Piezoelectric MEMS

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Outline

- Transducers and transduction principles
- Piezoelectricity
  - Notations
  - History
  - Piezoelectric transducers
- MEMS
- Key Piezoelectric Materials
- Applications:
  - Actuators
    - Micropumps
  - Energy harvesters
  - Resonators
  - Sensors
Transducers
**Transducers**

- Transducers: convert a signal from one signal domain into another using a transducer effect.
- We are especially interested in transducers and transducer effects converting:
  - A non-electrical signal in an electrical signal.
  - An electrical signal in a non-electrical signal.
- The transducer can be:
  - **Single-Step** Transducer: 
    - ex. Photodiode converting a photon flux in a photocurrent.
  - **Multi-Step** Transducer:
    - ex. Acceleration sensor converting an acceleration first into the deflection of a microstructure and then in an electric signal.
# Electro-mechanical transducers

<table>
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<th>Input signal</th>
<th>Output signal</th>
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<tr>
<td>Electrical</td>
<td>Electrical Conduction</td>
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<td>Piezoelectricity</td>
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<td>Electrostatics</td>
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<td>Tunneling Inductive effect</td>
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<td>Pneumatics</td>
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<td>Hydraulics</td>
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<td>Acoustics</td>
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<td></td>
<td>Resonance</td>
</tr>
</tbody>
</table>

## Electrical

- Logic elements
- MEMS actuators
- MEMS resonators
- Acoustic wave devices

## Mechanical

- Pressure sensors
- Accelerometers
- Gyroscopes
- Force sensors
- Flow sensors
- Cantilever beams
- Membranes
- Gears
- Resonators
- Microfluidic devices
Transducers

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What is piezoelectricity?

- Ability of certain materials to develop an electric charge proportional to a mechanical stress (direct effect)

\[ \frac{\partial D_i}{\partial T_{jk}} = d_{ijk}^E \]

- Development of a geometric strain (deformation) proportional to the applied electric field at zero stress (converse effect)

\[ \frac{\partial S_{jk}}{\partial E_i} = d_{ijk}^T \]

\[ S_{jk} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \]

- Variables:
  - \( D_i \): dielectric displacement [C/m²]
  - \( T_{jk} \): stress [N/m²]
  - \( d_{ijk}^E \): piezoelectric tensor [C/N]=[m/V]
  - \( d_{ijk}^E = d_{ikj} \)
  - \( S_{jk} \): strain
  - \( E_i \): electric field [N/m²]
  - \( u \): cartesian component of infinitesimal displacement
  - \( x \): cartesian coordinate
  - \( \varepsilon_0 \): permittivity of free space = 8.854 \times 10^{-12} \text{ F/m}
  - \( P_i \): dielectric polarization
  - \( D_i = \varepsilon_0 E_i + P_i \)
### Piezoelectric constitutive equations

<table>
<thead>
<tr>
<th>Equation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( S_{ij} = s_{ijkl}^E \cdot T_{kl} + d_{kij} \cdot E_k )</td>
<td>Dielectric displacement</td>
</tr>
<tr>
<td>( T_{ij} = c_{ijkl}^E \cdot S_l - e_{kij} \cdot E_k )</td>
<td>Stress</td>
</tr>
<tr>
<td>( D_i = d_{ikl} \cdot T_{kl} + \varepsilon_{ik}^T \cdot E_k )</td>
<td>Strain</td>
</tr>
<tr>
<td>( E_i = -g_{ikl} \cdot T_{kl} + \beta_{ik}^T \cdot D_k )</td>
<td>Electric field</td>
</tr>
</tbody>
</table>

\( c_{pr}^E \cdot s_{qr}^E = \delta_{pq} \)

\( c_{pr}^D \cdot s_{qr}^D = \delta_{pq} \)

\( \beta^S_{ik} \cdot \varepsilon^S_{jk} = \delta_{ij} \)

\( \beta^T_{ik} \cdot \varepsilon^T_{jk} = \delta_{ij} \)

\( i, j, k, l = 1, 2, 3 \)

\( p, q, r = 1, 2, 3, 4, 5, 6 \)

\( \delta_{pq}, \delta_{ij} = \text{identity matrices} \)

Subscripts indicate boundary conditions:

- “free”: constant stress, \( T \)
- “clamped”: constant strain, \( S \)
- “short circuit”: constant field, \( E \)
- “open circuit”: constant displacement, \( D \)
Piezoelectric tensors: short notations

\[
\begin{align*}
S_{ij} &= S_p & \text{When } i = j, \ p = 1, 2, 3 \\
2S_{ij} &= S_p & \text{When } i \neq j, \ p = 4, 5, 6 \\
T_{ij} &= T_p & c_{ijkl} = c_{pq} \\
E_{pq} &= E_{ijkl} & i = j \text{ and } k = l, \ p, q = 1, 2, 3 \\
2E_{pq} &= 2E_{ijkl} & i = j \text{ and } k \neq l, \ p = 1, 2, 3 \text{ and } q = 4, 5, 6 \\
4E_{pq} &= 4E_{ijkl} & i \neq j \text{ and } k \neq l, \ p, q = 4, 5, 6 \\
D_{iq} &= D_{ikl} & k = l, \ q = 1, 2, 3 \\
2D_{iq} &= 2D_{ikl} & k \neq l, \ q = 4, 5, 6 \\
E_{ikl} &= E_{ip} & h_{ikl} = h_{ip}
\end{align*}
\]

