Effect of substrate orientation on CdS homoepitaxy by molecular dynamics

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1. Abstract

CdS homoepitaxy growth was performed by molecular dynamics using different substrate orientations and structures in order to analyze the CdS crystallinity. As anticipated from thermodynamics of homoepitaxy, highly crystalline films with only point defects were obtained on substrates with rectangular surface geometries, including $[11\bar{2}]$ zinc blende (ZB), $[10\bar{1}0]$ wurtzite (WZ), $[11\bar{2}0]$ WZ, $[110]$ ZB, $[010]$ ZB, and $\left[\frac{1}{10}1\frac{1}{10}\right]$ ZB. In contrast, films grown on substrates with hexagonal surface geometries, corresponding to the $[0001]$ WZ and $[111]$ ZB growth directions, showed structures with a large number of defects including; anti-sites, vacancies, stacking faults, twinning, and polytypism. WZ and ZB transitions and grain boundaries are identified using a lattice identification algorithm and represented graphically in a structural map. A dislocation analysis was performed to detect, identify, and quantify linear defects within the atomistic data. Systematic simulations using different temperatures, deposition rates, and substrate polarities were performed to analyze the trends of dislocation densities on $[0001]$ WZ direction and showed persistent polytypism. The polytypism observed in the films grown on the substrates with hexagonal surface geometry is attributed to the similar formation energies of the WZ and ZB phases.

Keywords: A1. Molecular dynamics; A3. Homoepitaxy growth; A1. Defects; A2. Single crystal growth; B1. Cadmium sulfide.

2. Introduction

Cadmium sulfide (CdS) is a II-VI semiconductor material widely used in photovoltaic solar cells [1, 2] due to its direct band gap of 2.48 eV and absorption coefficient of $4 \times 10^6 \text{ m}^{-1}$ (at 500 nm) [3]. Additionally, CdS nanowires [4] and quantum dots [5] have attracted much attention for optical and electronic applications such as: light-emitting diodes [6], photodetectors [7], lasers [8], waveguides [9], logic circuits [10], and transistors [11]. Due to the potential of CdS to be used as a building block in future electronics, a variety of synthesis and deposition techniques have been investigated including: metal-organic chemical vapor deposition [12], physical vapor deposition (PVD) [4], electrodeposition [13], thermal evaporation [14], electrochemical synthesis [15], close space sublimation [16], and chemical bath deposition (CBD) [17].

CdS is stable in the wurtzite (WZ) and cubic zinc blende (ZB) crystal structures [18]. ZB and WZ CdS nanostructures have been reported to grow along different orientations with varying degree of crystallinity. A distinction in the degree of crystallinity emerges depending on the polarity and surface geometry. In particular, growths on polar surfaces with hexagonal geometry do not always result in highly crystalline [12], [19], [20] structures. For example, Ouyang, et al. reported that chemical deposition of CdS nanorods grown along $\langle 0001 \rangle$ WZ direction were defected with stacking faults (SF), exhibiting polytypism with a mixture of ZB and WZ phases [21] similar to previous reports [22], [23], [24]. Along the ZB polar $\langle 111 \rangle$ orientation, CdS quantum dots deposited via chemical co-precipitation were reported to contain SF, twinning, and polytypism by Kumar, *et al.* [5].

Strikingly, growths reported on surfaces with rectangular atomic surface geometry seem to indicate only highly crystalline structures. For example, along the $[10\bar{1}0]$ and $[11\bar{2}0]$ directions, single crystal

growth of WZ nanocrystals have been reported by Berrelet, *et al.* [25] and Ma, *et al.* [26] via chemical vapor deposition (CVD). These works indicate that the geometry of the CdS surface has a strong influence on the crystallinity of the overgrown homoepitaxial CdS; however a systematic study of this influence is lacking. In this work, the homoepitaxial growth of CdS along different orientations was simulated via high fidelity molecular dynamics (MD). CdS was deposited on WZ and ZB CdS substrates with different crystal orientations. Thereafter the resultant structures were analyzed to detect, identify, and quantify linear defects and their dependence on surface geometry. Lastly, simulated growths at different deposition conditions were employed to study their influence in film crystallinity by observing dislocation density trends.

