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Electrical Activity of Defects in CdTe Solar Cells via Aberration-corrected STEM

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CdTe is a near perfect material for low-cost, high efficiency thin-film solar cells [1]. However, there is still a considerable efficiency difference between the current best research cell (18.3%) [2] and the Shockley-Queisser limit of 32% [3]. A major limitation is the low average minority carrier lifetime, induced by carrier recombination at defects. But the physical behaviors of different defects, both grain boundaries (GB) and intra-grain dislocations, are still unclear. Moreover, $CdCl_2$ heat treatment greatly improves cell efficiency, while the detailed mechanism is not understood. Therefore direct correlation between structure and carrier recombination on the scale of individual defects is highly desirable.

Scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy (EELS) have been used to determine the atomic structure of intra-grain dislocations and GBs in CdTe. We resolved single Cd and Te atomic columns at 30˚ Shockley partial dislocation cores where stacking faults terminate into the perfect crystal, as shown in Fig. 1 (a). Movies of the Cd and Te partial pairs at the two ends of the intrinsic stacking fault show their annihilation and regeneration under the electron beam, indicating a low formation energy. Atomic structure models have been constructed based on the structure observed in STEM. Density functional theory (DFT) calculations show these intra-grain dislocation pairs do not create deep states inside the band gap (Fig. 1 (b, c)). Furthermore, due to charge transfer between the two partial dislocation cores, a significant energy band bending is induced, which could help separate electrons and holes, reducing recombination.

EELS has been used to determine the chemical composition of intra-grain partial dislocations and GBs in the $CdCl_2$ heat treated CdTe. No Cl enrichment has been detected at simple partial dislocation pairs such as shown in Fig. 1. However Cl clearly segregates at the junctions of stacking faults, which we refer to as complex partials. Fig. 2 (a) shows such a complex partial at the junction of two intrinsic faults, which has a $CdTe_3$ configuration at its core. The junction of two extrinsic faults, which are two layer faults, has two units of a Cd_3Te configuration (Fig. 2 (b)). The same core structures have been seen at a GB. Fig. 2 (c) shows a row of Cd_3Te dislocation cores along a $\Sigma 9$ coincident site lattice GB. The composition profile across this GB indicates a significant Cl enrichment of ~25% at the GB plane, while Te reduces by a similar amount, Fig. 2 (d). Cl enrichment and Te depletion have also been found at random grain boundaries, as shown in Fig. 3. The electrical activity of the dislocation structures will be studied via DFT calculation. Furthermore, to directly study the properties of specific dislocations, we have developed an integrated EELS, cathodoluminescence (CL) and electron beam induced current (EBIC) system for an aberration corrected VG Microscopes HB601 STEM. This combination system will provide a direct correlation between the atomic structure, the presence of impurities and the photovoltaic properties of individual defects in CdTe solar cells. Initial results will be presented [4].

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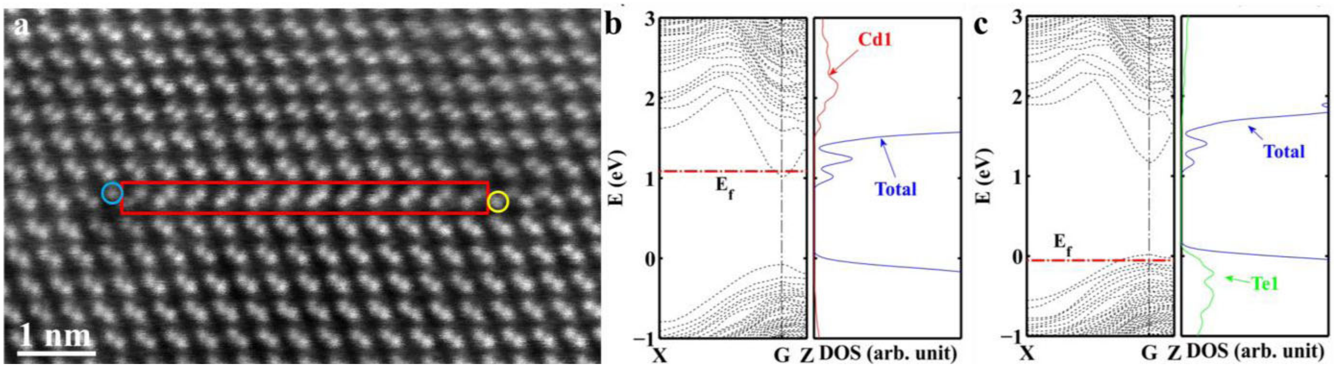

