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**Citation:** YU, M. and KENNY, S.D., 2017. Modelling the deposition process on the CdTe/CdS interface. Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 412, pp. 66–70.

### **Additional Information:**

- This paper was published in the journal Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms and the definitive published version is available at <https://doi.org/10.1016/j.nimb.2017.09.012>.

**Metadata Record:** <https://dspace.lboro.ac.uk/2134/26552>

**Version:** Accepted for publication

**Publisher:** © Elsevier

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# Modelling the deposition process on the CdTe/CdS interface

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## Abstract

CdTe is an excellent material for low-cost, high efficiency thin film solar cells and holds the record for Watts/\$ performance [1, 2]. Defects such as grain boundaries and dislocations lower the efficiency of CdTe solar cells [3], thus it is important to do research on how these defects are formed during the growth process, especially on the interfaces of different materials.

In this work we use computer simulation to predict the growth of a sputter deposited CdTe thin film on the CdS surfaces. Single deposition tests have been performed, to study the behaviour of deposited clusters under different conditions.

We deposit a  $\text{Cd}_x\text{Te}_y$  ( $x, y = 0, 1$ ) cluster onto the wurtzite (111) Cd and S terminated CdS surfaces with energies ranging from 1 to 40 eV. More than 1,200 simulations have been performed for each of these cases so as to sample the possible deposition positions and to collect sufficient statistics. The results show that Cd atoms are more readily sputtered from the surface than Te atoms and the sticking probability is higher on S terminated surfaces than Cd terminated surfaces. They also show that increasing the deposition energy typically leads to an increase in the number of deposited atoms replacing surface atoms and tends to decrease the number of atoms that sit on the surface layer, whilst increasing the number of interstitials observed.

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## 1. Introduction

With the development of modern society, the world's energy demands are increasing, therefore the security and supply of energy is a key problem. Conventional non-renewable resources, such as coal, oil, natural gas and nuclear, are still the main energy sources, but the reserves of these non-renewable resources are limited, and also the usage of these resources could cause many environmental problems.[4] People need to find more environmentally friendly, renewable energies, and solar power is one of the most promising renewable energies.

Electricity is one of the most common sources of energy for daily use. The majority of electricity is generated by conventional non-renewable sources. Governments are taking efforts in developing renewable electricity stations. In the UK, renewables share of electricity generation was over a quarter in 2016 Q1, up 2.3 percentage points on the share in 2015 Q1 [5] and solar photovoltaics (PVs) have an important role to play in this [6].

Solar PVs is now the third most important renewable energy source in terms of globally installed capacity. By the end of 2015, its capacity increased 29 percent year-on-year to a running total of 229 GW worldwide, and 700 GW of total global installed solar power is possible by 2020. China alone installed 14% of newly installed solar power sectors in 2016. [7] By far, the most prevalent material for solar cells is crystalline silicon. But thin film PVs devices have great potential and are a cheaper technology than conventional Si based photovoltaic devices [8].

Cadmium Telluride (CdTe) is an excellent material for low-cost, high efficiency thin film solar cells, and it is the only thin film photovoltaic technology to surpass crystalline silicon PVs in the watt/cost measure and have promising efficiency [1, 2]. However the laboratory record efficiency of CdTe solar cells lags significantly behind the theoretical maximum for the material. This discrepancy is often attributed to defects such as grain boundaries and intra-grain

dislocations [3]. Thus it is important to do research on how these defects are  
30 formed during the growth process, especially on the interface of two materials,  
and therefore reduce them.

In the laboratory, many interesting process are unable to be captured di-  
rectly during an experiment due to the extremely short time and size scale. In  
materials science, scientists usually use atomistic simulations as an outstanding  
35 partner with experiment in addressing problems. By changing the parameters in  
the simulations, we can simulate different experimental methods for producing  
thin film cells, e.g. magnetron sputtering [9] and close space sublimation [10].  
We use computer simulation to gain knowledge and predict the growth of the  
sputter deposited thin film PVs.

40 Molecular dynamics (MD) is one of the atomistic simulation techniques used  
in material sciences. In this method, an appropriate interatomic potential is  
chosen to describe the atomic forces, and the motion of atoms can be simulated  
by solving Newton's equations of motion. One can model the dynamics by  
integrating the equations of motion numerically.

45 MD follows the actual dynamical evolution of the system. The technique  
has been able to model many interesting processes, such as sputtering [11],  
crack propagation [12] and nanoindentation [13]. Resolving individual atomic  
vibrations requires a time step of the order of femtoseconds (fs) to integrate of  
the equations of motion.

