Purpose: To assess and optimize spectral properties of pyroelectric x-ray sources for potential imaging and therapy applications. As pyroelectric sources are inherently flux limited, efficient x-ray production is necessary for practical applications. A Monte Carlo simulation is created for the electron-photon transport process of an experimental pyroelectric x-ray source. Electron acceleration energy is determined through spectral fitting between simulation and experimental results. Determined electron energy is used to predict anode composition and thickness resulting in maximum flux in directional and transmission geometries.

Methods: A polarized z-cut lithium tantalate crystal measuring 1 cm³ was thermally cycled across 140Â°C in a vacuum of 7x10⁻³ Torr. Measurements of electron flux and x-ray spectrum were recorded and averaged for 5 thermal cycles. Simulations for reflection and transmission geometry x-ray emitters were conducted using EGSnrc Monte Carlo simulation package. Electron energies from 30 to 120 KeV were simulated for electron-photon conversion using gold, silver, tungsten, molybdenum, and copper targets of various thicknesses. Spectral comparison between simulated models of experimental conditions and recorded experimental spectra was performed using goodness-of-fit analysis. Anode target thickness and composition related to maximum x-ray generation was determined for tested electron target materials.

Results: A monoenergetic electron beam at 85 KeV best approximated overall spectral shape of the experimental setup at 0.22% RMS error between the observed and simulated spectrum. For transmission anodes simulated, copper produced the best electron-photon conversion ratio of 1.02% at 8.5 microns thickness at 100 keV. Likewise, copper significantly outperformed other materials with respect to flux in directional geometry.

Conclusions: The complex emission properties of pyroelectric x-ray source can be accurately approximated using spectral fitting methods. Practical device configuration can be easily modeled using empirical approximations to improve flux and maximum beam energy.