

Abstract Submitted
for the DAMOP16 Meeting of
The American Physical Society

Uranium doped LiSAF as a precursor for a ^{229}Th nuclear clock experiment EDMUND MEYER, MARKUS HEHLEN, BEAU BARKER, LEE COLLINS, XINXIN ZHAO, Los Alamos National Lab — We experimentally and numerically study the simple idea of growing ^{233}U doped LiSAF crystals. The micro-pulling-down technique is used to grow U:LiSAF single crystals with a high number density of U ions. The crystals are in the shape of rods that are geometrically well matched for imaging onto the spectrophotometer input slit. Growth is performed in an RF-heated chamber under argon inert atmosphere at elevated pressure. This reduces the evaporation of LiF and AlF₃ from the melt and crystal surface during growth which otherwise tends to degrade the crystal quality. Through physical arguments and robust numerical calculation we determine the oxidation state of the U ion to likely be trivalent and occupying the Sr site. Charge compensation is numerically studied through F interstitials and Li vacancies. We determine the energetically most favorable state for U:LiSAF and investigate the effects upon α -decay of ^{233}U to ^{229}Th , which $\approx 2\%$ of the time is in the excited isomeric state. Additional charge compensation mechanisms are needed to accommodate the Th^{4+} ground oxidation state and we investigate F interstitial as well as Li vacancy. The band structure is calculated and analyzed for select cases.

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Date submitted: 30 Mar 2016

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