50 Early research studies the energetic impacts of individual  $\text{Cd}_x\text{Te}_y$  ( $x, y =$   
 $0, 1$ ) clusters and the growth process on the CdTe surfaces. [14, 15] These  
research helps us understanding the growth of CdTe thin films. It is quite inter-  
esting to do more research on the growth process on the CdTe/CdS interface,  
since these two materials have different lattice constant, and therefore more  
55 likely to form defects. In this report, we use the MD to simulate the impact of  
individual  $\text{Cd}_x\text{Te}_y$  ( $x, y = 0, 1$ ) clusters on the CdS surfaces. These energetic  
impact tests are helpful to understand how the atoms behave during the deposi-  
tion process in different situations, and therefore helpful to find the appropriate  
growth conditions [16, 17].

## 60 2. Methodology

We use the MD to simulate the individual energetic impact tests, which generally last for a few picoseconds (ps). The MD code we are using for the simulations is the LAMMPS package (Large-scale Atomic/Molecular Massively Parallel Simulator [18, 19]), an open source code using classical MD.

65 To simulate the impacts on the CdTe systems, we use Stillinger-Weber (SW) potentials [20] for the II-VI elements [21]. The SW potentials are the most widely used semiconductor interatomic potentials. They use an energy penalty for non-tetrahedral bond angles to ensure the tetrahedral structure as the lowest energy structures. All II-VI compounds, including CdTe and CdS, exhibit  
70 either a zinc-blende or wurtzite structure in the stoichiometric conditions. As observed in experiments, only zinc-blende or wurtzite structure occurs during growth simulations under stoichiometric conditions, thus the SW potential may realistically reveal the defect formation mechanisms.

The lattice structure of CdS is wurtzite as shown in Figure B.1. The grey  
75 spheres represent the Cd atoms and yellow spheres the S atoms. The lattice constants for the CdS in our systems are chosen to be  $a = 4.126 \text{ \AA}$  and  $c = 6.737 \text{ \AA}$ , which are the optimal lattice constants using the SW potentials. In the experiments, CdTe are deposited on the wurtzite (111) CdS surfaces. Since the wurtzite (111) surfaces have the same hexagonal structure as the zinc-blende  
80 structure, CdTe would grow in (111) or (100) directions due to the different lattice constants, which are most common types of zinc-blende type of surfaces observed in the experiments. We simulate individual  $\text{Cd}_x\text{Te}_y$  ( $x, y = 0, 1$ ) cluster impact simulations on two different surfaces: the Cd-terminated (111) surface and the Te-terminated (111) surface.

85 The side view and top view of a wurtzite (111) S-terminated CdS surface are shown in Figure B.2. Bigger yellow spheres represent S atoms, and smaller green spheres represent Cd atoms. It is clear that the lattice has a double-layer structure, and the surface atoms are in a hexagonal shape. The red triangle areas in Figure B.2b indicate the smallest repeatable regions on the surface,

90 and the impact simulations are done within this region.

We model 6 double-layers of atoms, in total of 960 atoms, for both (111) Cd-terminated surface system and (111) S-terminated surface system. The bottom double-layer is fixed, and the next double-layer above the fixed zone are thermalised.

95 The growth conditions vary for different experimental techniques. We model the growth of CdTe thin films by magnetron sputtering deposition, which is a widely used technique for CdTe thin film production. In sputtering room temperature deposition is the most common, but elevated temperatures can be used to optimise performance. [22] Thus in our impact simulations, the temperature  
100 is set to be 350 K. We use the Berendsen thermostat [23] to thermalise the system.

A single  $\text{Cd}_x\text{Te}_y$  ( $x, y = 0, 1$ ) cluster, namely a single Cd atom, a single Te atom or a single CdTe cluster, is deposited onto the lattice at the height of approximately 10 Å above the surface. The atom or cluster is given a velocity  
105 perpendicular to the surface, which is equivalent to be given a deposition energy of 1 eV, 10 eV, 20 eV or 40 eV. The position of the deposited cluster is chosen randomly within the smallest area of each surfaces (the red regions shown in Figure B.2b). We perform the MD simulation for 4 ps to allow the impact to fully equilibrate. We then analyse the behaviour of the deposited cluster.

110 We did the impact simulations of 3 different species/clusters onto 2 surfaces with 4 different impact energies respectively, in total 24 cases. For each of these cases, we performed more than 1,200 impact simulations at random positions and rotations so as to sample the possible deposition positions and to collect sufficient statistics.