3. MD simulation details

A total of 8 substrates with different structures and surface orientations were created. Two of them had polar hexagonal surface symmetries corresponding to the [0001] WZ and [111] ZB growth directions. The other six substrates had polar and non-polar rectangular surface symmetries corresponding to the following growth directions: $[10\bar{1}0]$ WZ, $[11\bar{2}0]$ WZ, $[110]$ ZB, $[010]$ ZB, and $[\frac{1}{10}1\frac{1}{10}]$ ZB (equivalent to a $[100]$ ZB tilted by $\sim 8^\circ$ representing a miscut). The simulations were performed with the Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code [27] using the Stillinger-Weber potential developed in ref. [28]. The lattice parameters were $a=4.12597\text{\AA}$ and $c=6.73768\text{\AA}$ for the WZ substrates and $a=5.8350\text{\AA}$ for the ZB substrates. Due to limited computational resources, a fast deposition rate of $\sim 0.48\text{ nm/ns}$ was utilized to grow enough material for the analysis within tractable nanosecond windows. However, the effect of unrealistically high deposition rate is mitigated by using a high temperature of 1200 K to accelerate the dynamics of the growth. On the other hand, we emphasize that the objective of the MD studies is to show qualitative trends that agree with experimental results as a way to gain insights into growth mechanisms. The Nose-Hoover [29] algorithm was used to approximate isothermal growth conditions. During deposition, individual Cd and S atoms are randomly added at equal frequencies so that over time they give a 1:1 ratio of Cd to S atoms. Free boundary condition was employed in the growth direction and periodic boundary conditions in the orthogonal directions. The position of the atoms within the bottom two monolayers was fixed throughout each of the simulations to prevent crystal drift due to adatom momentum transfer. Following deposition, the film and substrate were subjected to a three step post-deposition treatment simulation. No more adatoms were added during this treatment. The first step consisted of an annealing stage in which the samples were heated at the deposition temperature for $\sim 8\text{ ns}$ in order to provide the system time and energy to find a stable configuration. During the second step the system temperature was ramped down from the deposition temperature towards 50 K over a period of $\sim 8\text{ ns}$. The third step involved minimizing the energy of the system (to approximate 0 K conditions). The last two steps reduce thermal effects (such as atomic vibration) to improve the clarity of the data and increase the accuracy of the lattice structure and defect analysis algorithms.

4. Results and discussions

Atomistic visualizations of the eight simulated CdS homoepitaxial growths are presented in Figures 1 and 2, which were rendered using the OVITO software tool [30]. Figure 1 contains the CdS grown on the six nonpolar surfaces with rectangular symmetry which include: $[10\bar{1}0]$ WZ, $[11\bar{2}0]$ WZ, $[110]$ ZB, $[010]$ ZB, $[\frac{1}{10}1\frac{1}{10}]$ ZB, and $[11\bar{2}]$ ZB. In each case, an atomic icon representative of the surface geometry is provided as a guide. With one exception, all the nanostructures grown on the nonpolar surfaces with rectangular symmetry showed a high degree of crystallinity with only point defects being present in the form of anti-sites and vacancies; no dislocations were observed. The exception was $[11\bar{2}]$ ZB; in this orientation a low density of stacking faults was observed in addition to point defects. However no twinning or polytypism were found. These results are in good agreement with experimental observations reported in the literature for rectangular surfaces. For example, growth

in $[10\bar{1}0]$ WZ and $[11\bar{2}0]$ WZ orientations have been experimentally shown to result in single crystals [25] [26].

An additional simulation was performed which uses a reconstructed (010)-(2x1) ZB surface. The simulated growth was similar to the non-reconstructed (010) ZB surface. Since these simulations use Newton's law and interatomic potentials, the reconstructed surface is always relaxed to the lattice structure when it is buried into the bulk. Similar phenomenon has been observed experimentally [31].

