Ambient Pressure Pyroelectric Ion Source for Harsh Environment Mass Spectrometry

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Summary

We present the construction and implementation of a compact ambient pressure pyroelectric ion source for harsh environment mass spectrometry based on thermally cycled pyroelectric lithium niobate or lithium tantalate. Thermal cycling alternately produces positive and negative ions at each face of the crystal. As constructed, basic species are detected as cations at the –z face upon heating, and acidic species are detected as anions at the –z face upon cooling. Electrical discharges are observed while cycling crystal temperature and are not correlated with ion production—rather, ions form during periods of electrical quiescence. The source is simple and robust, making it suitable for implementation in space exploration or demanding terrestrial environments.

Background

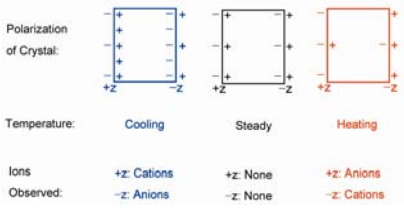
The origin of pyroelectricity is due to the fact that pyroelectric crystals are non-centrosymmetric and possess a maximum of one axis of rotation. A nonzero dipole for each unit cell imparts a net polarization to the bulk crystal. The change in polarization due to change in temperature (the pyroelectric effect) leads to an imbalance of charge in the crystal.

In a cut crystal of lithium niobate or lithium tantalate (common pyroelectric materials), the two faces orthogonal to the z crystallographic axis become oppositely charged. This results in a net electrical potential on each z face of the crystal unless it is compensated in some manner. The faces charge according to the following equation:

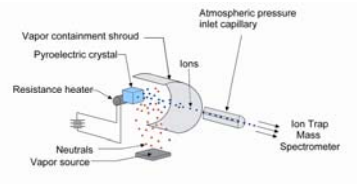
$$V=\varphi(\Delta T)d_{cr}(\varepsilon_{cr})^{-1}$$

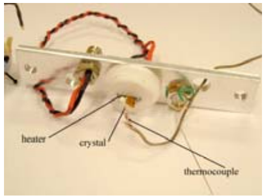
where V is the face potential, φ is the pyroelectric coefficient, ΔT is temperature change, d_{cr} is the thickness of the crystal along the z axis and ε_{cr} is the dielectric constant of the crystal along the z axis.

Positive and negative ions are alternately formed at a particular crystal face upon thermal cycling. The figure below shows the processes occuring at the crystal faces during such cycling. For example, at the –z face of a pyroelectric crystal cations are observed during heating, and anions during cooling.

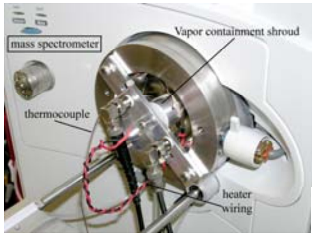


Design and Implementation





Schematic and photo of ion source. Ions are produced at the −z face of a pyroelectric crystal and travel through the vapor containment shroud to the atmospheric pressure inlet capillary of the mass spectrometer. The crystal is heated by a resistor cemented to the +z face.

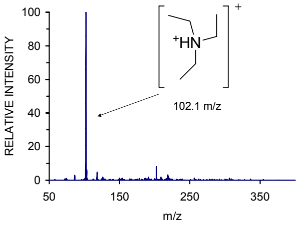


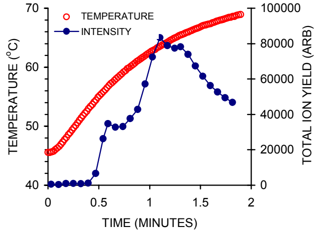
APPIS source mounted on ThermoFinnigan LCQ Deca XP ion trap MS.

The source is easily implemented in the laboratory and can be adapted for use with several different types of mass spectrometers. Small size and few parts allow for application in miniaturized and rugged systems for deployment where typical ionization sources are not able to be used. All that is required to produce ions is thermal cycling of the crystal. No high voltages, currents, or consumables are required for operation.

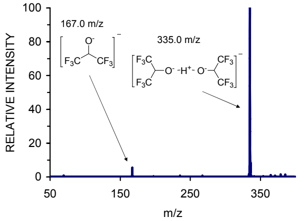
Results

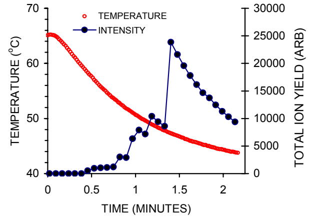
Heating yields cations at the –z face:

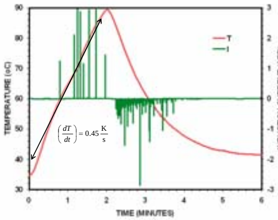


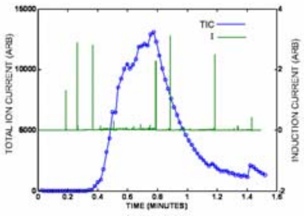


Cooling yields anions at the –z face:

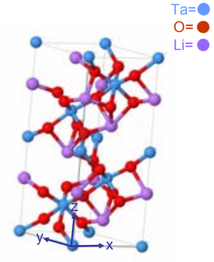








Electrical discharges are observed during heating and cooling. An inductive pickup monitors discharges as the temperature changes (left). Most ions are produced during periods of apparent electrical quiescence (right). Visible discharges are observed which correlate with the surges in induction current.



Unit cell of $LiTaO_3$, the pyroelectric material used in this work. This non-centrosymmetric structure has a non-zero dipole moment which contributes to a net polarization of the bulk crystal. Thermal excitation of atomic motion results in a decrease in the dipole which in turn gives rise to the pyroelectric effect.

Power Usage Analysis

Using **$q = (Cp)\rho(\Delta T)$** and **$P= q/T$** where Cp for $LiTaO_3$ = .06 cal g^{-1} $^oC^{-1}$ and ρ = 7.45 g cm^{-3}, 7.0 J are required to raise the temperature of a 5 x 5 x 5 mm LiTaO3 crystal 30 K. On the timescale of the experiment, typically 30 seconds, this corresponds to 230 mW, assuming 100% heat transfer efficiency, and no heat loss. This result indicates that in the current implementation the heat transfer and usage efficiency is approximately 30 %. Better heat transfer could be achieved through use of a thermoelectric device with proper thermal bonding.

Conclusions

The ambient pressure pyroelectric ion source is a simple device consuming very little power. Able to ionize acids and bases, common functionality observed in nature, the source should prove useful in a number of exploratory areas, including space environments and tasks on Earth involving unattended operation in harsh environments.

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