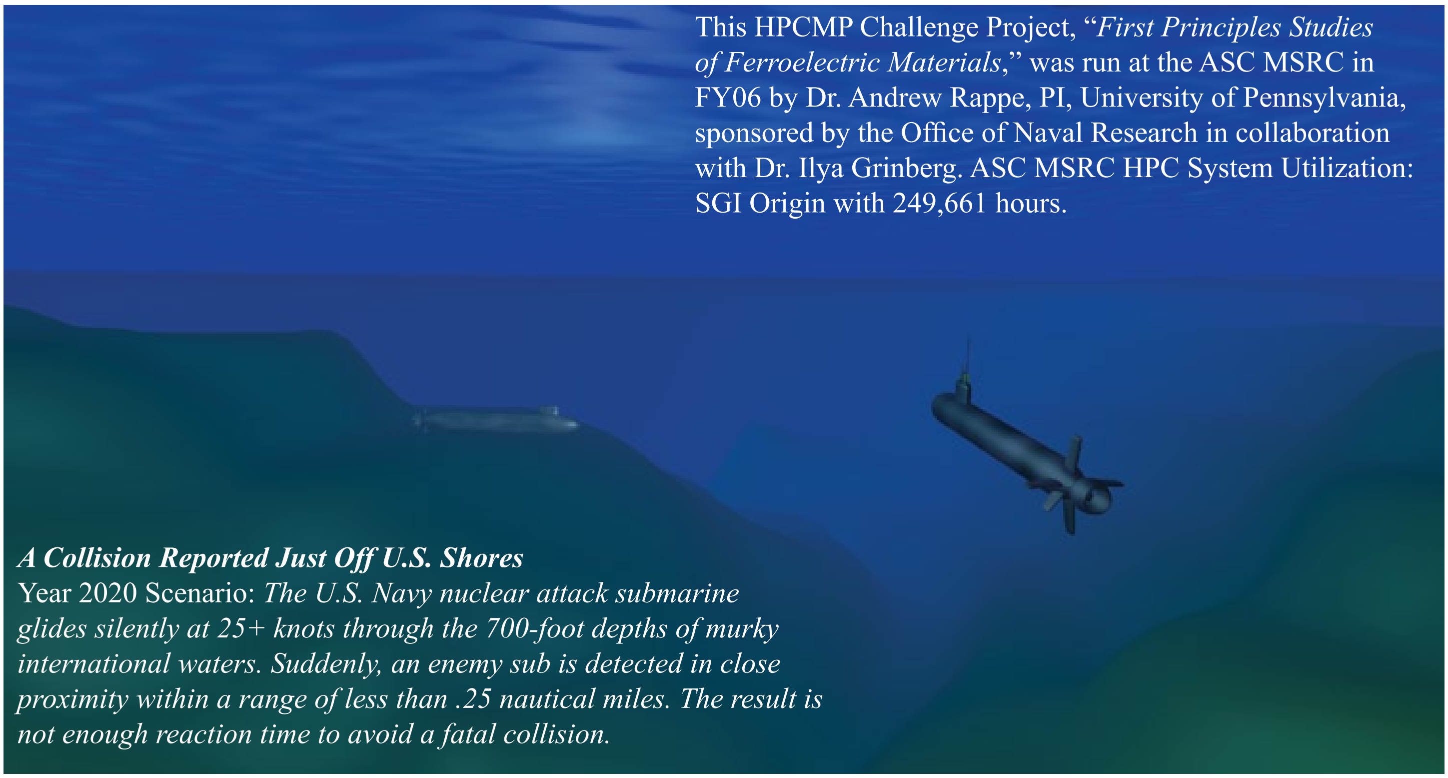
Ferroelectric Study Seeks to Improve Protection in the Ocean's Depths and Airwaves

By Gary Sivak and Dinah Luneke



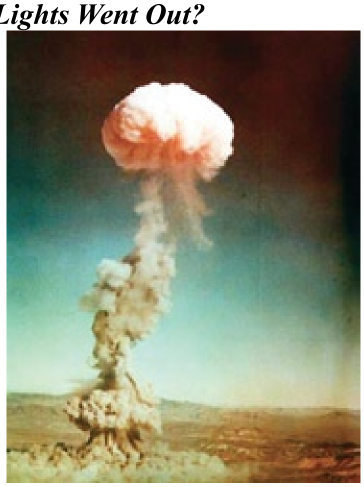
This HPCMP Challenge Project, "*First Principles Studies of Ferroelectric Materials*," was run at the ASC MSRC in FY06 by Dr. Andrew Rappe, PI, University of Pennsylvania, sponsored by the Office of Naval Research in collaboration with Dr. Ilya Grinberg. ASC MSRC HPC System Utilization: SGI Origin with 249,661 hours.