<table>
<thead>
<tr>
<th>$ij$ or $kl$</th>
<th>$p$ or $q$</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>1</td>
</tr>
<tr>
<td>22</td>
<td>2</td>
</tr>
<tr>
<td>33</td>
<td>3</td>
</tr>
<tr>
<td>23 or 32</td>
<td>4</td>
</tr>
<tr>
<td>13 or 31</td>
<td>5</td>
</tr>
<tr>
<td>12 or 21</td>
<td>6</td>
</tr>
</tbody>
</table>
Piezoelectric coefficients: relationships

**d_{ip} = \varepsilon_{ik}^T \cdot g_{kp}**

**g_{ip} = \beta_{ik}^S \cdot d_{kp}**

**e_{ip} = d_{iq} \cdot c_{qp}^E**

**h_{ip} = g_{iq} \cdot c_{qp}^D**

\[d = \left( \frac{\partial S}{\partial E} \right)^T = \left( \frac{\partial D}{\partial T} \right)^E\]

\[e = \left( - \frac{\partial T}{\partial E} \right)^S = \left( \frac{\partial D}{\partial S} \right)^E\]

\[g = \left( - \frac{\partial E}{\partial T} \right)^D = \left( \frac{\partial S}{\partial D} \right)^T\]

\[h = \left( - \frac{\partial T}{\partial D} \right)^S = \left( - \frac{\partial E}{\partial S} \right)^D\]
Electromechanical coupling factor

\[ k^2 = \frac{\text{electrical energy converted to mechanical energy}}{\text{input electrical energy}} \]

\[ k^2 = \frac{\text{mechanical energy converted to electrical energy}}{\text{input mechanical energy}} \]

- \( k^2 < 1 \rightarrow k < 1 \)
- Typical values for \( k \):
  - \( k \sim 0.10 \) : quartz
  - \( k \sim 0.40 \) : \( \text{BaTiO}_3 \) (ceramics)
  - \( k \sim 0.5-0.7 \) : PZT (ceramics)
  - \( k \sim 0.9 \) : Rochelle salt @ \( T_c = 24 \degree C \)

\[ d_{33} \]

Longitudinal mode

\[ d_{15} \]

Shear mode

\[ d_{31} \]

Lateral/transverse mode

\[ k_{33} = \frac{d_{33}}{\sqrt{S_{33}^E \cdot \varepsilon_3^T}} \]

\[ k_{15} = \frac{d_{15}}{\sqrt{S_{44}^E \cdot \varepsilon_1^T}} \]

\[ k_{31} = \frac{d_{31}}{\sqrt{S_{11}^E \cdot \varepsilon_3^T}} \]
History of Piezoelectricity

- Discovered by Pierre and Paul-Jacques Curie in 1880-81
  - External forces applied to single-crystal quartz, tourmaline, and Rochelle salt generated a charge on the surface of the crystal (proportional to the applied force)
  - Curie brothers observed the inverse effect within a year.
- 1880s-1910s → development of thermodynamics of piezoelectricity
- 1917 → WWI → Langevin and coworkers worked on ultrasonic submarine detector:
  - Thin quartz crystals with steel plates (50 KHz)
- 1920-1940 → development of microphones, accelerometers, signal filters, ultrasound transducers, actuators
  - Based on natural crystals
  - Start applications to NDT, elastic and viscous properties of liquids/gases, transient pressure measurements
- 1940-1965 → WWII → development of ferroelectric ceramics
  - Materials with perovskite structure (BaTiO₃, PZT)
  - Development of doping rationale
- 1965-1980s → Competitive collaboration between USA-Japan
  - Audio buzzers (smoke alarms), air ultrasonic transducers (TV remote control, intrusion alarms), SAW filter devices
**Piezoelectricity**

- 1980s → development of physical and chemical deposition techniques
- 1990s → development of dry etching techniques
- piezoMEMS developed in parallel to main stream MEMS processing
- 1989-1998 → strong development of ferroelectric memory devices
  - FeRAM (Ferroelectric Random Access Memory): low power/low voltage non-volatile memories

