SAND2012-9227P

ANL User facility proposal to be submitted by 26 October 2012
(http://nano.anl.gov/users/call_for_proposals.html)

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1. Describe the scientific or technical purpose and the importance of the proposed work. (500 word or 4000 characters)
Measuring high voltage (HV) (> 10 kV) impulses is important to many systems common to the DOE mission from defense technologies to protecting infrastructure and homes from lightning. The current technology available to measure HV impulses mostly relies on resistive and capacitive dividers to reduce a high voltage to a low voltage (< 10 V) that can then be read with a digitizer. The most common devices perform well for DC and AC (< 1 kHz) voltage measurements, but are limited in abilities for impulse measurements. Other techniques have been proposed such as a Pockels cell which was not pursued beyond fundamental calculations/estimations. All current traceable measurements are limited to having an uncertainty greater than a NIST developed artifact on permanent loan to Sandia National Laboratories Primary Standards Laboratory. This artifact has an uncertainty of only 0.8% (k=3). Initial calculations indicate it is possible to improve this measurement uncertainty by at least an order of magnitude if not two.

In the proposed work, fundamental material properties and phenomena of piezoelectric crystals when exposed to high voltage will be explored and documented. Currently, very little literature is available documenting the changes in piezoelectric crystals when exposed to high voltages. Direct implications of this work will be a better understanding of crystalline and piezoelectric materials at high voltages, and more specifically impulses. Additionally, knowledge will be gained in order to understand the effects of impulses on electronics, for example what happens to an oscillator crystal when there is a power surge, or static electricity discharge.

2. Provide a statement of the scope of the work to be carried out at CNM and expected outcomes. (1000 characters)
Finite Element Modeling (FEM) and simulation using the HPC Cluster at ANL will be used to study piezoelectric materials under high voltage (10 kV-300 kV) impulses. This work will expand the fundamental knowledge base that can be used for a broad range of applications, including development of new measurement techniques for high voltage impulses as well as safeguarding materials and electronics from high voltage impulses.

3. Why do we need CNM for this research ?(1000 characters)
The High Performance Computing Center allows the unique opportunity to utilize a mutliphysics model to experiment on a complex system safely and within practical time constraints. This work is not feasible using ordinary workstations for simulation and experimental work cannot provide the same level of physical understanding. Additionally, CNM has world experts with related work that are willing to collaborate to ensure the best results are had in a timely manner.

4. Why do you need the equipment/capabilities chosen? (1000 characters)

The HPC facility is unique with the hardware and available codes/software that will enable this work. In particular, we will use Comsol for FEM modeling of piezoelectric materials. Although this is a common commercial software, the ability to run very large simulations on common computer hardware is not practical. Simulations can take over 5,000 core hours, which equates to over a month of time on a standard system. The same calculation using the HPC cluster at ANL can be completed in days. Comparable capabilities have not been found without significant investment to expand existing hardware and software.

5. Describe the participants previous experience relevant to the proposal and describe the research results obtained. (500 words or 1000 characters)
Stefan Cular has worked for many years utilizing piezoelectric materials for sensors. Most of his work has focused on applying bulk and surface acoustic waves (SAW) for chemical and biological sensor applications. The most notable work so far accomplished was the development of SAW sensor that capitalized on the piezoelectric material properties to simultaneously sense anti-body/anti-gen binding while removing non-specifically bound material from the sensors surface. This subject was collaborative explored utilizing both experimental and modeling and simulation to better understand the physics of the SAW interactions with the binding materials. Utilizing the FEM models developed for the prior work, new structures were investigated solely with simulations that showed significant improvements to SAW sensor sensitivity with the addition of micro-cavities etched into the sensor surface and filled with a low density material.
Currently the PI is the AC Electrical Project lead for the Primary Standards Laboratory at Sandia National Laboratories with responsibilities for maintaining the NIST artifact for high voltage pulse measurements. Within the Project are necessary experimental facilities to test and verify physics found through the proposed modeling and simulation work.

6. Describe the proposed research (including samples and procedures if applicable) and explain the basis for the estimated time requested.

A number of simple FEM simulations will be configured and tested prior to running the desired full model to ensure the results are realistic and comparable with experimental data. The first simulation will model the effects of a static potential across a piezoelectric crystal. Once the model matches the experimental data, a wave propagating orthogonal to the applied potential will be added to the model. The third simulation model to be developed will apply an impulse potential that will be measured with the orthogonal wave.

With an 8-core system, we have seen a 100,000 node model simulate for 200 nanoseconds take roughly 8 hours of computation time. The simulated time of interest for this work is 2 microseconds, which equates the model to about 1000 core hours per simulation. For the highest voltages, the model may reach a node count over 1,000,000 which we estimate to require about 6,000 core hours. A total of 10 simulations are required to provide enough data to establish a data baseline. We estimate the total need of core hours to be 25,0000.

7. References, including relevant publications (1000 characters)

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R. Arora, W. Mosch, High voltage and electrical insulation engineering, IEEE Press, A John Wiley & Sons, Inc., 2011.

K. Hidaka, *Proc. IEE High Voltage Eng. Symp.*, Aug. 1999, pp. 2.1–2.14.

Y. Liu, F. Lin, G. Hu, and M. Zhang, *IEEE Trans. Instrum. Meas.*, vol. 60, no. 3, pp. 996–1002, Mar. 2011.

J.-L. Liu, B. Ye, T.-W. Zhan, J.-H. Feng, J.-D. Zhang, and X.-X. Wang, *IEEE Trans. Instrum. Meas.*, vol. 58, no. 1, pp. 161–166, Jan. 2009.

S. S. Bruce, “Scope of Accreditation to ISO/IEC 17025:2005, Sandia National Laboratory, Primary Standards Laboratory,” 2011.

G. J. FitzPatrick and E. F. Kelley, *J. Res. Nat. Inst. Stand. Technol.*, vol. 101, no. 5, pp. 639–658, Sep./Oct. 1996.

Cular, Stefan, Subramanian KRS Sankaranarayanan, and Venkat R. Bhethanabotla. "Enhancing effects of microcavities on shear-horizontal surface acoustic wave sensors: A finite element simulation study." Applied Physics Letters 92.24 (2008): 244104-244104.

Sankaranarayanan, S. K., Cular, S., Bhethanabotla, V. R., & Joseph, B. Flow induced by acoustic streaming on surface-acoustic-wave devices and its application in biofouling removal: A computational study and comparisons to experiment. Physical Review E, 77(6), 2008.

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8. Describe briefly the outcome of the prior accepted proposals to the CNM. (1000 Characters)

No previous proposals have been submitted.