A Collision Reported Just Off U.S. Shores

Year 2020 Scenario: *The U.S. Navy nuclear attack submarine glides silently at 25+ knots through the 700-foot depths of murky international waters. Suddenly, an enemy sub is detected in close proximity within a range of less than .25 nautical miles. The result is not enough reaction time to avoid a fatal collision.*

Where Were You When the Lights Went Out?

Broadcast Scenario: *A high-altitude explosion has just occurred over our Eastern seaboard. You are not in any imminent danger of fallout from the blast, but you will need to take immediate action to backup your computers' data. Be aware of a pending blackout as all utilities, phone services and transportation – all electronic communications – will cease.*



Nuclear Upper Atmosphere Explosion

The broadcast transmission goes dead, just as all unprotected computer data is wiped throughout the entire region. Communication, as we know it, comes to an abrupt halt.

Project Justification

In order to assure Naval submarines continue to maintain cutting-edge technology, it is imperative that scientists and researchers study and develop the best materials known to mankind to help our Naval crews outperform, out-maneuver and out-stealth all other undersea warfighters. These new technologies will be able to identify an enemy or friendly submarine outside the current detection range. The key to this undersea SONAR advantage is the development of better piezoelectric materials that can detect the pressure waves generated by a passing vessel, and then broadcast specific signals at longer distances.

An additional direction of research within this Navy-funded program is the development of ferroelectric materials for nonvolatile ram with significantly higher density. It is vitally important to assure our massive amounts of computer storage in military use, largely based on magnetic media data, will not erase if hit by an Electromagnetic Pulse (EMP), which could compromise operational capability.

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Developing hardened memory to store data in a more reliable way that would be invulnerable to an EMP is advantageous to both military and civilians.

Research Goals Serve the DoD Mission

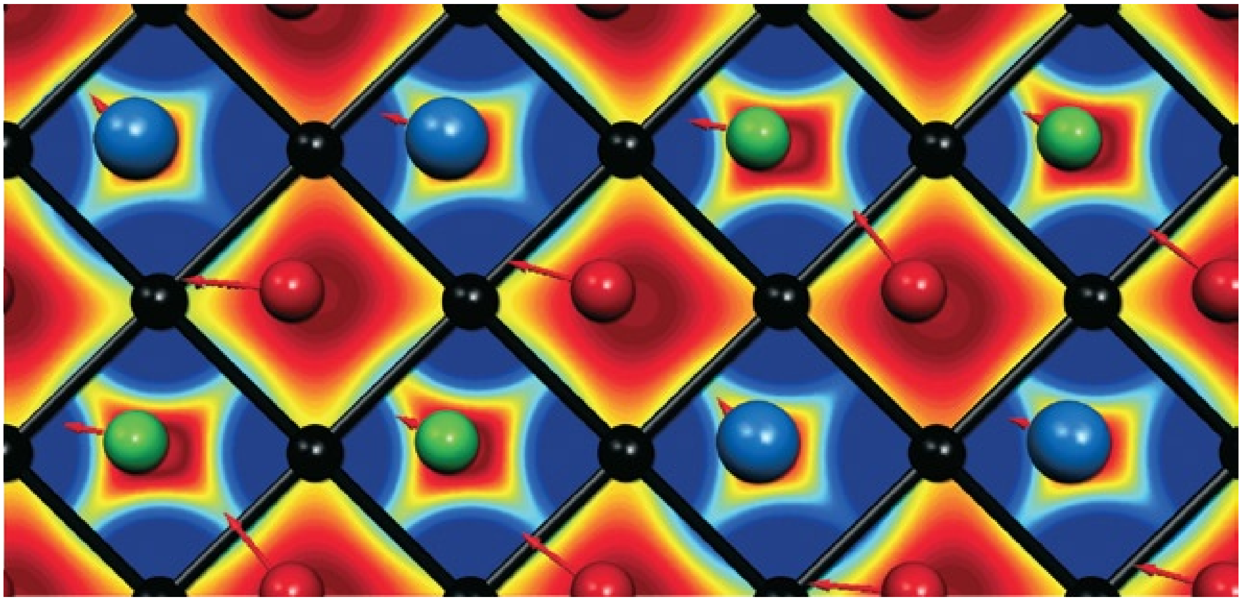
The primary research goal is to understand the phenomena of ferroelectricity and piezoelectricity so better materials can be designed for Naval SONAR and non-volatile ram applications. The goal is to understand, at an atomic level, what makes an oxide a ferroelectric or piezoelectric in order to propose new material compositions. This produces the discovery of new resources to provide enhanced piezoelectrics response. The results ultimately provide the Navy with more sensitive SONAR detection, longer usable lifetime of SONAR materials in the water without changing their response properties, and more environmentally friendly SONAR materials that do not rely on poisonous elements.