**Bulk piezoelectric transducers’ advantages:**
- Strong forces or alternatively, large displacement in bending structures
- Low operating voltage (due to high dielectric constant)
- High efficiency in energy conversation and low noise detection
- High speed and high frequency operation
- High acoustic quality (not in multidomain ferroelectrics)
- Linear behavior (not when large extrinsic contributions)
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<th>Innovation field</th>
<th>Materials and shaping</th>
<th>Main application</th>
</tr>
</thead>
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<tr>
<td>Frequency control and signal processing</td>
<td><strong>Frequency-/time standards</strong></td>
<td>Quartz single crystal plates</td>
<td>Precise frequency control</td>
</tr>
<tr>
<td></td>
<td>Mechanical frequency filters</td>
<td>Ceramic plates of specifically tailored PZT</td>
<td>Inexpensive frequency control and filtering</td>
</tr>
<tr>
<td></td>
<td>Surface acoustic wave (SAW) devices</td>
<td>LiNbO₃, LiTaO₃, Quartz single crystal substrates</td>
<td>Passive signal processing for wireless communication, identification, sensing, etc.</td>
</tr>
<tr>
<td>Sound and ultrasound (US)</td>
<td>Bulk acoustic wave (BAW) devices</td>
<td>Ceramic plates of hard PZT AlN, ZnO thin films</td>
<td>Sonic alerts</td>
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<tr>
<td></td>
<td>Buzzer</td>
<td>Ceramic tapes of soft PZT</td>
<td></td>
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<tr>
<td>Microphones and speakers</td>
<td></td>
<td>Ceramic tapes of soft PZT PZT thin films</td>
<td>Telephone, blood pressure</td>
</tr>
<tr>
<td>Ultrasonic (US) imaging</td>
<td></td>
<td>Diced plates of soft PZT or of PZNT single crystals PZT thin films</td>
<td>Medical diagnostics</td>
</tr>
<tr>
<td>Hydrophonics</td>
<td></td>
<td>Hard PZT of various shapes soft PZT composites</td>
<td>Sources and detectors for sound location</td>
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<tr>
<td>High power transducers and shock wave generation</td>
<td></td>
<td>Ceramic discs of hard PZT</td>
<td>Machining, US cleaning, lithotripsy</td>
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<tr>
<td>Atomizer</td>
<td></td>
<td>Ceramic discs of soft PZT</td>
<td></td>
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<tr>
<td>Air ultrasound</td>
<td></td>
<td>Ceramic discs of soft PZT</td>
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</thead>
<tbody>
<tr>
<td>Actuators and motors</td>
<td>Printers</td>
<td>Bars, tubes, multilayer ceramics of soft PZT</td>
<td>Needle drives and inkjet</td>
</tr>
<tr>
<td></td>
<td>Motors and transformers</td>
<td>PZT thin films</td>
<td>Miniaturized, compact motors and transformers</td>
</tr>
<tr>
<td></td>
<td>Bimorph actuators</td>
<td>PZT multilayer ceramics</td>
<td>Pneumatics, micropumps, braille for the blind</td>
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<td></td>
<td>Multilayer actuators</td>
<td>Multilayer stacks of soft PZT</td>
<td>Fine positioning and optics</td>
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<td>Injection systems</td>
<td>Multilayer stacks of soft PZT</td>
<td>Automotive fuel valves</td>
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<td>Sensors</td>
<td>Acceleration sensors</td>
<td>Rings, plates of soft PZT</td>
<td>Automotive, automation, medical</td>
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<td>Pressure and shock-wave sensors</td>
<td>LiNbO₃ substrates</td>
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<td>Flow sensors</td>
<td>PVDF foils</td>
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<td>Mass sensitive sensors</td>
<td>Soft PZT discs</td>
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<td></td>
<td>Ignition</td>
<td>Quartz discs, Quartz substrates ZnO, AlN thin films</td>
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<tr>
<td>Adaptronics</td>
<td>Ignition</td>
<td>Hard PZT cylinders</td>
<td>Gas and fuel ignition</td>
</tr>
<tr>
<td></td>
<td>Adaptive devices</td>
<td>Various shapes of soft PZT, multilayer stacks of soft PZT</td>
<td>Active noise and vibration cancellation, adaptive control, airtail filter control</td>
</tr>
</tbody>
</table>

**GeorgiaTech**

**Creating the Next**
MEMS devices

• Most commercial MEMS devices are:
  • based on electrostatic actuation
  • leverage Si, SiO$_2$, Si$_x$N$_y$, SiC, etc.

• Industrial push towards:
  • smaller size,
  • increased integration density,
  • increased speed,
  • larger range of motion,
  • more powerful actuating elements

MEMS devices compared to bulk:
• Thinner active material
• Smaller dimensions $\rightarrow$ smaller operating voltages
• Weaker forces
• Smaller displacements
• Higher resonance frequencies
PiezoMEMS vs. electrostatic MEMS

- PiezoMEMS (based on AlN) offer high-T, high resonance, with excellent T and resonance stability
  - ubiquitous in high frequency filters
  - wireless technology
- Piezoelectric effects develop in presence of mechanical excitation
  - does not require additional power supply
  - low-power devices with low noise floors and broad dynamic ranges
- Piezoelectricity can be used for local power generation/harvesting
  - low power wireless sensor nodes → IoT
- PiezoMEMS actuators have higher energy density (linear rather than square dependence on E)
  - ~10x lower driving voltage actuators
  - can be driven by CMOS (better integration)
- Excellent scaling (down) properties
  - More useful work at smaller volumes
Key PiezoMEMS Materials
Wurtzite structure: AlN, ZnO