### 115 3. Impact results

From all the impact results, we have studied the behaviour of the deposited cluster, i.e. where is the deposited cluster at the final state and how does it affect the surrounding atoms. We categorize the final states into seven cases as

illustrated in Figure B.3 and described in Table 1.

Case 1	Bounce off	The deposited cluster bounces off the surface;
Case 2	Sputter out	The deposited cluster collides and other atoms are ejected from the surface;
Case 3	Replace	The deposited cluster replace one of the surface atoms and push it onto the surface.
Case 4	Sit on	The deposited cluster sits on the surface as a new layer;
Case 5	Join first layer	The deposited cluster joins the first layer and forms defects in the surface layer;
Case 6	Penetrate	The deposited cluster penetrates the surface and becomes interstitials;

Table 1: Classification of impact results.

120 Percentage bar charts with errors are generated for each of the 24 cases shown in Figures B.4.

The results show that on the Cd-terminated surface, increasing the deposition energy typically leads to a decrease in the number of atoms that sit on the layer. It also tends to increase the number of atoms sputtered from the system, 125 replace the surface atoms or even penetrate the surface. On the S-terminated surface, the results show a similar trend, except there is almost no penetration nor joining of the surface layer.

The behaviours of the deposited cluster at low energies are less complex than ones at higher energies as expected. The deposited clusters with higher energies 130 could penetrate the surface and displace other atoms to other sites, while ones with lower energies usually lose their energy in the impact and stick on the surface.

The results show that, it's more difficult for the cluster to penetrate the S-terminated surfaces than the Cd-terminated ones. The Cd atoms are more

135 likely to be reflected on the Cd-terminated surface, while the Te atoms are more likely to be reflected on the S-terminated surface. The results also show that on the S-terminated surfaces, the surface atoms are more easier to be replaced by the deposited atoms.

When the CdTe cluster is deposited, it usually dissociates. The statistical 140 results are shown in Figure B.5. Over half of the CdTe cluster dissociates during the deposition. One of the dissociated atoms usually stick on the surface, while the other one may either be reflected or replace surface atoms.

For cases where the atoms leave the surface (including both reflected and sputtered), we counted the number of each species to leave the surface over all 145 deposition energies. The bar chart of the average number of sputtered atoms per deposition is shown in Figure B.6.

The results show that Cd atoms are more readily sputtered from the surface than Te and S atoms. The number of atoms sputtered from the Cd-terminated surfaces is 1.5 times larger than the S ones. They highlight that the sticking 150 probability is higher on S-terminated surfaces than Cd ones. The number of S atoms sputtered are almost the same for two kinds of surfaces. The number of Cd atoms sputtered from the Cd-terminated is 2.4 times larger than the S ones, while the number of Te atoms sputtered is 1.3 times less. The Cd atoms are 3 times easier to be sputtered on the Cd-terminated surface than the Te atoms, 155 while they are almost the same on the S-terminated surface.

#### 4. Conclusion

The energetic impact simulations of small  $\text{Cd}_x\text{Te}_y$  ( $x, y = 0, 1$ ) clusters onto the wurtzite (111) Cd and S terminated surfaces at 1, 10, 20 and 40 eV have been simulated.

160 The results show that Cd atoms are more readily sputtered than Te and S atoms, especially on the Cd-terminated surfaces. The deposited clusters are more likely to be reflected than sputtered. The sticking probability is higher for the S-terminated surfaces than the Cd-terminated ones. The Cd-terminated



surfaces more likely to be penetrated or create interstitials in the surface layer  
165 than S ones. There are high possibilities for the deposited cluster to sit on the  
surface at low energies, while it is more likely to replace surface atoms at high  
energies. The CdTe cluster usually dissociate during the deposition.

Mechanisms to allow CdTe to growth on the CdS surfaces are not observed  
from the energetic impact simulations. It's not clear from the impact simulations  
170 alone how further layers of CdTe would grow. Further work using long time scale  
dynamics simulations are underway to gain knowledge of the growth process of  
CdTe layers.

## Appendix A. References

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## Appendix B. List of Figures

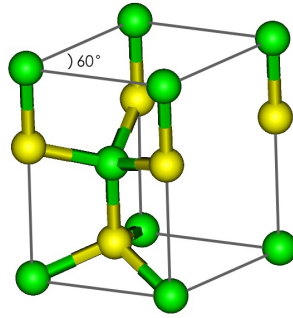


Figure B.1: The wurtzite structure of CdS, the green spheres represent the Cd and yellow ones the S atoms.

