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AbInitio Nonlinear Piezoelectric Model for Single Crystals

U.S. ARMY RDECOM

ARL open campus

S&T Campaign: Materials Research

Tier 2 High Strain Rate & Ballistic Materials

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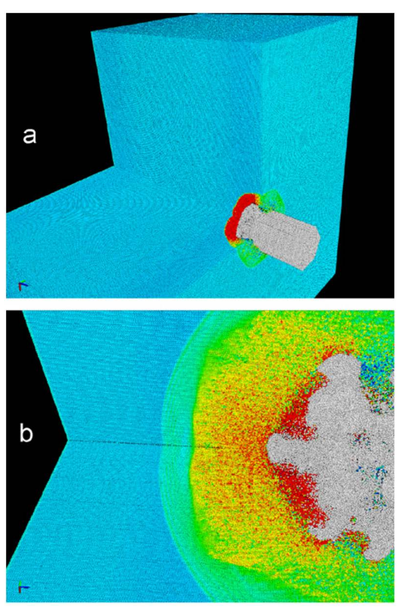
Research Objective

- Formulate novel piezoelectric materials from a more complete and fundamental understanding of how fully coupled fields influence both the deformation and electromagnetic response of this class of materials



Simulating Impact on Piezoelectric media

Challenges

- Simulations of armor-grade piezoelectrics (e.g. SiC and AlN) neglect full coupling of Maxwell's equations with the mechanical equations of motion
- Radiated EM fields influence deformation and failure of piezoelectric ceramics
- Full coupling of the field equations is needed to understand how transient mechanical waves can generate radiated electromagnetic power, (power harvesting from vibrating mechanical devices)

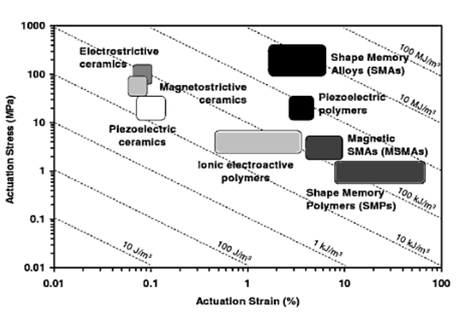


Fig. 1.1. Actuation energy density diagram indicating typical ranges of actuation stress, actuation strain, and the actuation energy densities of different active materials that exhibit direct coupling.

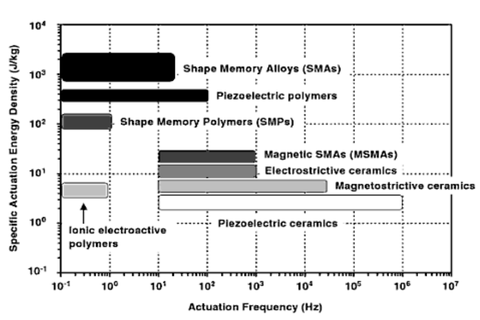
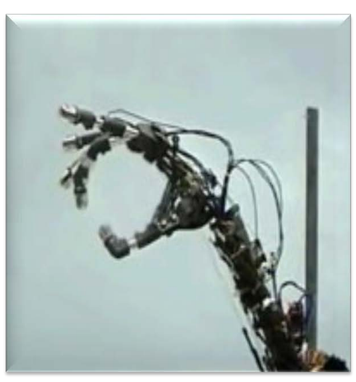


Fig. 1.2. Actuation frequency diagram comparing the actuation frequency ranges of different active materials that exhibit direct coupling.

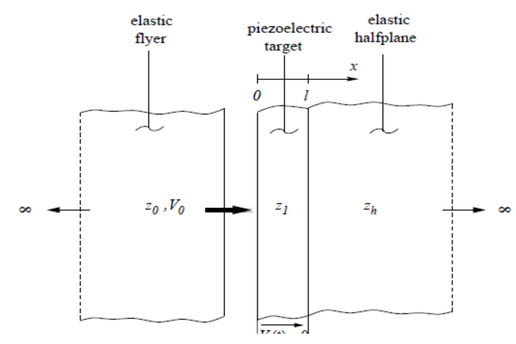


Develop modeling capabilities for wide range of applications

ARL Facilities and Capabilities Available to Support Collaborative Research

- Provides access to HPC resources
- Allows access to COTS/GOTS software provided on HPC and ARL systems
- Recent results presented for electromagnetomechanics comprise two reports:
  - "A Convective Coordinate Approach to Continuum Mechanics with Application to Electrodynamics," ARL-TR-6298, January, 2013.
  - "On the Proper Formulation of Maxwellian Electrodynamics for Continuum Mechanics," Continuum Mechanics and Thermodynamics, Volume 26, Issue 3 (2014), Page 387-401
- ARL researchers have extensive expertise in CEM/CSM modeling and software development

IMPACT INDUCED PLANE WAVES IN A PIEZOELECTRIC TARGET



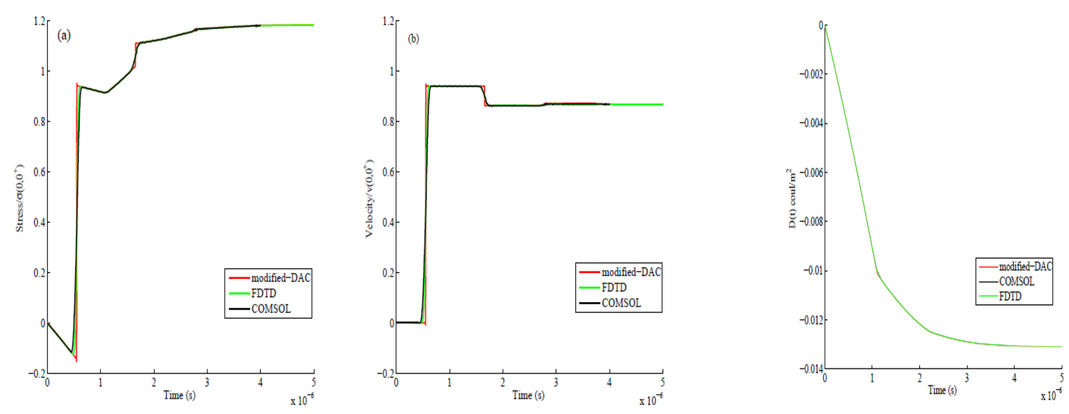
$$\rho \frac{\partial^2 u(x,t)}{\partial t^2} = \frac{\partial \sigma(x,t)}{\partial x}$$

Stress/Voltage

$$\sigma(x,t) = C^D \frac{\partial u(x,t)}{\partial x} - hD(x,t)$$
$$\mathcal{E}(x,t) = -h\frac{\partial u(x,t)}{\partial x} + D(x,t)/\varepsilon$$

Stress/Charge

$$\sigma(x,t) = C^E \frac{\partial u(x,t)}{\partial t} - e\mathcal{E}(x,t)$$
$$D(x,t) = e\frac{\partial u(x,t)}{\partial t} - \epsilon\mathcal{E}(x,t)$$



Complementary Expertise/ Facilities/ Capabilities Sought in Collaboration

- This class of materials (piezoelectrics) requires development of sophisticated multiscale material models that are consistent with temporally disparate <u>multiphysical</u> fields (electromagnetic and mechanical)
- Requires cross-disciplinary skills in solid mechanics/electromagnetics/physics and expertise in CSM/CEM
- Verification and validation of theory requires comparison with carefully conducted Kolsky bar, plate impact & other experiments which are specially calibrated to simultaneously measure transient electromagnetic and mechanical fields

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