- Stress along the c axis results in deformation of the N-Al-N bond, w/o bond length change
- Polarity is “embedded” in the crystal and polar axis reorientation would require bond breaking → no ferroelectricity
- Requires single crystalline quality thin films, with all crystallites oriented along the c axis
- Stable piezoelectric coefficients as a function of amplitude and frequency of $E$ and $T$
Perovskite structure: PZT

- Are often ferroelectric
- Can be “poled” post-processing to increase the average $P$, and hence the effective $d_{ij}$
- Piezoelectric contributions from:
  - Polarization rotation
  - Polarization extension
  - Domain wall motion
- Extrinsic contributions result into:
  - Higher $d_{ij}$ compared to non-ferroelectric compositions
  - Higher nonlinearities, $f(E, \omega, T)$
Key Perovskite-Based Piezoelectric Materials

Ferroelectrics: La-doped PZT

Ultra-soft Ferroelectrics: Ba(Sn,Ti)O$_3$

Electrostrictors: Pb(Mg$_{1/3}$Nb$_{2/3}$)O$_3$

Antiferroelectrics: Nb-doped Pb(Zr, Sn, Ti)O$_3$

\[ S_{ij} = s_{ijkl}^E . T_{kl} + d_{kij} . E_k + M_{ijkl} . E_k . E_l \]

\[ M_{ijkl}: \text{electrostriction} \]

For high permittivity materials:

\[ S_{ij} \sim Q_{ijkl} . P_k . P_l \]
Piezoelectric thin films clamped on substrates

- Clamping of piezoelectric thin films on passive substrates results in an “effective” response:

\[
d_{33,f} = d_{33} - 2d_{31} \frac{S_{13}^E}{S_{11}^E + S_{12}^E} \quad \text{and} \quad e_{31,f} = d_{31} \frac{1}{S_{11}^E + S_{12}^E}
\]

1.9 μm thick PZT films on 750 Si μm thick substrates, measured via double beam interferometry

\[
\int 2T_{1,s} dz + \int T_{3,s} \frac{s_{33,s}}{s_{13,s}} dz \frac{1}{\int T_{1,p} dz} = -f(r) \quad \Rightarrow \quad d_{33,f,\text{meas}} = d_{33,f} + f(r)s_{13,s}e_{31,f}
\]

PiezoMEMS Actuators
## Solid State Actuators

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>Piezoelectric</th>
<th>Electrostrictive</th>
<th>Magnetostrictive</th>
<th>Shape memory</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ferroic class</td>
<td>Ferroelectric</td>
<td>Ferroelectric</td>
<td>Ferromagnetic</td>
<td>Ferroelastic</td>
</tr>
<tr>
<td>Switching force</td>
<td>Electric field</td>
<td>Electric field</td>
<td>Magnetic field</td>
<td>Thermal stress</td>
</tr>
<tr>
<td>Maximum strain (%) (Ref.)</td>
<td>0.1 (Jaffe et al. 1971; furuka and Uchino 1986)</td>
<td>0.1–0.2 (Cross et al. 1980; Uchino et al. 1980)</td>
<td>0.1–0.2 (Hathaway and Clark 1993)</td>
<td>7–10 (Wayman and Shimizu 1972)</td>
</tr>
<tr>
<td>Fastest response</td>
<td>μs</td>
<td>μs</td>
<td>μs</td>
<td>s</td>
</tr>
<tr>
<td>Generative force (N/cm²)</td>
<td>3,500</td>
<td>5,000</td>
<td>3,500</td>
<td>20,000</td>
</tr>
<tr>
<td>Efficiency (%)</td>
<td>50</td>
<td>50</td>
<td>80–90</td>
<td>3</td>
</tr>
<tr>
<td>Example</td>
<td>Pb(Zr, Ti)O₃</td>
<td>Pb(Mg₁/₃, Nb₂/₃)O₃</td>
<td>(Tb, Dy)Fe₂</td>
<td>Ni₁₋ₓ Tiₓ</td>
</tr>
</tbody>
</table>
Piezoelectric modes

- $d_{15}$ is the highest piezoelectric coefficient, but difficult to implement in MEMS and thin film-based devices
- Requires high applied $V$ (wide distance b/w electrodes reduces resulting $E=V/thickness$), but low displacement (thin films)

- The deposition technologies of PZT thin films have greatly progressed in the last 20 years (based on random access memory (FeRAM))
- Major differences of PiezoMEMS actuators with FeRAM
  1. No $P$ reversal → unipolar driving in an actuator,
  2. prepared on a movable structure (sensing or actuating)
  3. larger thickness:
     - FeRAM $\sim$100 nm vs. PiezoMEMS $\sim$2 µm
  4. larger element size:
     - FeRAM $<$500nm vs. PiezoMEMS $>$100 µm

Piezoelectric actuation modes

- Many different actuation modes → borrowed from bulk actuator design
- Stress and strain (displacement) offered in trade-off
- Blocking force is also limited by mechanical depoling threshold for the piezoelectric element in ferroelectric based device