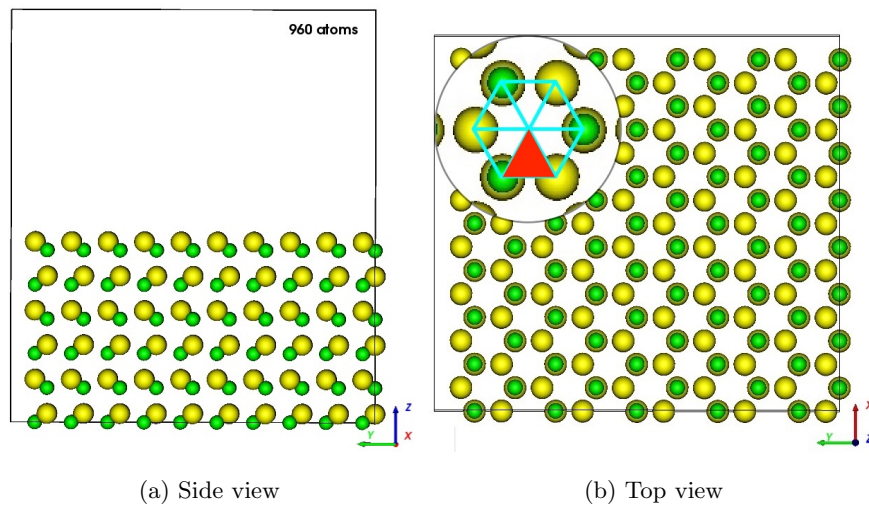


Figure B.2: Side view and top view of a wurtzite (111) S-terminated CdS surface. Bigger yellow spheres represent S atoms, and smaller green spheres represent Cd atoms. The CdS lattice stacked in double-layers. Atoms in each double-layer are in a hexagonal shape. The red triangle areas in (b) indicate the smallest repeatable regions on the surface.

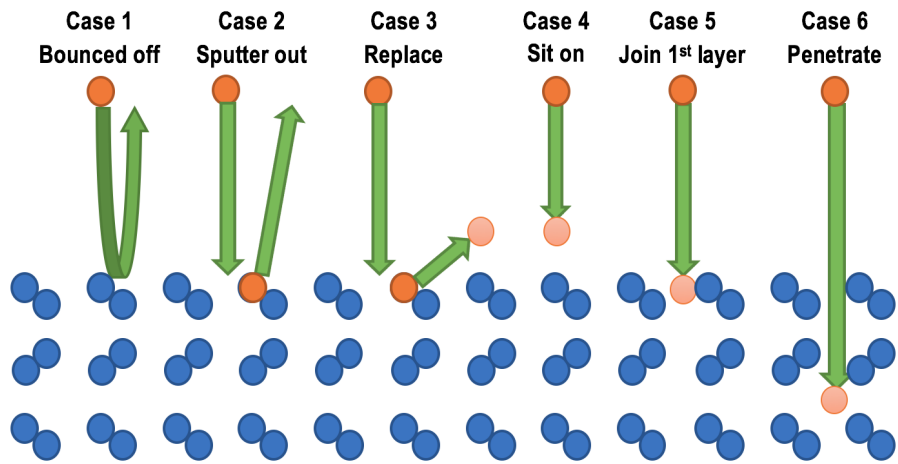


Figure B.3: The illustration graph for the 6 cases of the final states after impact as described in Table 1

