

Column-by-Column Imaging of Dislocation Slip Processes in CdTe

Chen Li^{1,2}, Yelong Wu³, Andrew R. Lupini¹, Naba Paudel³, Yanfa Yan³ and Stephen J. Pennycook⁴

¹ Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA

² Department of Chemistry, Vanderbilt University, Nashville, TN, USA

³ Department of Physics and Astronomy, The University of Toledo, Toledo, OH, USA

⁴ Department of Materials Science and Engineering, University of Tennessee, Knoxville, TN, USA

The migration of dislocations affects many material properties including deformation, plasticity and electronic properties. In order to understand the mechanism of the motion of dislocations, both experimental and theoretical studies have been performed [1]. It is known that full dislocations such as edge or screw dislocations can dissociate into Shockley partial dislocations, which have higher mobility than full dislocations. However, direct observation of the Shockley partial dislocation movements at the atomic level has not been achieved before.

In this research, we use 5th order aberration-corrected scanning transmission electron microscopes (STEM) with sub-Å resolution to identify the atomic structure of different types of dislocations in CdTe solar cell materials [2]. The STEM Z-contrast image in Fig. 1 (a) shows a pair of 30° Shockley partial dislocations at the two ends of an intrinsic stacking fault, which are likely to have dissociated from a screw dislocation [2]. Unpaired Cd and Te columns have been resolved in each core. Based on the STEM images, an atomic model has been built and relaxed with density-functional theory (DFT), and the structure along the dislocation line can be understood [3]. Different from the cases of Si and diamond [1], no dimer has been found along the dislocation core (Fig. 1(c)). Kinks along the dislocations can also be located in three dimensions using through-focus imaging. Similar unpaired Cd or Te columns have been observed at both 30° and 90° Shockley partial dislocations associated with extrinsic stacking faults. Fig. 2 (a) shows two unpaired Cd columns in a 90° Shockley partial dislocation associated with an extrinsic stacking fault. However, instead of unpaired columns, CdTe-TeCd or TeCd-CdTe bonding has been observed at 90° Shockley partial dislocations associated with an intrinsic stacking fault.

Moreover, we have been able to directly watch the dislocation movement by stimulating the dislocation with the electron beam, meanwhile the low beam energy (60 KV) and low-current mode can protect the samples from being damaged. Several movies will be shown in the presentation. One movie shows the 90° Shockley partial dislocation of Fig. 2(a) gliding back and forth along the stacking fault. Three continuous frames were cut from the movie, demonstrating the glide mechanism column by column (Fig. 2 (b-d)). The Cd₀ column in fig. 2(b) was unpaired, while Cd₁-Te₁ and Cd₂-Te₂ form two dumbbells. But in fig. 2(c), the bonding between Cd₂ and Te₂ has been broken. Te₂ reformed a dumbbell with Cd₀, leaving Cd₂ as a new unpaired column. In fig. 3(d), Te₂ broke the bonding with Cd₀, and re-bonded with Cd₂. A similar movement happened simultaneously on another unpaired Cd column. This movie clearly demonstrates the glide mechanism is bond-breaking and bond-exchange. However, instead of the unpaired columns, the columns which actually move are the ones nearby. Shockley partial dislocations with unpaired columns all show a similar glide mechanism. Nevertheless, the 90° Shockley partial dislocations associated with intrinsic stacking faults, without unpaired columns in the dislocation cores, do not move under the electron beam. Another movie shows that 30° Shockley

partial dislocation pair associated with intrinsic stacking fault can not only glide, but also annihilate and reappear (Fig. 3). The stacking fault between the dislocation pairs can even change directions. This movie might demonstrate the dissociation process of a screw dislocation into partial pairs in different directions. These dislocation motions not only affect the plasticity but also the photovoltaic properties of CdTe solar cells, because states in the bandgap depend on the bonding at dislocation cores. [4]

References:

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 [4] This research was sponsored by the US DOE, Office of Energy Efficiency and Renewable Energy, Foundational Program to Advance Cell Efficiency (CL, YW, NP, YY, SJP), the Office of DOE-BES, Materials Science and Engineering Division (ARL), and a user project supported by ORNL's Center for Nanophase Materials Sciences (CNMS), which is also sponsored by DOE-BES.