1. Direct extensional actuators:
   - Expansion/contraction of piezoelectric element used directly for displacement
   - Low strain but can produce the highest stress

2. Externally leveraged actuators:
   - Direct extension is amplified by an external mechanism (lever, Moonie)
   - Enhanced displacement at the cost of blocking force

3. Internally leveraged actuators:
   - “Amplification” mechanisms based on bending of actuator itself
Piezoelectric actuation modes for MEMS devices

- Direct extensional modes are difficult to implement in MEMS devices:
  - Thin films’ piezoelectric response $\sim 10^5$-$100^8$ pm/V
  - Multilayer stacks are substantially more challenging to process and integrate at microscale
  - Slowest response times

- piezoMEMS devices are more often based on internally leveraged amplification

![Diagram of piezoelectric actuation modes for MEMS devices](image-url)
• Stiffness of the piezoactuator and the external structure is coupled
  → Operational frequency of actuator is often limited by mechanical resonance frequency of the structure.
  → Additional factors: kinetic energy of the mass + energy stored in the spring
• Vibrating mass cannot follow the excitation signal as the frequency increases → phase difference b/w input signal and response
Flextensional Transducers

Require 3D fabrication and patterning approach → less MEMS friendly

MEMS friendly due to planar-compatible fabrication requirements
Piezoelectric Micro-Pumps

- Particularly of interest for biomedical applications
- Piezoelectrics act faster than other actuators, they exert moderate pressure against low energy consumption
- Complex systems of inlet valve, chamber (with pump), and outlet valve
- In microfluidic applications, non-moving-parts (Tesla, nozzle/diffuser) valves are preferred:
  - **Advantages:**
    - Simple structure,
    - miniaturization,
    - no need for external control,
    - high efficiency,
    - simple operating principle,
    - low cost
  - **Challenges**
    - Design based on fluid properties for diodicity (forward flow, preventing backflow)
    - Suffer from some backflow and clogging
- Fluid displacement is performed through a diaphragm
  - Passive element
  - Mobile and fully clamped at edges
  - Deflection shape will dominate the "residual" chamber volume

Mohith, S., Karanth, P. N. & Kulkarni, S. M. Mechatronics (2019)
Piezoelectric Micro-Pumps

- Balancing the diaphragm thickness to the piezoelectric material:
  - Thinner diaphragms are more flexible →
    - Higher displacement
    - Lower pressure
  - Rule of thumb:
    - piezoelectric thickness > membrane thickness
    - stiffness to be balanced by the diaphragm diameter
    - Operate at higher field amplitude (higher displacement) and (often) resonance frequency
- Additional changes can be imparted by design of the piezoelectric actuation and chamber, example include:
  - Bimorph piezoelectric actuator → increased fabrication complexity
  - Double diaphragm actuation (top and bottom) → increased fabrication complexity
  - External multi-layer piezoelectric actuator → limited miniaturization
  - Operation at resonance → mechanical structure resonance frequency does not coincide with the piezoelectric element’s
  - Peristaltic pumps → often operated as multi-chamber flow
Piezoelectric Micro-Pumps

- Multi-unit piezoPumps
  - Single piezoelectric element with standing waves on a single membrane
  - Multiple piezoelectric elements on a single membrane
  - Single or multiple piezoelectric elements working with phase shifts (open/close options) on separate membranes

- Compared to single-chamber configuration, multi-unit ones offer:
  - Reduced alternated flow rate
    → Reduced backflow
  - Backflow can be further tuned through use of designed valves
  - Combinations of nozzle/diffusers and Tesla valves
PiezoMEMS Energy Harvesters
Energy harvesting from the environment

Micro and sub-micron scale energy harvesting:

- ~1–100 μW
- Self-supported portable or embedded sensor and communication networks
- Mechanical energy sources, i.e. vibration generated from:
  - industrial machines,
  - human activity,
  - vehicles,
  - structures,
  - environment sources

<table>
<thead>
<tr>
<th>Human Body</th>
<th>Vehicles</th>
<th>Structures</th>
<th>Industrial</th>
<th>Environment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Walking, arm motion, finger motion, jogging, swimming, eating, talking</td>
<td>Aircraft, unmanned air vehicle, helicopter, automobiles, trains</td>
<td>Bridges, roads, tunnels, farm house structures</td>
<td>Motors, compressors, chillers, pumps, fans</td>
<td>Wind, solar, temperature gradient, daily temperature</td>
</tr>
<tr>
<td>Breathing, blood pressure, exhalation, body heat</td>
<td>Tires, tracks, peddles, brakes, shock absorbers, turbines</td>
<td>Control switch, heating ventilation and air conditioning systems, ducts, cleaners, etc.</td>
<td>Conveyors, cutting and dicing, vibrating machine</td>
<td>Ocean currents, acoustic waves, electromagnetic waves, radio frequency signal</td>
</tr>
</tbody>
</table>
Energy harvesting from the environment

