Contribution ID: **38** Type: **Invited talk (30 min + 5 min discussion)**

Positron Annihilation Lifetime Spectroscopy (PALS) studies of thin film Solar Energy Materials using PLEPS

Thursday, 8 December 2022 13:05 (35 minutes)

Orthorhombic Barium di-silicide (BaSi2) is an emerging sun light conversion material for thin film solar cells, owing to its suitable bandgap, high light absorption coefficient, and long minority-carrier lifetime. Moreover, Ba and Si are very abundant and environmentally benign materials. The nature of defects in BaSi2 thin films grown by Molecular Beam Epitaxy (MBE), Thermal Evaporation (TE), and RF-sputtering is examined by PALS. Comparison with ab-initio calculations indicates that Si mono-vacancies are present inside grains of MBE grown BaSi2 films, that have been successfully applied in p-type BaSi2/n-type c-Si heterojunction solar cells. A grain boundary trapping model is employed to unravel the annihilation channels inside the grains and at the grain boundaries, in combination with POSWIN analysis. PALS demonstrates that larger open volume defects, Ba mono-vacancies or di-vacancies, are present in TE-deposited BaSi2 films. BaSi2 films deposited by RF-sputtering will also be discussed. Face-to-Face-Annealing (FTFA) annealing of these films produces orthorhombic BaSi2 and prevents to a large degree near-surface oxidation.
A second class of rapidly emerging thin film solar cells is based on hybrid organic-inorganic lead halide perovskites, that show great prospects for application in perovskite/c-Si tandem cells. PALS studies of formamidynium-based lead halide (FAPI) perovskite absorber layers will be presented and compared to other perovskite studies.

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Session Classification: Positrons

Track Classification: Positrons