Experiment Brief

Cathodoluminescence in the TEM

Title

Mapping the electronic band gap of semiconductor compounds with milli-electron volt accuracy

Gatan instrument used

Gatan's cathodoluminescence (CL) products enable optically-coupled transmission electron microscopy (TEM) to reveal and correlate nanoscale structural, optical, and electronic properties of materials

Background

The energy band gap (E_{gap}) is an important feature of semiconductors that determines their use in electronics and optoelectronics applications. Through control of a semiconductor's band gap, scientists and engineers can design novel devices and optimize device designs. However, with the explosion in nanotechnologies, determining E_{gap} at a meaningful spatial resolution is increasingly complex. The device has a graded E_{gap} formed by sulfur (S) diffusion into the CdTe absorber during thermal processing. Here we demonstrate how to reveal the change in E_{gap} by analyzing the photons emitted due to radiative recombinations after the sample is excited by the focused electron beam of a TEM.

Materials and methods

A cross-sectional TEM sample was prepared using focused ion beam lift out before the grain structure was revealed using TEM and STEM imaging modes (Figure 1a and 1b); E_{gap} was then mapped using CL spectrum imaging. CL spectrum imaging records a full CL spectrum – intensity versus wavelength (or energy) – at each location of the electron beam. The non-linear least squares fitting routine of DigitalMicrograph® software was used to determine the center of the dominant peak (corresponding to the A°X exciton) at each pixel, enabling the variance in E_{gap} to be mapped (Figure 1c).

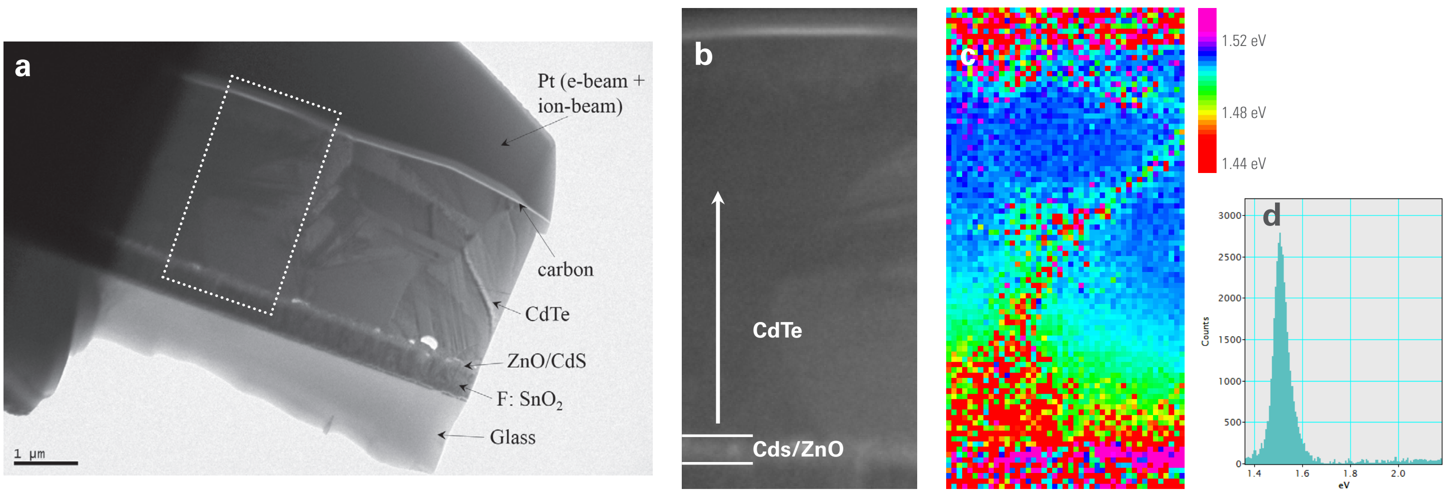

Figure 1. a) TEM image of a polycrystalline CdS/CdTe solar cell. b) and c) show correlated TEM image and band gap map. The band gap map was extracted from a CL spectrum image of the region indicated by the rectangle in a). A typical CL spectrum from the spectrum image is displayed in d) from which the band gap at each pixel was determined using the non-linear least squares method. An alloy with 17% S was observed immediately adjacent to the CdS layer (Egap reduced by 83 meV), and S was found to diffuse >1.45 µm into the grain centers. However, enhanced S diffusion at grain boundaries resulted in through-thickness diffusion of S with grain boundaries at the backside of the device exhibiting a band gap reduction of 13 meV, corresponding to an S content ~1%.

Summary

The band gap of the compound semiconductor CdTe1-xSx was mapped in the TEM by measuring the band-to-band luminescence using cathodoluminescence. Reduction in the local band gap was observed associated with sulfur diffusion during thermal processing. Due to the intrinsically low background of CL and the high energy (wavelength) offered, the band gap could be determined with better than 10 meV resolution.

Credit(s)

Special thanks to Prof. Ken Durose, University of Liverpool for providing the sample and Dr. Ashley Howkins and the Experimental Technique Centre (ETC), Brunel University, London.

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EB-OpticalTEM-Bandgap-CA-FL2-DEC23