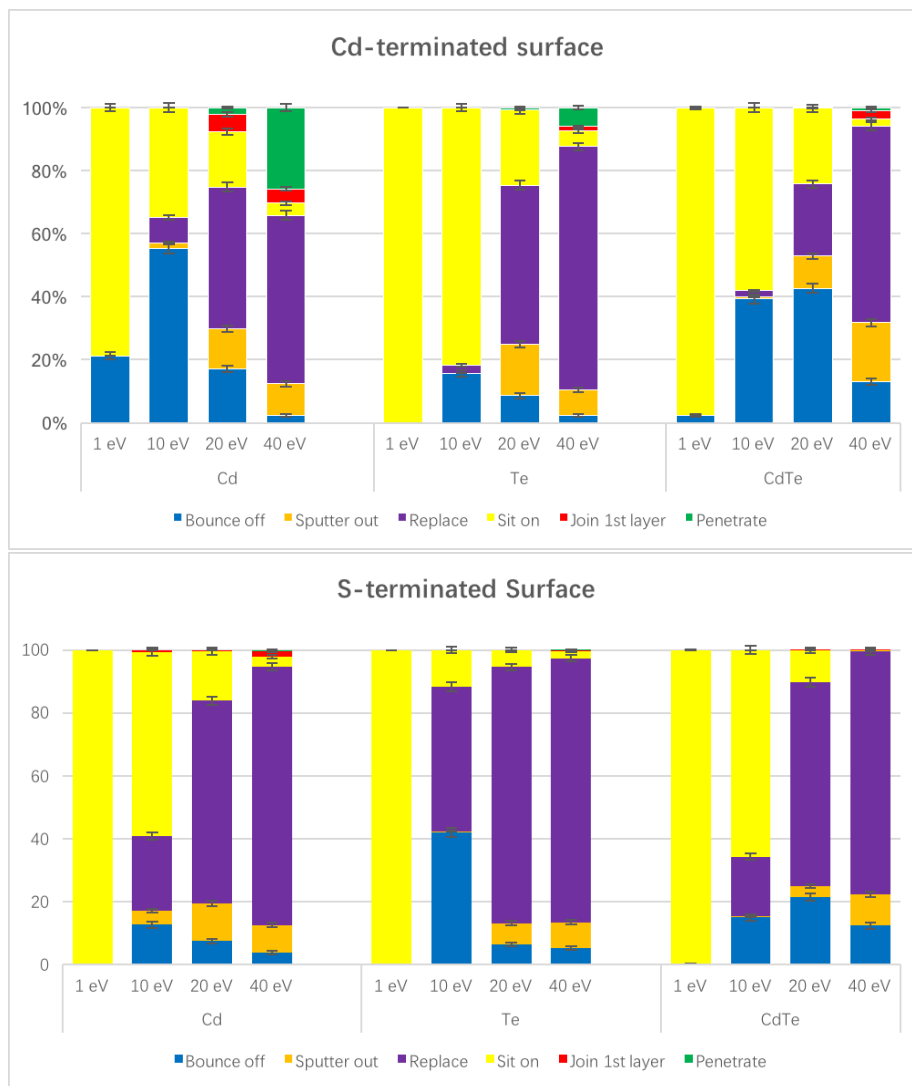


Figure B.4: Energetic impact results of small  $Cd_xTe_y$  ( $x, y = 0, 1$ ) clusters on wurtzite (111) Cd-terminated and S-terminated CdS surfaces. The 6 cases of the final states are illustrated in Figure B.3

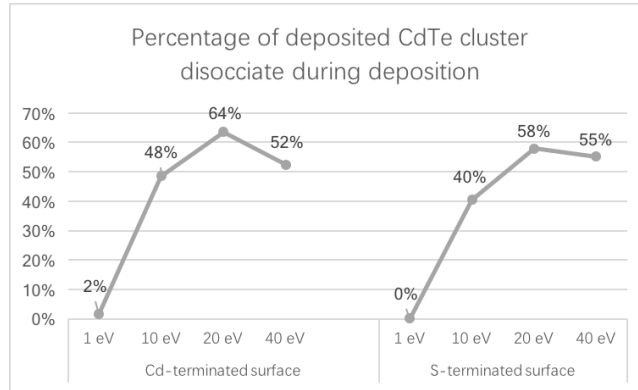


Figure B.5: Line graph for the percentage of deposited CdTe cluster dissociated during deposition.

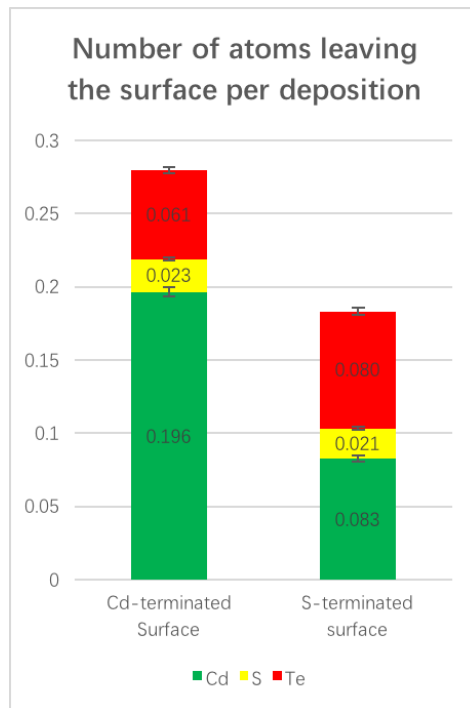


Figure B.6: Bar chart for the average number of atoms leave the surface per deposition.