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Passivation of Defects in CdZnTe Crystals in Hydrogen Atmosphere

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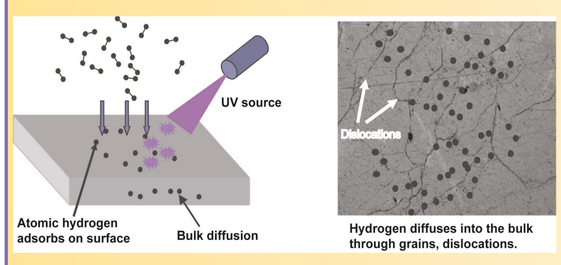
Introduction

CdZnTe (CZT) devices generally experience sub-optimal charge-transport properties that limit the performance of the detectors. Such deleterious effects in CZT crystals derive from various bulk defects like Cd vacancies (V_{Cd}), impurities, dislocations, and inclusions. These material-related problems are associated with crystal-growth conditions and cannot be easily resolved in the near future. Our objective is to increase the charge carriers' lifetimes by reducing or inactivating the existing defects in currently available CZT detector-grade crystals. We explored a technique of hydrogenation to reduce such material defects by exposing the crystals to atomic hydrogen at a temperature range of 250 °C – 400 °C, which is below the melting point of Te. Hydrogen is a unique element that easily diffuses into the crystal's bulk, and since the zinc-blende structure of CZT crystal possesses an open lattice, atomic hydrogen will dissolve therein and quickly diffuse interstitially. Diffused hydrogen passivates the electrically active dangling bonds [1-2] without adversely affecting the material's properties, and shifts the energy levels of the defects out of the band-gap, so resulting in lower trapping and electrical passivation of the defects. Furthermore, hydrogen bonded with a cation vacancy to form an H–V_{Cd} complex behaves as a single acceptor dopant and is expected to lead to an increase in the carrier's lifetime. Moreover, our UV-assisted hydrogenation system will ensure the enhancement of hydrogen diffusion into the bulk of the CZT crystals.

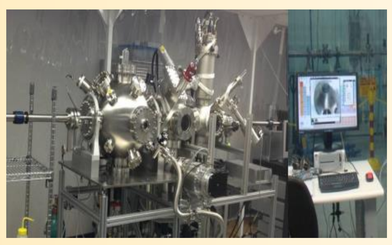
Mechanism & Experiment

Hydrogenation Mechanism

- Surface exposure to hydrogen;
- Molecular dissociation and adsorption on surface;
- Transition from surface adsorption to bulk absorption;
- UV-assisted hydrogenation: enhances H/H_2 ratio in gas;
- Fast diffusion along short-circuit paths, i.e. dislocations and grain boundaries;
- Mobile H saturates trapping centers, i.e. dangling bonds.



Hydrogen adsorption and diffusion mechanism



UV-assisted hydrogenation system

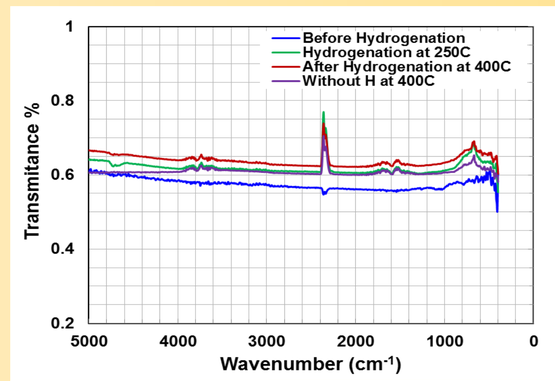
Hydrogen Treatment

- Two neighboring CZT samples (6x4x2 mm³) were selected for this experiment.
- One sample was treated by hydrogen at 400°C for 5 hours. Another sample was treated by hydrogen at 250°C for 5 hrs.
- Measurements of IR transmittance were taken by FTIR, photoluminescence (PL) at 4 K, and electrical resistivity before and after treatment.