Micro and sub-micron scale energy harvesting:

• $\sim 1\text{–}100 \, \mu\text{W}$
• Self-supported portable or embedded sensor and communication networks
• Mechanical energy sources, i.e. vibration generated from:
  • industrial machines,
  • human activity,
  • vehicles,
  • structures,
  • environment sources
• Is piezoelectric better than electromagnetic transduction?
• Based on constitutive equations:
  • Power generated by electromagnetic approach $\sim \nu^2$
  • Power generated by piezoelectric approach $\sim \nu^{3/4}$
  • Crossover at $\nu_{\text{critical}} \sim 0.5 \, \text{cm}^3$
  • For $\nu < \nu_{\text{critical}}$:
    • $\text{Power}_{\text{electromagnetic}} < \text{Power}_{\text{piezoelectric}}$
    • Challenging assembly of the conductive coil and magnetic layer becomes challenging
PiezoMEMS energy harvesters

1. **Phase 1**: source excitation converted into cyclic oscillations via mechanical assembly.
   → some energy loss due to:
     • unmatched mechanical impedance,
     • damping,
     • backward reflection.

2. **Phase 2**: cyclic mechanical oscillations converted into cyclic electrical energy through the piezoelectric effect.
   → Energy loss due to:
     • Piezoelectric transduction → $k^2$
     • Figure of Merit = $d \cdot g$

3. **Phase 3**: generated electrical energy is conditioned by rectification and dc/dc conversion.
   → Energy losses due to:
     • power consumption by the circuit
     • Unmatched electrical impedance

- To increase $P$ density:
  • maximize **trapping of mechanical energy**
  • reduce **mechanical loss** due to mismatch in mechanical impedance
  • reduce electromechanical loss (increase $k$)
PiezoMEMS energy harvesters

- Most piezoMEMS energy harvesters based on resonator beams
- Unimorph or bimorph structures with a proof mass
  - Amplify the ambient vibrations
  - Adjust the (center) resonant frequency to the available environmental frequency, normally <100 Hz
  - Need for wide resonance bandwidth (to accommodate the range of natural resonances in the environment)
- All resonator have natural damping;
- Piezoelectric resonators have
  - Mechanical damping
  - Electrical damping

\[ P = \frac{\zeta_{\text{electr}}}{4\omega_n(\zeta_{\text{electr}} + \zeta_{\text{mech}})^2} m A^2 \]

\[ V_{31} = T_{xx} \cdot g_{31,f} \cdot t_{xx} \]

- \( t_{xx} \): thickness of piezoelectric layer
- \( T_{xx} \): stress
- \( g_{31,f} \): effective \( g_{31} \)

- \( P \): power
- \( \omega_n \): natural frequency of system
- \( \zeta_{\text{electr}} \): electrical damping ratio
- \( \zeta_{\text{mech}} \): mechanical damping ratio
- \( m \): mass
- \( A \): acceleration
Maximum power extracted from a piezoresonator

- Basic mass-spring-damper model:

\[
P = \frac{\zeta_{\text{electr}}}{4\omega_n(\zeta_{\text{electr}} + \zeta_{\text{mech}})^2} m A^2
\]

- Extractable \( P \) is inversely proportional to the resonance frequency, \( \omega \), at a fixed acceleration, \( A \) 
  → design for the lowest possible frequency → to achieve the highest power

- Extractable \( P \) is proportional to acceleration \( A \)
  → Low accelerations will limit any designed device

- Extractable \( P \) is proportional to proof mass, \( m \)
  → Maximizing proof mass increases the extractable energy

- Extractable \( P \) is maximized at \( \zeta_{\text{electr}} \approx \zeta_{\text{mech}} \)

- Maximum extractable \( P \) that can be dissipated in the electrical load, if piezoelectric is not limiting factor:

\[
P_{\text{max, electrical}}(\omega_n) = \frac{m A^2}{16\omega_n \zeta_{\text{mech}}} = \frac{m Y^2 \omega_n^3}{16 \zeta_{\text{mech}}}
\]

- \( P \): power
- \( \omega_n \): natural frequency of system
- \( \zeta_{\text{electr}} \): electrical damping ratio
- \( \zeta_{\text{mech}} \): mechanical damping ratio
- \( m \): mass
- \( A \): acceleration

- \( Y = \frac{A}{\omega_n} \): proof mass deflection
More performance parameters: $K^2$ vs. $k_{33}^2$

- Power generation performance of the vibration harvester is represented by $K^2$:
  - $K^2$: Generalized Electromechanical Coupling (GEMC) factor:
    \[
    K^2 = \frac{\omega_{\text{short}}^2 - \omega_{\text{open}}^2}{\omega_{\text{short}}^2}
    \]
    - $\omega_{\text{short}}$: resonance frequency in short circuit
    - $\omega_{\text{open}}$: resonance frequency in open circuit

