

The energetic impact of small Cd_xTe_y clusters on Cadmium Telluride

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Abstract

Cadmium Telluride (CdTe) is an excellent material for low-cost, high efficiency thin film solar cells. It is important to do research on how these defects are formed during the growth process, since defects lower the efficiency of solar cells. In this work we use computer simulation to predict the growth of a sputter deposited CdTe thin film. Single deposition tests have been performed, to study the behaviour of deposited clusters under different conditions. We deposit a Cd_xTe_y ($x, y = 0, 1$) cluster onto the (100) and (111) Cd and Te terminated surfaces with energies ranging from 1 to 40 eV. More than 1,000 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 Te terminated surfaces than Cd terminated surfaces. They also show that increasing the deposition energy typically leads to an increase in the number of atoms sputtered from

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the system and tends to decrease the number of atoms that sit on or in the surface layer, whilst increasing the number of interstitials observed.

Keywords: Modelling; CdTe; Energetic impact

1 Introduction

Energy security and supply is a key problem in the coming years. More and more energy is required, while reserves in coal, oil, natural gas and other non-renewable resources become smaller due to human consumption. People need to find more environmentally friendly, renewable energy. Solar power is one of the most promising renewable energies.

Electricity is one of the most common sources of energy for daily use. Nowadays most electricity is generated by non-renewable sources, such as coal, gas and nuclear. Governments are taking efforts in developing renewable electricity stations. In the United Kingdom, renewables share of electricity generation was a record 19.4% in the first quarter of 2014, up 6.9 percentage points on the share in the first quarter of 2013 [1] and solar photovoltaics (PVs) have an important role to play in this [2].

Solar PVs is now the third most important renewable energy source in terms of globally installed capacity. In 2013, its capacity increased by 38 percent to a running total of 139 GW worldwide [3]. 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 [4].

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 [5, 6]. 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 [7]. Thus it is important to do research on how these defects are formed during the growth process and

therefore reduce them.

Atomistic simulation is widely used as an outstanding partner with experiment in addressing problems in materials science. By changing the parameters in the simulations, we can simulate different experimental methods for producing thin film cells, e.g. magnetron sputtering [8] and close space sublimation [9]. We use computer simulation to gain knowledge and predict the growth of the sputter deposited thin film PVs.

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.

MD follows the actual dynamical evolution of the system. The technique has been able to model many interesting processes, such as sputtering [10], crack propagation [11] and nanoindentation [12]. Resolving individual atomic vibrations requires a time step of the order of femtoseconds (fs) to integrate of the equations of motion.

In this report, we use the MD to simulate the impact of individual Cd_xTe_y ($x, y = 0, 1$) clusters on the CdTe surfaces. These energetic impact tests are helpful to understand how the atoms behave during the deposition process in different situations, and therefore helpful to find the appropriate growth conditions [13, 14].

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 [15, 16]), an open source code using classical MD.

To simulate the impacts on the CdTe systems, we use analytical bond-order potentials (BOPs) [17, 18] for the CdTe binary system [19, 20]. The BOPs are

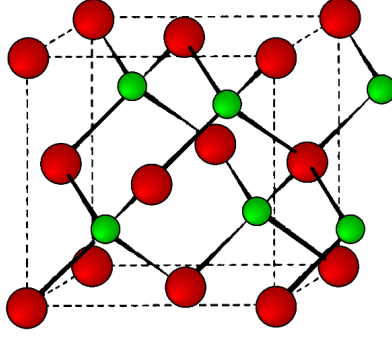


Figure 1 Zinc-blende structure.

Red bigger spheres represent the Te atoms and green smaller spheres the Cd atoms.

based upon quantum-mechanical theories and can offer a more accurate description of interatomic interactions compared to Tersoff [21] and Brenner [22] types of potentials. The Tersoff and Brenner types of potentials only consider the σ bonding with a second-moment approximation, while the BOP incorporating both σ and π bondings with a more advanced four-moment approximation.

