, mainly because the additional complexity introduced by the treatment of electromagnetic fields requires the development of specialized methods and codes that can capture the coupling between the mechanical and electronic aspects of the problem. To date, two main avenues of solution have been considered: 1) using a continuum Poisson solver to compute the external field and Gauss law to infer induced charges on atoms [4], and 2) introducing an external field in fully-atomistic charge-equilibration (qEq) techniques [5]. In order to leverage existing simulation code-bases as much as possible, we opt for the second approach. Fundamentally, qEq is very simple: charge should be redistributed on every atomic nucleus so as to minimize the total electrostatic energy of the system, subject to the constraint of global charge conservation. In this setting,

$$V_{electro} = \sum_i V_{external}(x_i)\ q_i + V_{self}(q_i) + \frac{1}{2}\sum_{j\neq i} V_{Coulomb}(q_i, q_j, r_{ij}),$$

where V_{self} is a self-energy term that represents the energetic cost of modifying the charge state of an atom, $V_{external}$ is the potential due to externally applied field, and $V_{Coulomb}$ the interaction energy between a pair of charges. Due to their light masses, electrons equilibrate extremely rapidly on atomic vibration timescales; charges are therefore assumed to be in constant equilibrium with respect to the instantaneous position of the atoms, in a classical equivalent of the Born-Oppenheimer approximation. In practice this approach requires carrying out a self-consistent qEq procedure at every timestep of the simulation, which significantly adds to the computational cost. qEq techniques have a long history of application in chemistry [6], where they are primarily used to model short-range covalent charge exchanges between bonded atoms. However, with applications to conducting surfaces under electric fields, the Coulomb energy cannot be truncated at short range as it is common in chemical applications, but has to be fully accounted for in order to insure global charge equilibration.

For our model, we parameterize V_{self} in order to approximate the behavior of specific materials, in particular copper. Our approach is to parameterize V_{self} so that the classical model reproduces the electrostatic energy of training systems whose response to an external electric field was evaluated with density functional theory [7], the most popular quantum calculation technique in materials science. For single component systems, the first non-trivial term in V_{self} is quadratic in q_i. Adjusting the coefficient of the quadratic term produces a very good agreement with the quantum reference values for perfect surfaces, with less than a few percent error at high fields (~2 GeV), c.f. Fig. 1. Essentially perfect agreement can be achieved by introducing virtual charge acceptors/donors tied to each atom by a spring, which is equivalent to introducing polarization in the classical model. For defective surfaces (e.g., a surface with an adatom or a vacancy), the agreement is still good, but the model fails to capture the quantum asymmetry with respect to reversal of the external field. As highlighted by a recent study, this stems from the lack of intrinsic dipole in the classical model [8]. Our team is currently working on addressing this limitation.

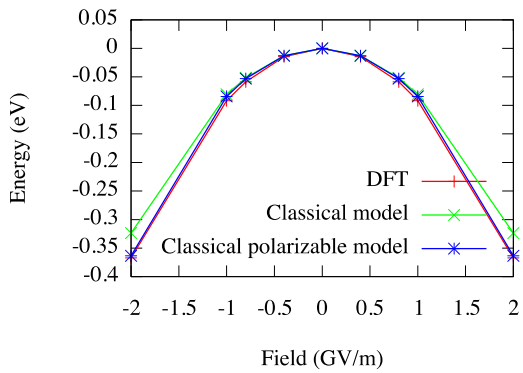

Figure 1: Comparison of the energy of a (100)-oriented copper slab, obtained by density functional theory and by two classical models. Other surfaces show similar agreement with the same set of parameters.

In spite of its current limitation, the qEq model can capture non-trivial coupling between the surface microstructure and the induced charges. As shown in Fig. 2, charges accumulate at protrusions, such as step edges, and then shield less prominent neighbor atoms. Running molecular dynamics simulations on this model at very high fields demonstrated that one should expect breakdown by ion emission from the surface following from the spontaneous formation of nano-tips. Nano-tip features locally enhance the field, which promotes their further growth until field-emission finally occurs. However, we noted that this process is only observed at fields that are much larger than those applied in actual accelerating structures. This observation, which is also clearly established experimentally [9,10], strongly suggests that other mechanisms first create surface structures that act as focal enhancement points for the field which enables their further growth and eventually

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leads to breakdown. Searching for such mechanisms is currently an area of significant interest for many groups. We believe that atomistic simulations could provide novel insights on the problem that are hard to obtain experimentally.

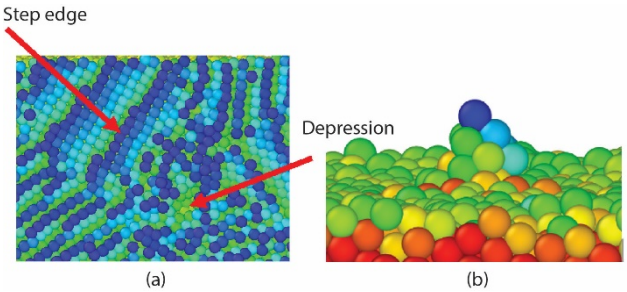

Figure 2: (a) Field-induced charge distribution at a polycrystalline surface in classical molecular dynamics simulations. Large amounts of excess charge (blue) accumulates at protruding features, such as step edges. Very little charge (green) accumulates in depressions or down from protrusions. (b) Spontaneous formation of a surface nano-tip under a very high electric field (10 GV/m). Ions are emitted from the tip soon after.

In summary, atomistic simulations have potential to yield novel insights on the mechanisms that lead to RF breakdown, and hence on the development of mitigating strategies. While important steps have been taken, challenges remain on how to best make connection with experiments while accurately capturing the relevant physics. In our opinion, this will require a concerted modeling and experimental effort in order to constrain the potential investigation avenues and insure the efficient transfer of information between scales.

HIGH GRADIENT TESTING SYSTEM

A crucial part of this work is the installation, and commissioning of the C-band high-gradient test facility at LANL. The RF test station will be built around a 50 MW 5.712 GHz Toshiba klystron. The klystron system produces 1 microsecond RF pulses with up to 300 pulses per second, suitable for the fast conditioning of the structures. The RF system will be installed and operational before the end of the calendar year 2019. The system will immediately be suitable for the high gradient tests of the room-temperature normal conducting accelerator structures. Next, structures cooled to 77 K with liquid nitrogen will be tested. Later additions to the test stand will include cryo-coolers for operation at low temperatures, as low as 20 K.

CONCLUSIONS AND FUTURE PLANS

In summary, a new project has been started at LANL with a major goal of establishing a new high performance RF structure engineering and experimentation capability. The project is possible due to unique intersection of LANL expertise in RF engineering, material science, and advanced manufacturing, and the national importance. We plan to conduct large-scale molecular dynamics simulations to identify effects of pulse heating and local surface modifications on development of the RF breakdown. We will identify particular features of alloys that make them more or less prone to breakdown and design new alloys with improved breakdown limitations. We will fabricate and test coupons of new materials and prototype NCRF cavities. We plan to look into novel fabrication, joining, and surface preparation methods to produce RF cavities operating with low probabilities of breakdown. We will commission a high gradient test station, which will be the first high gradient C-band test stand in the United States. The test station will have options for cryo-cooled operation of the normal-conducting structures. We will use the new experimental setup to test RF cavities at high gradient and long pulse length and we plan to make it available to collaborators.

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