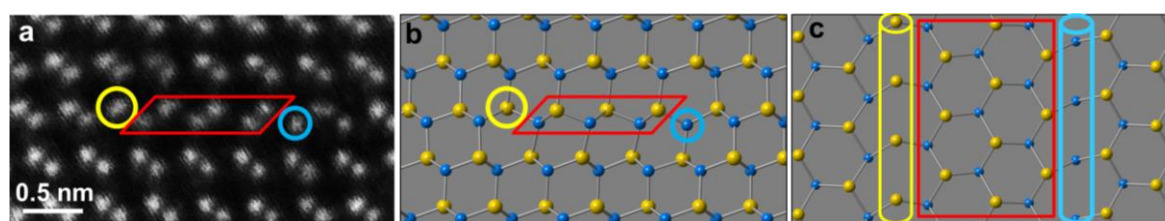


Figure 1. (a) STEM Z-contrast image showing unpaired Cd (blue circle) and Te (yellow circle) columns in the dislocation pair associated with an intrinsic stacking fault. (b) Corresponding model built with DFT. (c) The side view of the dislocation plane shows that no dimer is formed along the dislocation. The red frames indicate the intrinsic stacking fault.

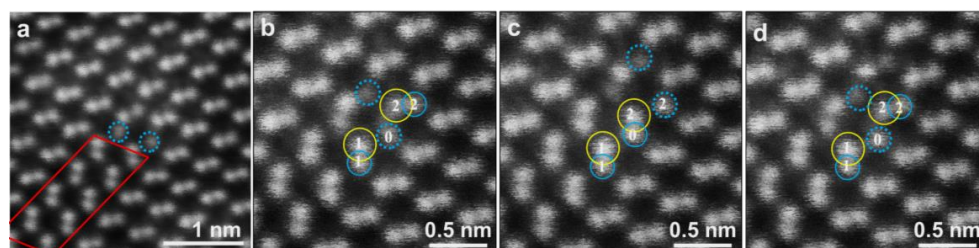


Figure 2. (a) STEM Z-contrast image shows two unpaired Cd (blue dashed circles) in a 90° Shockley partial dislocation associated with an extrinsic stacking fault (red frame). (b-d) 3 continuous frames from a movie showing the partial dislocation gliding back and forth along the stacking fault. The blue and yellow circles indicate Cd and Te columns, respectively (submitted for publication).

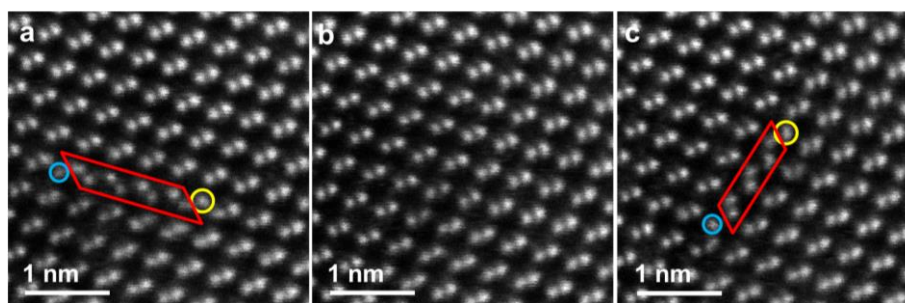


Figure 3. (a) STEM Z-contrast image shows unpaired Cd (blue circle) and Te (yellow circle) columns in a dislocation pair associated with an intrinsic stacking fault (red frame). The dislocation pair can (b) annihilate and (c) reappear with a stacking fault in another direction (submitted for publication).