The lattice structure of CdTe is zinc-blende as shown in Figure 1. The red bigger spheres represent the Te atoms and green smaller spheres the Cd atoms. The lattice constant in our systems is chosen to be 0.683 nm, which is the optimal lattice constant using the BOPs. The (100) and (111) surfaces are most common types of zinc-blende type of surfaces. We simulate individual Cd_xTe_y ($x, y = 0, 1$) cluster impact simulations on four different surfaces: the Cd-terminated (100) surface, the Cd-terminated (111) surface, the dimerised Te-terminated (100) surface and the Te-terminated (111) surface.

For the Te (100) surfaces there are two surface reconstruction that have been proposed, namely the (2×1) and the $c(2 \times 2)$, both involving Te dimerisation on the Te-terminated (100) surface [23]. We choose the (2×1) dimerised Te-terminated (100) surface for our impact simulations, because the (2×1) dimerisation has a lower system energy than $c(2 \times 2)$ dimerisation within our description.

Illustrations of the four different surfaces used in the impact simulations are shown in Figure 2. Circles and diamonds represent the two different species, and the

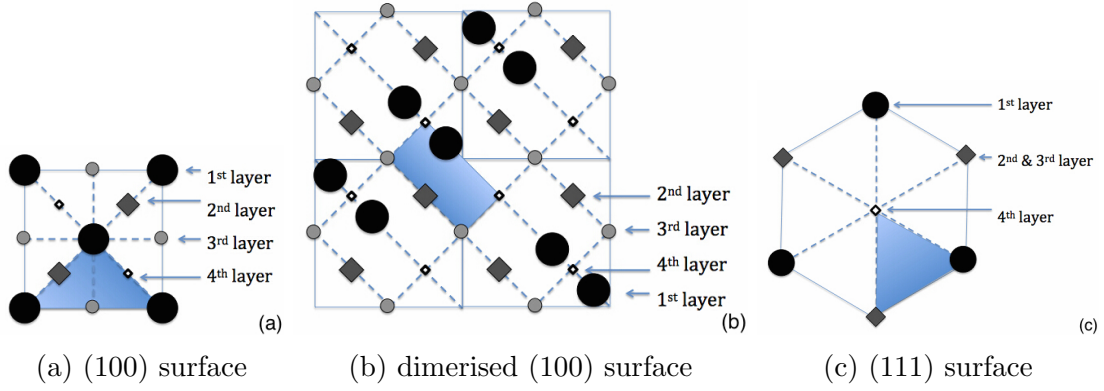


Figure 2 Illustration of different surfaces used in the impact simulations. These graphs are top views of the first 4 layers on the CdTe surfaces. Circles and diamonds represent the two different species. Sizes represent the different layers. Blue areas are the smallest repeatable regions on the surface.

different sizes represent the atoms in different layers. Shaded triangle or rectangle areas are the smallest repeatable regions on the surface, and the impact simulations are done within these regions.

We model 12 layers of atoms, in total of 864 atoms, for the (100) surface systems; and 6 double-layers of atoms, in total of 960 atoms, for the (111) surface systems. The bottom 2 layers (or 1 double-layer) are fixed, and the next 2 layers (or 1 double-layer) above the fixed zone are thermalised.

We simulate the deposition of magnetron sputtering, which usually done at room temperature. Thus in our impact simulations, the temperature is set to be 300 K. We use the Berendsen method [24] to thermalise the system where both the heat bath coupling constant and the time step are set to be 1 fs. A single Cd_xTe_y ($x, y = 0, 1$) cluster, namely single Cd atom, single Te atom or single CdTe cluster, is deposited onto the lattice at the height of approximately 1 nm above the surface. The atom or cluster is given an velocity 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 deposited cluster is chosen randomly within the smallest area of each kind of surfaces (the shaded areas shown in Figure 2). We perform the MD simulation for 4 ps, which is enough for the temperature of the impact area to become stable after the impact and the system to reach a metastable state. We then relax the system and analyse

