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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 1000 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 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.

1. Introduction

Energy security and supply is a key problem in the coming years. More and more energy is required, whilst 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, renewable share of electricity generation was a record at 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 are now the third most important renewable energy source in terms of globally installed capacity. In 2013, its capacity increased by 38% to a running total of 139 GW worldwide [3]. By far, the most prevalent material for solar cells is crystalline silicon. But thin film PV 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 has 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 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].

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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 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, whilst 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 Fig. 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 the 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 reconstructions that have been proposed, namely the (2×1) and the $c(2\times2)$, 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 $c(2\times2)$ dimerisation within our description.

Illustrations of the four different surfaces used in the impact simulations are shown in Fig. 2. Circles and diamonds represent the two different species, and the 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, with a total of 864 atoms, for the (100) surface systems; and 6 double-layers of atoms, with a 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 is usually done at room temperature. Thus in our impact simulations, the temperature is set to be at 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 a velocity perpendicular to the surface, which is equivalent to being 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 Fig. 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 reach a metastable state. We then relax the system and analyse 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 a total of 48 cases. For each of these cases, we performed more than 1000 impact

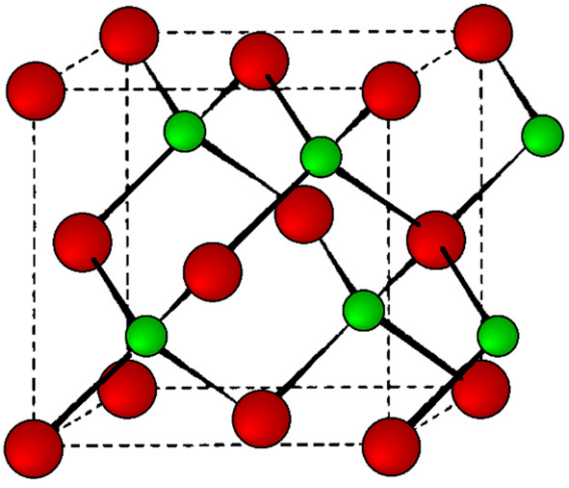

Fig. 1. Zinc-blende structure. Red bigger spheres represent the Te atoms and green smaller spheres the Cd atoms.

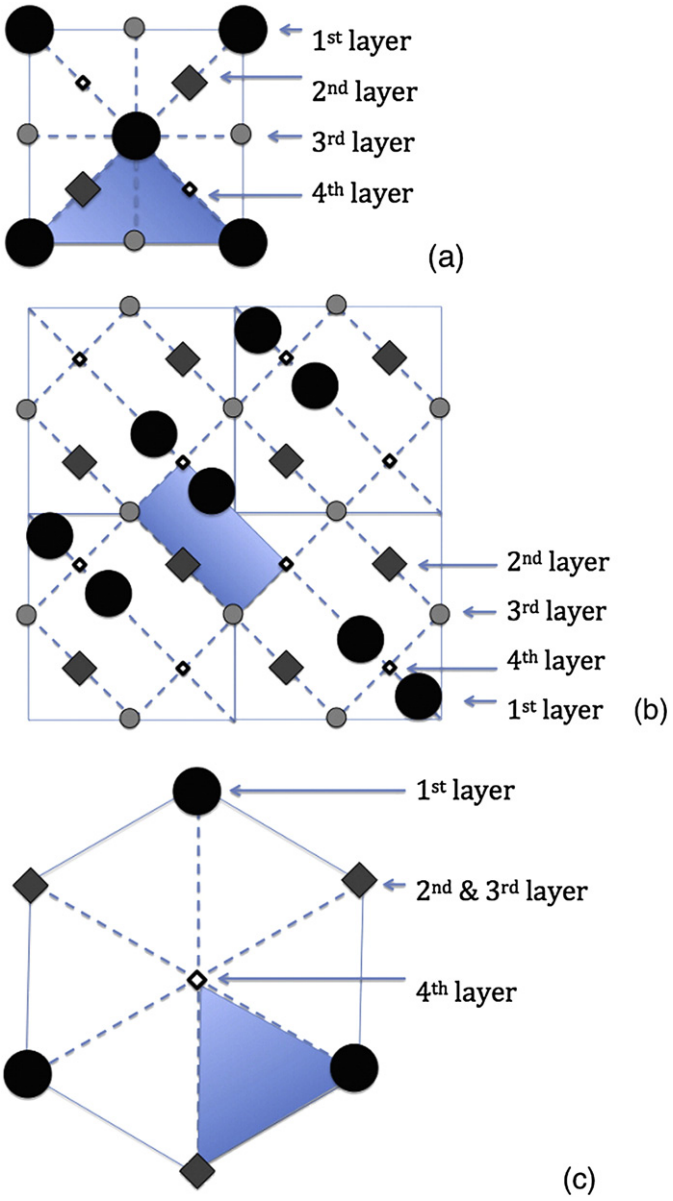

Fig. 2. Illustration of different surfaces used in the impact simulations. These graphs are top views of the first 4 layers on the CdTe surfaces. Circles and diamonds represent the two different species. Sizes represent the different layers. Shaded triangle or rectangle areas are the smallest repeatable regions on the surface. (a) (100) surface, (b) dimerised (100) surface, and (c) (111) surface.