Growth on two polar surfaces with hexagonal symmetry, (0001) WZ and (111) ZB, showed a large number of defects including: anti-sites, vacancies, stacking faults, twinning, and polytypism (existence of multiple phases). Atomistic visualizations of the MD simulated growths are shown in Figure 2 where twinning, stacking faults, and ZB and WZ domains are marked in red. In order to highlight the ZB and WZ domains and corresponding grain boundaries, a structural analysis was performed as shown in Figure 3 using the common neighbor analysis algorithm for diamond (ZB case) and hexagonal diamond (WZ case) lattices included within OVITO [30]. In Figure 3, the atoms are color coded in order to more easily identify the different crystal domains. Red atoms indicate the WZ structure whereas blue atoms correspond to ZB. Atoms that were not recognized to be in either WZ or ZB structure are shown in yellow. Therefore, the yellow atoms identify grain boundaries and possibly dislocations. Plane and cross-sectional view images are provided for each simulated growth on the $[0001]$ WZ and $[111]$ ZB oriented substrates. The plane view images are located at ~ 80 Å and ~ 100 Å from the bottom of the substrate, for $[0001]$ WZ and $[111]$ ZB respectively, and show a quasi-hexagonal network of grain boundaries connecting WZ and ZB domains as typically observed in polycrystalline films [32]. The cross-sectional images showed that the domain boundaries are typically normal or with some angle, between 20° to 35° , to the direction of growth. Both growths showed similar polytypism with a significant number of WZ and ZB domains. Similar CdS polytypism has been reported experimentally by Ouyang [21] and Kumar [5] in nanowires and quantum dots.

Table 1 summarizes and compares the results of this work with results reported for nanostructures in the literature. Even though the nanostructure formation has other factors that are not considered in our simulations, there is a similar trend of the defect types with respect to growth directions. This indicates that the substrate orientation is an important factor for single crystal growth.

The dislocations in the simulated growths on the $[0001]$ WZ and $[111]$ ZB substrates were analyzed using a dislocation extraction algorithm for ZB [33] [34] and WZ [35] lattices. Figure 4 shows color coded line representations of the dislocation networks. The dislocations were classified according to their ZB or WZ Burger's vector family. Seven different Burgers vectors were identified in the ZB and WZ families. The Burger's vectors are listed and color coded in the legends of Figure 4. For clarity, separate images are provided for the ZB and WZ families of dislocations. Overall the dislocations are uniformly distributed within the overgrowths but no dislocations were detected in the substrates. By far the most prevalent dislocations are the Shockley partials with a Burger's vector of $1/6 \langle 112 \rangle$. Similar dislocations were identified experimentally by Li [36] in ZB CdTe. Full dislocations with a Burger's vector of $\langle 0001 \rangle$ are also present with significant density, as shown in Figures 4 (e) to (h). Other dislocations as listed in the legend were also present in lower density.

These results indicate a general tendency in which homoepitaxy growth of CdS on substrate orientations with rectangular surface geometry lead to single crystal films. In contrast, growth on hexagonal geometry resulted in polytypism. In order to investigate whether this general tendency persists or the results could be attributed to other factors, growth simulations were performed at various temperatures and deposition rates on a Cd-terminated CdS $[0001]$ substrate. Figure 5(a) plots the dislocation density at different temperatures. Here the dislocation density is defined as the summation of the total dislocation line length divided by the heterostructure's volume. While the dislocation density decreased with increasing temperature, polytypism persisted. Similarly Figure 5(b) shows that the deposition rate affected the dislocation density (at the higher temperature), but the dislocation density was not reduced to zero. Finally, in order to observe the effect of substrate termination, growth was simulated on a S-terminated CdS $[000\bar{1}]$ substrate as shown in the inset of Figure 5(b). In general the dislocation density was higher on the S-terminated substrate with polytypism

persisting. The simulation results are in good agreement with literature data and indicate the same dependence of polytypism on substrate orientation. The existence of polytypism in the films grown on the hexagonal substrates is attributed to the small difference in the structural energy associated with the WZ and ZB phases [18]. Since both WZ and ZB phases contain the exact same hexagonal surface geometry and similar structural energy, it is equally favorable to nucleate either structure.