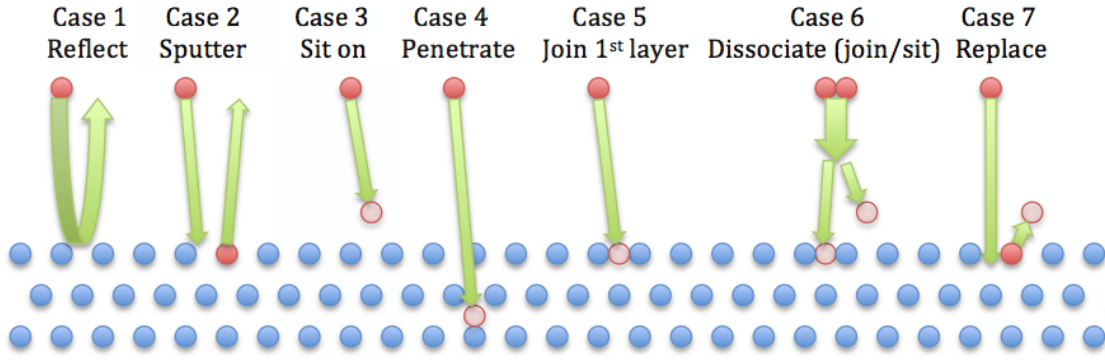


Figure 3 Illustration of 7 cases of the final states after impact.

the behaviour of the deposited cluster.

We did the impact simulations of 3 different species/clusters onto 4 surfaces with 4 different impact energies respectively, in total 48 cases. For each of these cases, we performed more than 1,000 impact simulations at random positions and rotations so as to sample the possible deposition positions and to collect sufficient statistics.

3 Impact results

3.1 Categorization of final states

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 3 and described in Table 1.

Percentage bar charts with errors are generated for each of the 48 cases shown in Figures 4 and 5.

The results show that increasing the deposition energy typically leads to an increase in the number of atoms sputtered from the system. It also tends to decrease the number of atoms that sit on or in the surface layer, whilst increasing the number of interstitials observed.

When the CdTe cluster is deposited, if it sticks on the surface it usually disso-