- Power generated in a $d_{33}$-mode unimorph cantilever harvester without passive layer:
  \[
  P_{\text{piezo}} = Vol_{\text{piezo}} \cdot YM_{\text{piezo}} \cdot S^2 \cdot \omega_{\text{excit}} \cdot k_{33}^2
  \]
  - $Vol_{\text{piezo}}$: volume of piezoelectric material
  - $YM_{\text{piezo}}$: Young’s Modulus of piezoelectric
  - $S$: strain
  - $\omega_{\text{excit}}$: excitation frequency

- $k_{33}^2$ in a $d_{33}$-mode unimorph cantilever harvester:
  \[
  k_{33}^2 = \frac{d_{33}^2 \cdot YM_{\text{piezo}}}{\varepsilon_{\text{piezo}}} = \frac{e_{33}^2}{\varepsilon_{\text{piezo}} \cdot YM_{\text{piezo}}}
  \]
  - $d_{33}$: electromechanical coupling coefficient of piezoelectric
  - $e_{33}$: dielectric permittivity of piezoelectric

- $K^2 < k_{33}^2$

\[
K^2 = \frac{\text{stored electrical energy}}{\text{total input mechanical energy}} = \frac{\text{stored electrical energy}}{\text{mechanical energy in elastic layer} + \text{mechanical energy in piezoelectric layer}}
\]
For $d_{31}$-mode energy harvesting cantilevers, use a Dimensionless Figure of Merit (DFoM):

$$DFoM = \left( \frac{k_{31}^2 Q_m}{S_{11}} \right)_{on-resonance} \cdot \left( \frac{d_{31} \cdot g_{31}}{\tan \delta} \right)_{off-resonance}$$

- $Q_m$: mechanical quality factor
- $1/Q_m$: mechanical loss

DFoM allows direct comparison of different materials for use in a specific energy harvesting design.

In general, to increase the DFoM:
- Increase piezoelectric coefficients
- Reduce (dielectric and mechanical) losses
- Ferroelectrics allow tailoring of properties
PiezoMEMS resonators
PiezoMEMS resonators

- RF devices require low mechanical and dielectric losses at high frequencies
  - Difficult to fulfill with ferroelectric compositions
  - Often leverage non-ferroelectric piezoelectrics (AlN)
  - However, compared to non-ferroelectrics, ferroelectric compositions (e.g., PZT) offer:
    - Larger piezoelectric coefficients
    - Larger electromechanical coupling factors
    - Wider resonance bandwidths
    - Lower motional resistance
    - Ferroelectricity enables control of properties to overcome processing-induced sample-to-sample variability
  - PZT-based MEMS remain still an excellent option for resonators

- Thin-film bulk acoustic resonator (TFBAR or FBAR)
  - Mostly based on non-ferroelectric materials (AlN)
  - Needs: temperature behavior, stability vs. time, strength and purity of the wanted resonance frequency
PiezoMEMS Sensors
PiezoMEMS chemical resonator sensors

- Chemical sensors classifies by 4S:
  - Selectivity
  - Sensitivity
  - Speed
  - Stability
- Very low mass, suspended resonators, functionalized through use of a chemically-selective coating
  → Change in resonator fundamental resonance by absorption of the chemical species
  → Sensitivity is directly proportional to adsorption coefficient of chemical onto the resonator film
- Limitations:
  - Polycrystalline films are substantially cheaper to process, but not as consistent in properties
  - Epitaxial films on single crystalline substrates are not cost-effective for mass production
- Advantages:
  - Very fast response compared to other approaches
  - Relatively temperature insensitive materials
  - Chemically stable in a range of atmosphere
  - Radiation-hard and non-sensitive to stray electromagnetic waves
PiezoMEMS: Fabrication and Integration Challenges
PiezoMEMS: Materials and Film Stacks

- Historically MEMS devices processed on Si, based on CMOS design knowledge and desired compatibility with CMOS devices for miniaturization
- Most recently push for non-traditional (non-Si) substrates:
  - Polymeric, flexible substrates → flexible electronics
  - Glass substrates → integrated functionalities into the electronic screens
- Biggest challenges:
  - High processing temperatures for perovskite ferroelectrics, often > 650 °C
    → Not compatible with CMOS, glass or polymeric substrates
    → Limitations on “bottom” layers: electrode materials (Pt, Ir/IrOₓ), adhesion layers, etc.
    → Requires alternative processing approaches:
      → Low temperature fast processing times
      → Localized processing and patterning
  - Chemical diffusion of cations into the substrate (Pb, Bi, Ba)
    → Required use of diffusion barrier layers: SiO₂
    → Metal to oxide adhesion layers required: Ti/TiOₓ (for Pt), Cr/CrOₓ (for Au)
## Piezoelectric Materials

