DEFECT ANALYSIS OF MBE REACTOR GROWN HgCdTe ON GaAs, GaSb, CZT SUBSTRATES THROUGH TNL-EPIGROW SIMULATOR

P. K. Saxena, P. Srivastava, A.Srivastava
Tech Next Lab Pvt Ltd,
Lucknow - 226003, India,
Email: a.saxena@technextlab.com,
Tel: (011) 522 404 1565, (011) 983 915 1284

Abstract

The paper reviews systematically the progress of HgCdTe materials grown via molecular-beam epitaxy (MBE) for IR detection in terms of atomistic approach including material physics, structure design, and fabrication. The state of the art of epitaxy process of $Hg_{1-x}Cd_xTe$ films over GaAs, GaSb, CdZnTe substrates by MBE (Molecular Beam Epitaxy) from an experimental and modeling perspective is analyzed. The most advanced kMC (kinetic Monte Carlo) MBE epitaxy model dependent on reactor geometry implemented in TNL-EpiGrow is benchmarked against experimental data. The efforts are carried out to reproduce the MBE reactor based epitaxial growth of $Hg_{1-x}Cd_xTe$ over GaAs, GaSb, CdZnTe substrates through TNL-EpiGrow^{TM} simulator at atomistic scale. TNL-EpiGrow^{TM} simulator is based on randomness and provide real time deposition environment of MBE reactor process. It is possible to extract the properties associated with of each and every atom involve in adsorb, diffusion and desorption processes over the lattice. It provides flexibility to map the various types of defects generated during the growth process layer-by-layer and island-mode. TNL-EpiGrow^{TM} Simulator provides an innovative and cost effective solution for MBE, CVD and MOCVD reactors including number of semiconductors based epitaxial growth processes with capabilities to distinguish the types of defects with its position on lattice, strain mapping layer-by-layer, surface roughness, lattice parameter etc. The vacancies and dislocation densities are reported here for three cases. The output results reveal that under similar conditions of MBE growth of $Hg_{1-x}Cd_xTe$, CdZnTe is the best suited option as compare to GaAs and GaSb substrates [2].

Numerical Technique

The fabrication of high performance HgCdTe infrared focal plane arrays (IRFPAs) requires high crystalline quality MCT films. The well known $Cd_{1-x}Zn_xTe$ (CZT) substrates with x=0.04 is the best suited substrates. However, the small wafer size, high cost, relatively poor quality, low mechanical strength, and low thermal conductivity properties of CZT substrate offer serious limitations. Therefore, alternative substrates are trialed in order to overcome the limitations offered by CZT substrate. In present work GaAs, GaSb and CZT are chosen for growth comparison of MCT to study growth behavior and achieve the deeper insight of MBE reactor process during growth. [1]. The kinetic Monte Carlo (kMC) technique including adsoption, diffusion and desorption processes under specified chamber pressure, temperature and substrate temperature is used for off-lattice MCT growth. Details of numerical method used here is given in our previous publications refer to reference [2-3].

To evaluate the growth morphology of MCT over GaAs, GaSb and CZT substrates under MBE reactor environment several experiments have run. The MBE reactor input conditions given in Table I. To reduce the defects densities, CdTe buffer layer is deposited over GaAs, GaSb and CZT substrates before the deposition of MCT layers. It is well known that CZT is well lattice matched substrate for MCT growth and no need for buffer layer deposition; however it also suffers with defects generation. The attempt is to study the microscopic behaviour of MCT monolayer deposition over the CdTe buffer layer, just assuming that Hg atoms diffuse into CdTe buffer and provide more stable atomic configuration for MCT growth. All results reported here are reproducible under similar input conditions.

Results & Discussion

TNL-EpiGrow^{TM} simulator shows great promise for epitaxial growth of II-VI and III-V materials based on various reactors geometries with potential capabilities to understand the underneath atomistic processes associated with each and every atom inside the MBE reactor [3-4]. The two steps growth processes i.e. CdTe buffer deposition followed by MCT deposition for each substrate case for 50 s each respectively over the 30x30 unitcell^2 of rectangular substrate's size. The input conditions are given in Table I. However, the atomistic arrangement of atoms of deposited CdTe buffer layers over GaAs followed by deposited $Hg_{1-x}Cd_xTe$ atoms are only depicted in Fig. 1.

$$1\,unitcell\ \times 1\,unitcell = lattice\ constant^2\ \dot{A}^2$$

Table I: Input growth conditions

Subst rate	Lattice Constant	Substrate (unit cells)	Substrate Temp.	Effusion Cell Cd	Effusion Cell Hg	Effusion Cell Te	Time	Process Steps
GaAs	5.65 A	30x30 A^2	200°C	200°C	35°C	200°C	50s each Step	2 Steps; CdTe & MCT
GaSb	6.095 A	30x30 A^2						2 Steps; CdTe & MCT
CZT	6.468 A	30x30 A^2						2 Steps; CdTe & MCT