As new materials move down the pipeline to become next-generation SONAR devices with enhanced sensitivity, "The Navy after Next" motto applies: *The fundamental design of materials today is needed to become the devices of the next decade.*

HPCMPO MSRC Utilization

The MSRCs that Dr. Rappe utilized for these Challenge Projects include: ERDC, Arctic Region Supercomputing Center (ARSC), Army High Performance Computing Research Center (AHPCRC), the Space and Missile Defense Command (SMDC) and the ASC MSRC. The primary CTA of this research is CCM. Dr. Rappe enjoys conferring with all the experts at the different sites on which computers have the fastest interconnect between CPUs and which ones would work best for his calculations.

"ASC has the resource, HPC11 – part of the Origin 3000 series – that seems to work well for parallel electronic structure applications. The human support we receive at ASC has resulted in a good working relationship. We also prefer the one-week-long run time queues that are used at the ASC versus a 24-hour paradigm. Our runs require large amounts of memory per CPU, and we certainly found that at the ASC machines. In considering ways of reformulating the algorithms and the hardware and the software to better take advantage of parallel architecture, the ASC and the other MSRCs can help as we work together to develop the roadmap for electronic structure for the future," Dr. Rappe says.



This image gives us important clues for the discovery of higher-performance, longer-lasting and more environmentally friendly US Navy SONAR materials.

Atom Color Key

** The O atoms (oxygen, black) form cages (black lines) that hold each metal atom.*

** The Pb atoms (lead, red) move away from the center of their cages (long red arrows) to improve bonding to O.*

** All metal atoms move up and to the left, but the exact direction of each Pb atom's motion is influenced by avoiding large Zr neighbors (zirconium, blue) and moving toward small Ti (titanium, green) neighbors.*

** The size differences between Ti and Zr are the key to making different Pb atoms move in.*

Homegrown Applications Save the Day
Dr. Rappe prefers homegrown applications, like ABINIT or Gnu-PL Type, which are publicly available software. One of the named codes used at ASC is DACAPO, which was developed by one of the major research groups in Denmark. These codes allow the chemistry to be performed to expand all the atomic orbitals, which are the regions around atoms where electrons are found. This allows the use of a Fast Fourier Transform, which is a great mathematical technique to help computers analyze signal data.

From Atoms to Electrons
Ferroelectric materials have a permanent electric dipole moment, which is the direction that can be switched between equivalent states by the application of an external electric field. As the material is compressed, all the atoms slightly shift. This causes the dipoles to rotate as voltage, across the sample, for the materials to respond electrically. Piezoelectricity is the ability of some materials to generate an electric charge in response to applied mechanical stress. “The point is that all ferroelectrics are automatically also piezoelectrics, to some extent,” Dr. Rappe says. “Of course, we are in the process of searching around in the space of ferroelectric materials for new piezoelectric materials that are even more improved.”

Controlling Electromagnetic Pulses
Magnetic forces are much weaker than electric forces. The strength of pulse needed to depolarize ferroelectric material with stored data is hundreds of times higher than needed to depolarize magnetic media. The point of this study is that the idea of ferroelectric memory does not seek to replace the ram in the core of the computer, but instead, could serve as the back-up of last resort where strategic information could be called back rapidly. Critical data would also be much less vulnerable to the EMP that can corrupt conventional magnetic data storage tape-to-disk.

As part of this massive push by the Navy to further this research, new materials have been identified and characterized within this last year by Dr. Rappe and his colleagues. “There are exciting new piezoelectrics we have identified with a ‘figure of merit,’ to summarize how good a material is for this application,” Dr. Rappe reports, “and is higher than anything we have seen previously. Nothing tells us that we are at the limit of our research. So, this is an ongoing search for continuing to help protect our country against an EMP attack on our computer data, as well as improving our ability to see underwater.”

For more information, please contact CCAC at www.ccac.hpc.mil or 1-877-222-2039.

In the future, using hardened ferroelectric memory, a terabyte of back-up could be stored onto a device as small as this portable thumb drive.