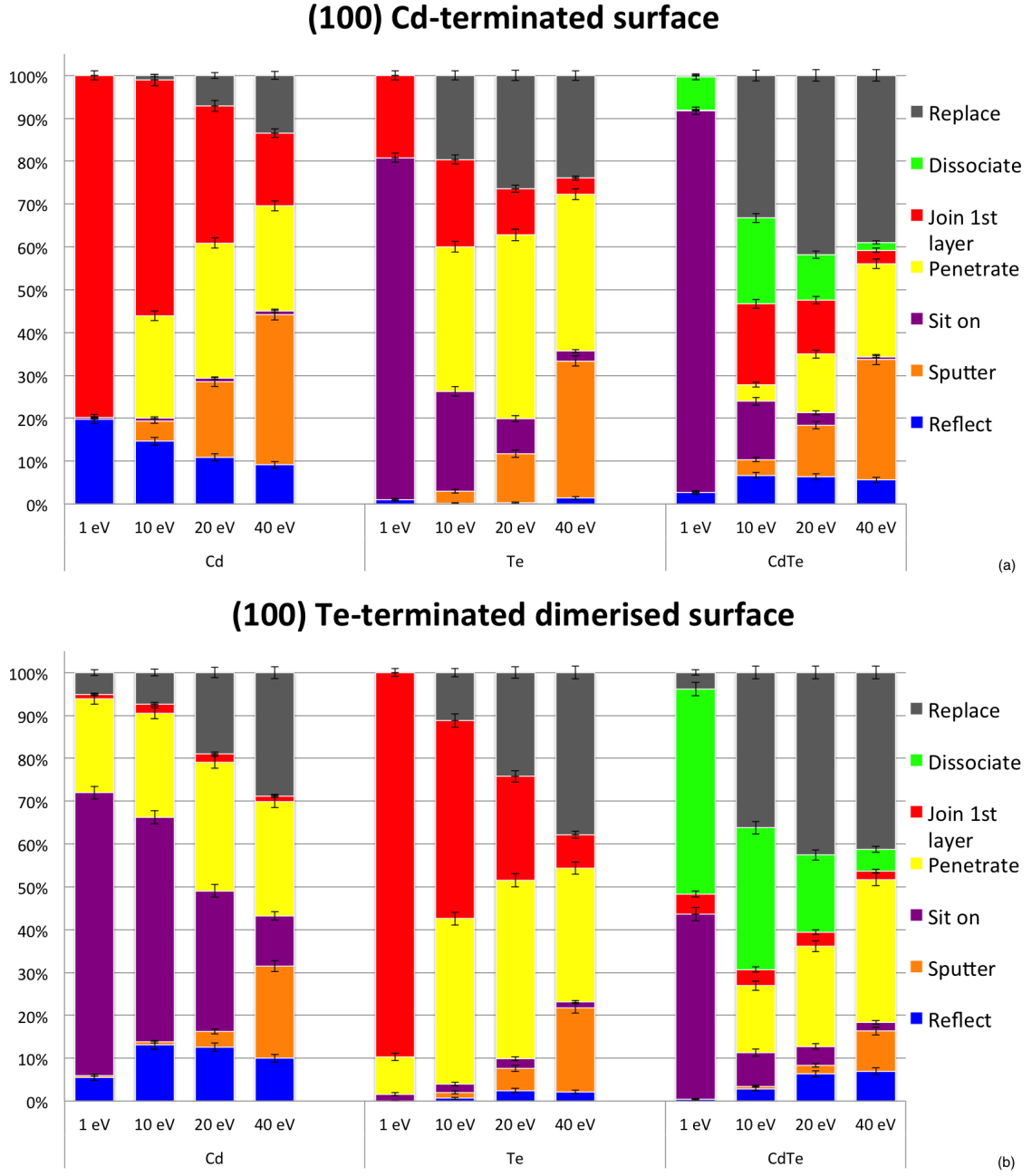


Figure 4 Energetic impact results of small Cd_xTe_y ($x, y = 0, 1$) clusters on (100) Cd-terminated and (100) Te-terminated surfaces. The 7 cases of the final states are illustrated in Figure 3