The comparison of extracted output data for the samples (GaAs/CdTe/HgCdTe, GaSb/CdTe/HgCdTe, CdZnTe/CdTe/HgCdTe) under similar growth conditions are depicted in Table II. In all the cases, the MCT is grown over the CdTe buffer layer however the difference in total number of deposited atoms in each case is attributed due to lattice mismatch of CdTe buffer layer to the GaAs, GaSb and CdZnTe substrates. The extracted lattice parameters of grown CdTe and MCT layers for each substrate case are tabulated in Table II. It is clearly reflected from Table II that the minimum defects density is obtained for the case where CZT substrate is used for epitaxial growth of MCT. The total number of vacancies and dislocation density extracted here for each case follow the similar trend of minimum values for CZT substrate against the GaAs and GaSb substrates.

The dislocation density in each monolayer is shown in Fig.2, Fig.3 and Fig.4 for GaAs, GaSb and CZT substrates respectively. For each substrate case the thickness of substrate is taken 9 monolayers over which atomistic deposition occurs depending upon the incoming flux of atoms. The algorithms of kMC method is designed such a way that each atom search itself the sitting position on to the lattice. The layer by layer dislocation density curves depicts the deposition process for each substrate case. Initially the dislocations are less prominent in each substrate case as the atoms try to occupy the beneath layer bonding position. Moving upward in growth direction the strain is increased and we have observed large dislocation density for CdTe buffer layers deposition. There are flexibility to map strain layer-by-layer and surface roughness in TNL-EpiGrow simulator along with extraction capabilities to get the information of each deposited atoms along with content of each material contents. The mole fraction of MCT is obtained by tracing number of atoms of Hg, Cd and Te.

Table II: Extracted Output Parameters

Parameters		**GaAs/CdTe/ HgCdTe**		**GaSb/CdTe/HgCdTe**		**CdZnTe/CdTe/HgCdTe**	
		CdTe	**HgCdTe**	**CdTe**	**HgCdTe**	**CdTe**	**HgCdTe**
Lattice parameter (^{o}A)	**a**	5.9594	5.9713	6.4495	6.9783	6.1489	6.4765
	b	5.9662	6.6454	6.3471	6.6695	6.0663	6.0995
	c	6.6470	6.4843	6.6167	6.4108	6.1512	5.7141
Total deposited atoms		604755		696705		776608	
Dislocation Density (/cm^2) (Ist / IInd Growth Steps)		CdTe$_{dis}$ = 6.78x10^{11} HgCdTe$_{dis}$ = 2.32x10^{12}		CdTe$_{dis}$ = 5.88x10^{11} HgCdTe$_{dis}$ = 2.13x10^{12}		CdTe$_{dis}$ = 1.69x10^{11} HgCdTe$_{dis}$ = 1.92x10^{12}	
Total Vacancies		20%		19%		18%	

Conclusions

The MBE reactor based MCT deposition process is replicate at atomistic scale. The growth rates are matched with the experimental growth rates. The output results suggest CZT substrate is ideal for MCT deposition whereas depends upon requirement one may chose bigger substrates i.e. GaAs and GaSb for MCT growth. There is still big room to optimize and improve the output results in terms to further reduce the defect densities. TNL-EpiGrow^{TM} simulator is capable to expedite the MBE, CVD, Lateral & vertical MOCVD reactors based epitaxial processes development by reducing cost and manpower consumptions. The MBE reactor process can be optimized to achieve high quality MCT films for MW & LW IR detection applications.