Results & Discussion

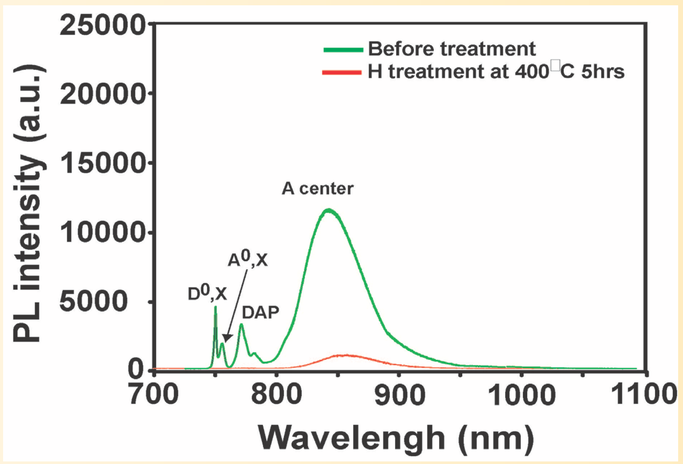
FTIR Measurements: IR Transmittance

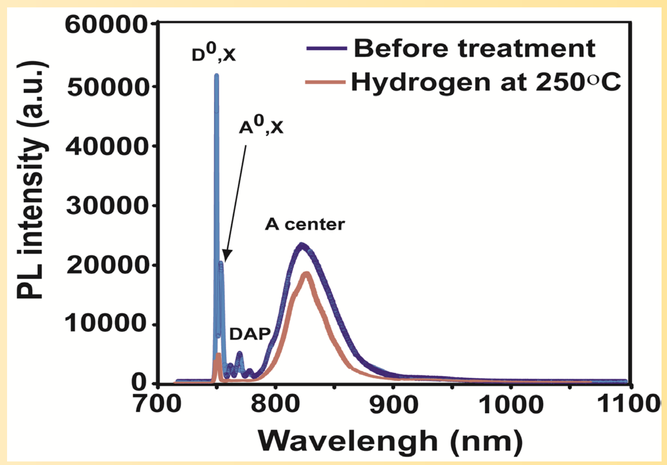
- IR transmittance of CZT crystals was measured at the MIR range by the FTIR method;
- Transmittance spectra were found fairly straight in the wave number region from 400 cm^{-1} to 5000 cm^{-1};
- The IR transmittance of CZT samples were increased about 5% after hydrogen treatment, which indicates an improvement of the quality of the crystals.



IR transmittance spectra of CZT crystals treated by hydrogen at different conditions

Photoluminescence (PL) Measurements





Before hydrogen treatment:
Donor-bound exciton peak (D^0,X), accepter-bound exciton peak (A^0,X), donor-acceptor pair (DAP) peak and A-center are well resolved.

After hydrogen treatment at 400°C for 5 hours:
No exciton peaks, only a weak A center band is observed.

Before hydrogen treatment:
D^0,X , A^0,X, DAP peaks and A-center are prominent.

After hydrogen treatment at 250°C for 5 hours,
Exciton peaks were weakened, but not fully compensated due to inadequate treatment; whereas the A^0, X peak appeared as stronger than the D^0,X. The DAP peak disappeared, and the A center band slightly decreased.

Absence of D^0,X: Likely hydrogen passivated Indium (In) donors by forming a neutral donor-hydrogen complex;

Absence of DAP: DAP attributes donors to In_{cd}^+ and acceptors to [$In_{Cd}^+V_{Cd}^{2-}$] [3]. The DAP disappeared at both treatment conditions, likely due to better passivation of donors and acceptors. Also, hydrogen reacts with acceptors more effectively [4], which causes the change in the of A^0,X peak;

A-center band: Attributed to radiative recombination of cadmium vacancy and indium donor complex (In-V_{Cd}) that decreased due to hydrogenation. Moreover, dangling bonds associated with dislocations are likely passivated by hydrogen atoms.

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Summary

- IR transmittance was increased noticeably after hydrogen treatment;
- PL results indicates that hydrogen effectively passivated various defects in CZT crystals;
- Hydrogen treatment method was found to be effective to improve the quality of the crystal;
- Need further study on the treatment parameters (e.g., temperature, exposure rate and time) for better understanding and optimizing the process.

Acknowledgement

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