5. Conclusions

MD simulations of CdS homoepitaxial growth were performed using different substrates orientations. The substrates can be subdivided in two groups: non-polar rectangular and polar hexagonal surface geometries. In general the rectangular cases showed highly crystalline films with only point defects. The exception was the growth along $[11\bar{2}]$ which showed a low density of stacking faults. In contrast the hexagonal cases displayed highly defected structures with presence of SF, twinning, and polytypism. A structural analysis was performed to identify the WZ and ZB domains and corresponding grain boundaries for the hexagonal growth. The dislocation analysis indicated that the most predominant dislocations are Shockley partials with a Burger's vector of $1/6 \langle 112 \rangle$ and full dislocations with a Burger's vector of $\langle 0001 \rangle$ for the ZB and WZ families respectively. In general the simulation results agree well with experimental data reported in literature predicting defective and single crystal growths on hexagonal and rectangular surfaces respectively. Lastly, different deposition conditions were explored to improve the film's crystal quality for $[0001]$ WZ case. The simulations showed that films grown at higher temperatures contained lower dislocation length densities. Low deposition rates and $[0001]$ substrate polarity also decreased the film's dislocation length densities, although these effects were only observed at high deposition temperatures. Polytypism observed in the films grown on the substrates with hexagonal surface geometry is attributed to the similar formation energies of the WZ and ZB phases.

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7. References

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Figures

Figure 1. Atomistic visualizations of MD simulations for CdS homoepitaxial growth along (a) $[10\bar{1}0]$ WZ, (b) $[11\bar{2}0]$ WZ, (c) $[110]$ ZB, (d) $[010]$ ZB, (e) $\left[\frac{1}{10} \frac{1}{10} \frac{1}{10} \right]$ ZB and (f) $[11\bar{2}]$ ZB, directions. Shaded regions represent the initial substrate.

Figure 2. Atomistic visualizations of MD simulations for CdS homoepitaxial growth along (a) $[0001]$ WZ (b) $[111]$ ZB, directions. Shaded regions represent the initial substrate.

Figure 3. Structural maps of CdS homoepitaxial growths on hexagonal surfaces. (a) Top and (b) cross-sectional views of CdS grown on [0001] WZ. (c) Top and (d) cross-sectional views of CdS grown on [111] ZB, shaded regions represent the initial substrate.

Figure 4. Cross sectional (left column) and top view (right column) visualization of dislocations in the films grown on the [0001] WZ and [111] ZB CdS substrates are shown. The images are grouped according to either ZB or WZ Burger's vector types as indicated by the color legends. (a), (b), (e) and (f) are dislocations in the CdS grown on [0001]CdS. (c), (d), (g), and (h) are dislocations in the CdS grown on [111]CdS.

Figure 5. Dislocation length density for (a) different temperatures at constant deposition rate and (b) different deposition rates at 1200 K and 2000 K. The inset is the dislocation length density for different polarities: [0001] and [000 $\bar{1}$] are Cd and S terminated respectively, at 1200 K and 2000 K.

Table 1. Comparison of our simulated results to experimental results reported in the literature.

Growth direction	Deposition Method	Crystallinity	Structures	Defect type	Ref
WZ [0001]	MD Simulations	Polycrystalline		SF, Twinning, polytypism	This work
	Electrochemical	Polycrystalline	Nanowires	Grain boundaries	[22]
	Chemical Bath Deposition	Polycrystalline	Nanorods	SF, polytypism	[21]
	Chemical Bath Deposition	Polycrystalline	Nanorods	SF, polytypism	[24]
	Chemical Bath Deposition	Polycrystalline		Screw, Hirth dislocation	[23]
	MOCVD	Single crystal	Nanorods, Nanowires		[12]
	Thermal evaporation	Single crystal	Nanorods, nanoneedles		[19]
ZB [111]	Thermal evaporation	Single crystal	Nanobelts		[20]
	MD Simulations	Polycrystalline		SF, Twinning, polytypism	This work
ZB [111]	chemical co-precipitation	Polycrystalline	Quantum Dots	SF, Twinning, polytypism	[5]
WZ [10$\bar{1}$0]	MD Simulations	Single crystal			This work
	CVD	Single crystal	Nanowires		[25]
WZ [11$\bar{2}$0]	MD Simulations	Single crystal			This work
	CVD	Single crystal	Nanowires		[26]
	CVD	Single crystal	Nanowires		[25]
ZB [110]	MD Simulations	Single crystal			This work
ZB [010]	MD Simulations	Single crystal			This work
ZB [$\frac{1}{10}$ 1 $\frac{1}{10}$]	MD Simulations	Single crystal			This work
ZB [112]	MD Simulations	Single-crystal		SF	This work