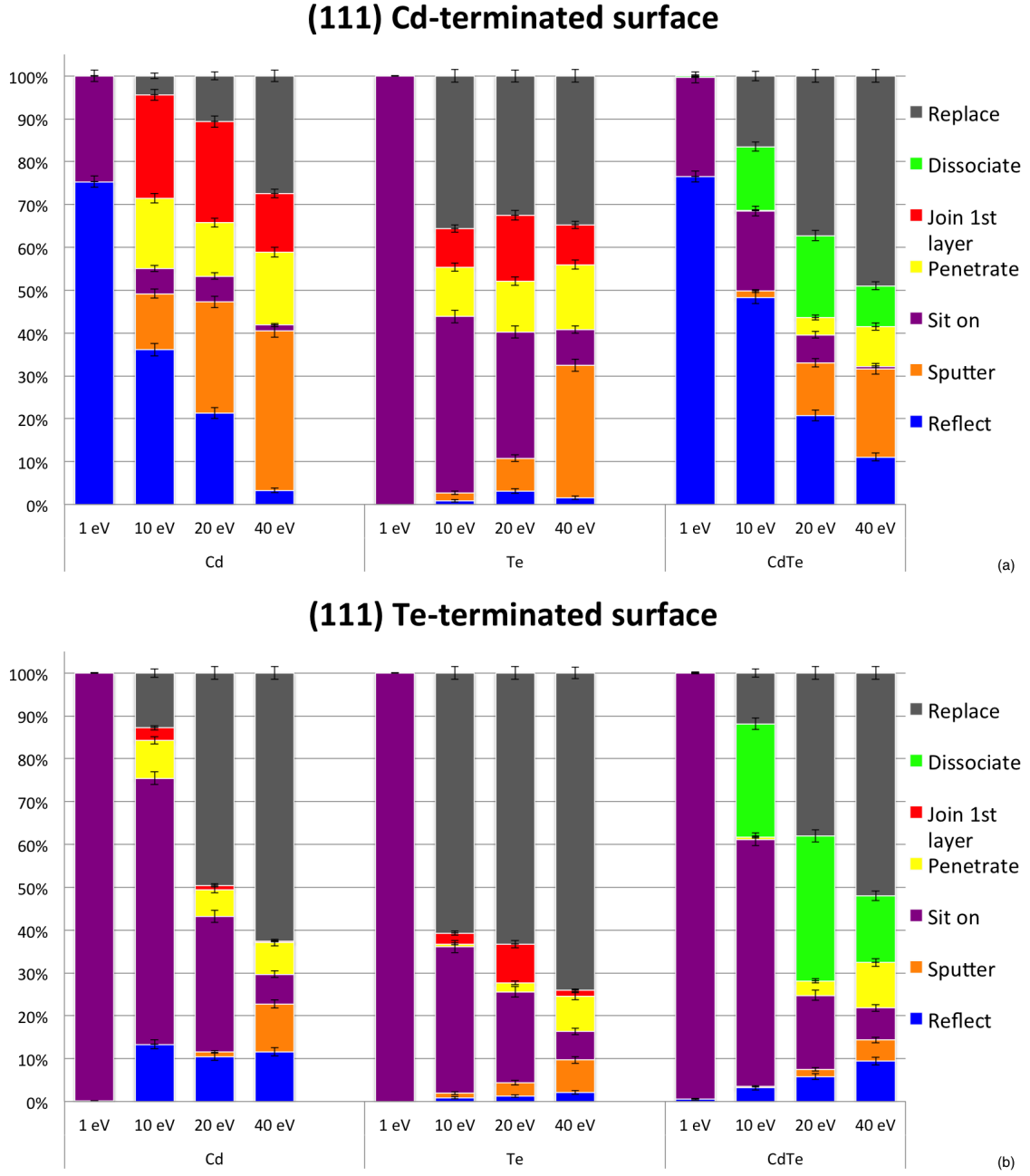


Figure 5 Energetic impact results of small Cd_xTe_y ($x, y = 0, 1$) clusters on (111) Cd-terminated and (111) Te-terminated surfaces. The 7 cases of the final states are illustrated in Figure 3

Case 1	Reflect	The deposited cluster leaves the surface;
Case 2	Sputter	The deposited cluster collides and other atoms are ejected from the surface;
Case 3	Sit on	The deposited cluster sits on the surface as a new layer;
Case 4	Penetrate	The deposited cluster penetrates the surface and becomes interstitials;
Case 5	Join first layer	The deposited cluster joins the first layer and forms defects in the surface layer;
Case 6	Dissociate	The deposited cluster dissociates, either joins the first layer or sits on the surfaces; (This case only occurs when depositing CdTe cluster.)
Case 7	Replace	The deposited cluster replace one of the surface atoms and push it onto the surface. (If depositing CdTe cluster, this case represents the cluster dissociates and replace.)

Table 1 Classification of impact results.

ciates at higher energies, while it prefers a soft-landing at low energies. This is not true for the (100) Te-terminated surfaces, where it also dissociates at low energies. When a single Cd/Te atom is deposited on a surface, the species of surface atoms affect the behaviour of the deposited atoms. On the surface, the probability to join the 1st layer is larger if we deposit the same species as the surface atoms than different. While the probability to sit on the surface is lower if we deposit the same species as the surface atoms than a different species.