Figure 1. (a) Z-contrast image shows Cd and Te single atom columns (blue and yellow circles) at two ends of an intrinsic stacking fault (red box). (b, c) The band structure and density of state (DOS) of the individual Cd-core and Te-core both show no deep gap states.

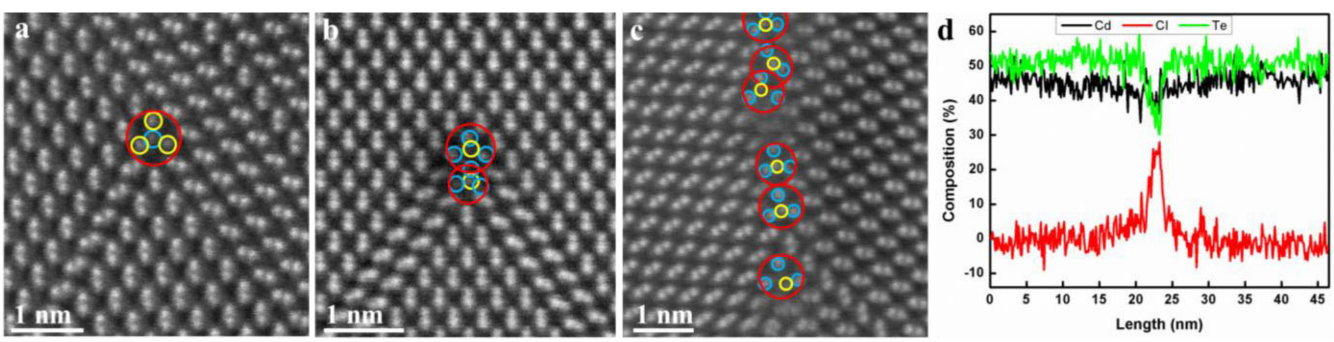

Figure 2. Similar dislocation core structures at (a) the junction of two intrinsic faults, (b) the junction of two extrinsic faults and (c) a Σ9 GB. Blue and yellow circles indicate Cd and Te columns, respectively. (d) Composition profile showing significant Cl enrichment and Te depletion at the GB plane in (c).

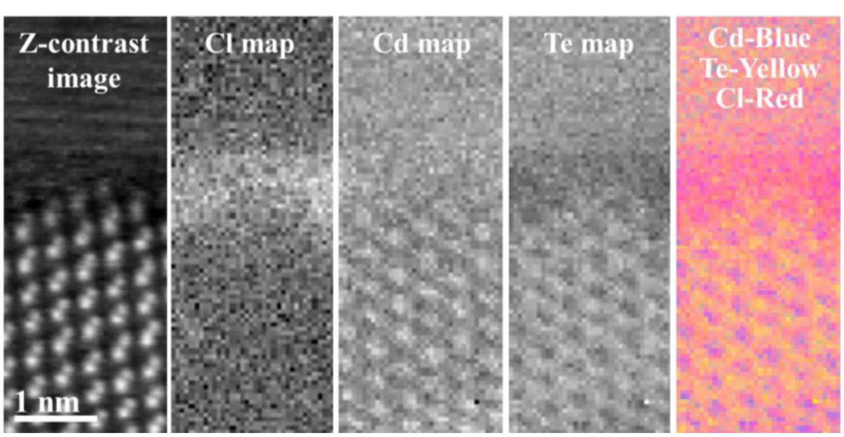

Figure 3. Spectrum images showing Cl segregation and Te depletion at a random GB.

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