<table>
<thead>
<tr>
<th>Materials</th>
<th>Advantages</th>
<th>Challenges</th>
<th>Major use</th>
</tr>
</thead>
<tbody>
<tr>
<td>Non-Ferroelectric: AlN</td>
<td>• Very low dielectric and electromechanical losses</td>
<td>• Lower piezoelectric coefficients&lt;br&gt;• Needs epitaxial growth for functionality</td>
<td>• Resonators and sensors</td>
</tr>
<tr>
<td>Ferroelectric Perovskites: PbZr&lt;sub&gt;1-x&lt;/sub&gt;Ti&lt;sub&gt;x&lt;/sub&gt;O&lt;sub&gt;3&lt;/sub&gt; (PZT) + dopants</td>
<td>• Very high piezoelectric coefficients&lt;br&gt;• Designer compositions</td>
<td>• High dielectric permittivity and losses</td>
<td>• Actuators and transducers</td>
</tr>
<tr>
<td>Electrostrictive Perovskites: PbMg&lt;sub&gt;1/3&lt;/sub&gt;Nb&lt;sub&gt;2/3&lt;/sub&gt;O&lt;sub&gt;3&lt;/sub&gt;</td>
<td>• High strains with low losses&lt;br&gt;• Limited hysteresis</td>
<td>• High dielectric permittivity&lt;br&gt;• Challenging processing</td>
<td>• Actuators with limited loss and hysteresis</td>
</tr>
<tr>
<td>Antiferroelectric Perovskit: PbZrO&lt;sub&gt;3&lt;/sub&gt;, La-PZT (+dopants)</td>
<td>• High auxetic strains and high forces&lt;br&gt;• No thermal depoling</td>
<td>• Challenging processing&lt;br&gt;• Often high actuation voltage</td>
<td>• Actuators with high blocking force and free displacement</td>
</tr>
</tbody>
</table>
Tailoring Properties: Solid Solutions and Orientation

- Ferroelectric materials’ properties can be modified through compositional changes
- Enhanced piezoelectric response at the morphotropic phase boundary

Defay, Integration of Ferroelectric and Piezoelectric Thin Films, 2013
Tailoring Properties: Modifying Internal Bias

- Internal bias can be created on-purpose (doping with Nb, Mn, ...) or by Pb-loss at the surface
- Internal bias is often accompanied by hard pinning sites
- In soft materials, judicious control of internal bias can result in:
  - Better aligned dipoles along the out-of-plane direction
  - Increased piezoelectric coefficients
  - Decreased dielectric permittivity

![Graph showing dielectric properties](image1)

![Graph showing remnant polarization](image2)

Pt/(001) 900 nm PMN-PT/Pt
Pt/(001) 900 nm PMN-PT/Cr-Au
Chemical Gradients in Solid Solutions

ToF-SIMS/EDS, 200nm PZT (52/48)

TEM EDX, 2μm PZT (53/47)


How to Deal with the Chemical Gradients?

- **In thick** films, chemical gradients result in substantial compositional excursions → should be avoided to enhance the electromechanical response

- **In thinner** films, chemical gradients can be used to advantage to create superlattice-like (SL) structures with enhanced properties → Not a cost-effective approach, as requires increased deposition steps

---

(100)-oriented, ~200 nm-thick PZT (SL: Λ = 32 nm) films

<table>
<thead>
<tr>
<th>Film</th>
<th>SL</th>
<th>MLA</th>
<th>Grad-free</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\varepsilon_r$</td>
<td>724 ± 22</td>
<td>590 ± 18</td>
<td>602 ± 13</td>
</tr>
<tr>
<td>$d_{33,f}$ (pm/V)</td>
<td>95 ± 5</td>
<td>65 ± 5</td>
<td>65 ± 5</td>
</tr>
</tbody>
</table>

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Patterning of Ferroelectric Thin/Thick Films

- Complex oxides often require complex patterning
- Can be affected by the film’s chemical gradients.
- In general, two approaches:
  1. Reactive Ion Etching and Ion Beam Etching
     - Poor selectivity over photoresist or metallic electrode;
       → Require timed control of the process
     - Low etch rates → not effective for thicker films
     - Material redeposition along side-walls
     - Ion Beam Removal can also damage the surface layer → often can be recovered by annealing at high temperature
  2. Solution Based Patterning
     - Good selectivity compared to photoresist and metal electrode
     - Often requires 2 or more etchants (ex. 1BOE:2HCl:3H₂O→50%HNO₃) in ultrasonic baths
     - Insoluble by-products → redeposit on walls and surface of sample
     - Often require additional etch to remove by-products of first etch
Ferroelectrics are **multifunctional** materials, enabling:

- sensing and actuation capabilities, (piezoelectric and pyroelectric functionalities)
- multilayer ceramic capacitors for microelectronic applications
- integrated switches and filters for radio systems,
- energy harvesting for self-powered devices,
- mechanical relays for low power embedded microcontrollers,
- photocatalytic applications.

“More than Moore” (MtM)

Compared to traditional electrostatic- and magnetic-based micro- and nano-electro-mechanical systems (MEMS, NEMS), offer:

- Lower voltage operation,
- Larger temperature range stability,
- Reduced sensitivity to electromagnetic fields,
- Greater scalability,
- Radiation-hard.

Applications:
- Unattended sensors
- Small scale robotics
- Ultra-low power GPS
- Pico- & nano-satellites

Courtesy of R. Polcawich, Army Research Lab
Questions?