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

The results show that, it's more difficult for the cluster to penetrate the (111) surfaces than the (100) ones. But on the other hand, it's easier to be reflected on the (111) surfaces than the (100) ones. We define that the surface is 'undamaged' if the deposited cluster either be reflected or become adatoms on the surface. The percentage of cases where surfaces are undamaged for the (111) surfaces is higher than (100) ones. These facts indicate that the double-layer structure in the (111)

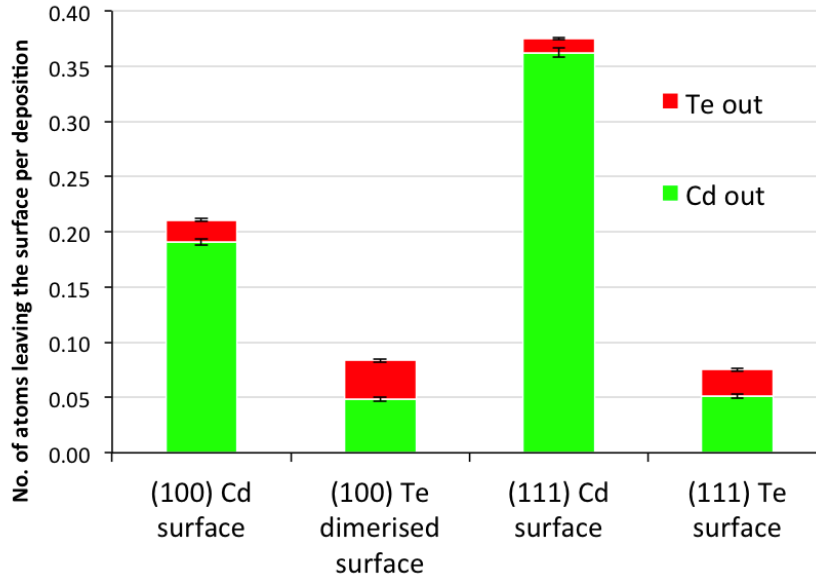


Figure 6 Average number of atoms leave the surface per deposition.

surfaces are more stable than the single layers structure in the (100) surfaces.

For cases where the atoms leave the surface (including both reflected and sputtered), we counted the number of each species to leave the surface. The bar chart of the average number of sputtered atoms per deposition is shown in Figure 6. The results show that Cd atoms are more readily sputtered from the surface than Te atoms. The number of atoms sputtered from the Cd terminated surfaces is 2.5 and 5 times larger than the Te ones for the (100) and (111) surfaces respectively. They highlight that the sticking probability is higher on Te terminated surfaces than Cd ones. The ratios of the Cd atoms sputtered v.s. the Te atoms sputtered for the Te terminated surfaces (1.4 for (100) surface and 2.1 for (111) surface) are much smaller than the ratios for the Cd terminated surfaces (9.5 for (100) surface and 28.3 for (111) surface).

4 Conclusion

The energetic impact simulations of small Cd_xTe_y ($x, y = 0, 1$) clusters onto the (100) Cd and Te terminated surfaces and (111) Cd and Te terminated surfaces at

1, 10, 20 and 40 eV have been simulated.

The results show that Cd atoms are more readily sputtered than Te atoms, especially on the Cd-terminated surfaces. The deposited clusters are more likely to be reflected than sputtered at lower energies. The sticking probability is higher for the Te-terminated surfaces than the Cd-terminated ones. This explains why the growth rate decays when the Cd concentration increases in the vapor in the work of C. Ferekides et al. using elemental vapor transport at atmospheric pressures [24].

The results also show that (100) surfaces are more likely to be penetrated or create interstitials in the surface layer than (111) surfaces. There are high possibilities for the deposited cluster to sit on the surface at low energies, and the CdTe cluster usually dissociate and replace surface atoms when deposited onto the surfaces.

We do not observe CdTe growth mechanisms from the energetic impact simulations. It's not clear from the impact simulations 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 surfaces.

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