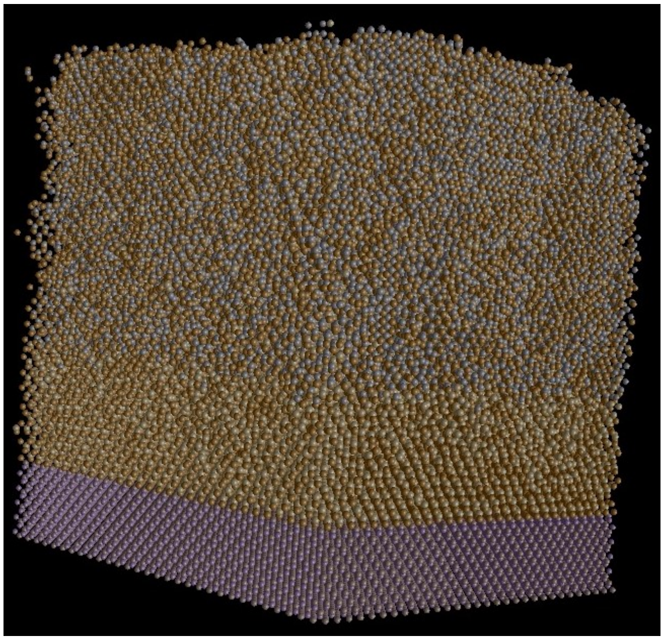

Fig. 1a: Atomistic growth of CdTe followed by MCT on GaAs substrate

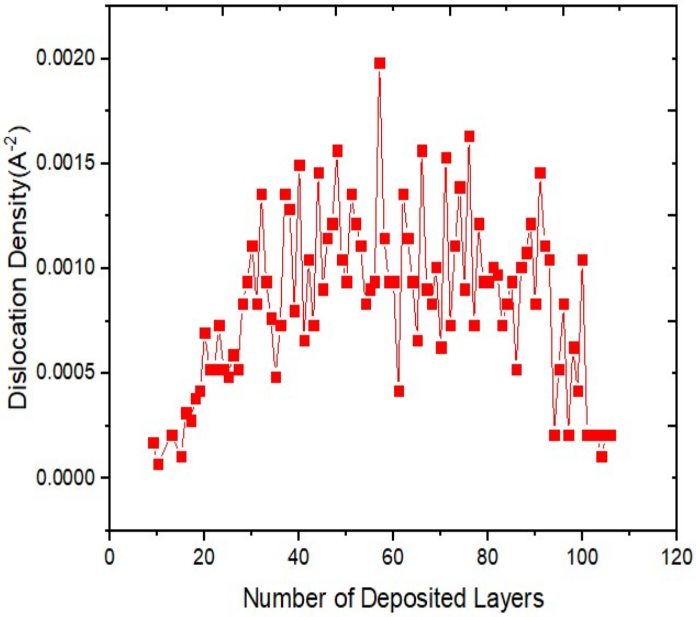

Fig.2 Dislocation Density with deposited layers over GaAs substrate

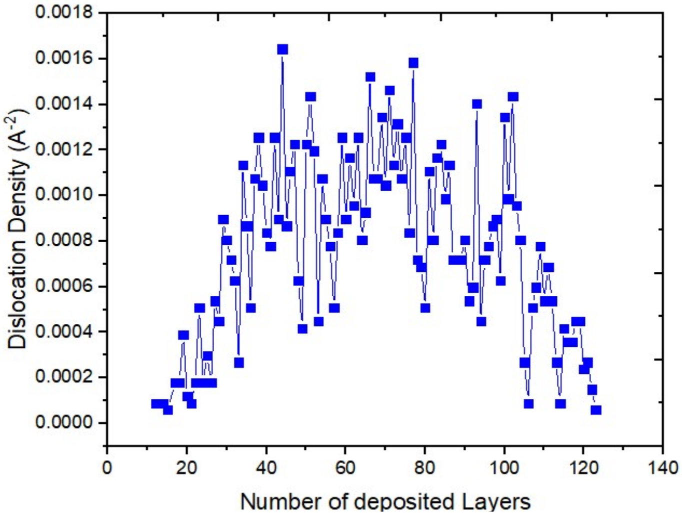

Fig.3 Dislocation Density with deposited layers over GaSb substrate

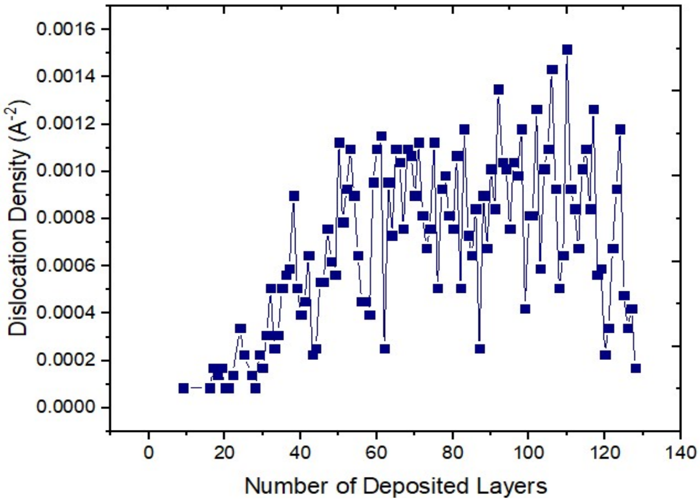

Fig.4 Dislocation Density with deposited layers over CdZnTe substrate

References

1. R. Gu, et. al., “MBE growth of HgCdTe on GaSb substrates for application in next generation infrared detectors”, *Journal of Crystal Growth* **468** (2017) 216-219.
2. User Manual, TNL-EpiGrow Simulator, (2023), Tech Next Lab Private Limited, http:www.technextlab.com.
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