Defects Analysis of MBE growth of HgCdTe on GaAs, GaSb, CZT substrates through Atomistic TNL-EpiGrow Simulator

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The fabrication of high performance HgCdTe (MCT) infrared focal plane arrays (IRFPAs) require nearly lattice matched substrate. The $Cd_{1-x}Zn_xTe$ (CZT) substrates with x=0.04 is the best suited substrates with negligible lattice mismatch with MCT. However, the small wafer size, high cost, relatively poor quality, low mechanical strength, and low thermal conductivity offer serious limitations. Therefore, alternative substrates are trialed by researchers in recent years in order to overcome the limitations offered by CZT. Main alternative substrates, (Si, Ge, GaAs and GaSb) have been studied in details for the mid-wave infrared detection applications. However, the industry trend towards development of smaller pixel size and high sensitivity detector arrays requires high quality MCT film. The Stress due to lattice and thermal mismatch in epitaxially-grown samples leads to mismatch defects e.g. dislocations act as effective recombination centers and degrade yield and electro-optical properties of the device [1]. In present work, HgCdTe MBE epitaxial growth on various substrates using TNL-EpiGrow™ Simulator is carried out under same input conditions given in Table I. The atomistic scale capabilities to extract the position of each and every atom on lattice provide flexibility to direct extract the dislocation densities and vacancies generated in each monolayer of each grown sample. TNL-EpiGrow™ Simulator provides an innovative and cost effective solution for MBE, CVD and MOCVD reactors based epitaxial growth with capabilities to distinguish type of defects with its position on lattice, strain mapping layer-by-layer, surface roughness, lattice parameter etc [2].

To evaluate the growth morphology of MCT over GaAs, GaSb and CZT substrates under MBE reactor environment several experiments have run. The innovative deposition technique used for epitaxial deposition process is detailed in reference [2-3]. The comparison of extracted output data for the samples grown (GaAs/CdTe/HgCdTe, GaSb/CdTe/HgCdTe, CdZnTe/CdTe/HgCdTe) are depicted in Table II. It is clearly reflected that the minimized defects density is obtained for the case where CZT substrate is used for epi-growth of MCT. The total number of vacancies also follows the similar trend of dislocation density. In all cases the MCT is grown over CdTe layer, however, the difference in total number of atom deposited in each case is attributed due to selection of different substrates. The atomistic deposited of CdTe over GaAs followed by $Hg_{1-x}Cd_xTe$ (x=0.34) is depicted in Fig. 1. TNL-EpiGrow™ 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 each and every atomistic processes inside reactor [3-4]. TNL-EpiGrow™ simulator helps to expedite the technology developments 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.

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.
3. P. K. Saxena et al. An innovative approach for controlled epitaxial growth of GaAs in real MOCVD reactor environment, *Journal of Alloys and Compounds* **809** (2019) 151752.
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Table I: Input growth conditions

Sub-strate	Substrate (unit cells)	Substrate Temp.	Effusion Cell Cd	Effusion Cell Hg	Effusion Te	Time	Process Steps
GaAs	30x30 A^2	800°C	200°C	35°C	200°C	50s for each Step	2 Steps; CdTe & MCT
GaSb	30x30 A^2						2 Steps; CdTe & MCT
CZT	30x30 A^2						2 Steps; CdTe & MCT

Table II: Extracted Output Parameters

Parameters		GaAs/CdTe/ HgCdTe		GaSb/CdTe/HgCdTe		CdZnTe/CdTe/HgCdTe	
Lattice parameter (°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 (/cm²) (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%	

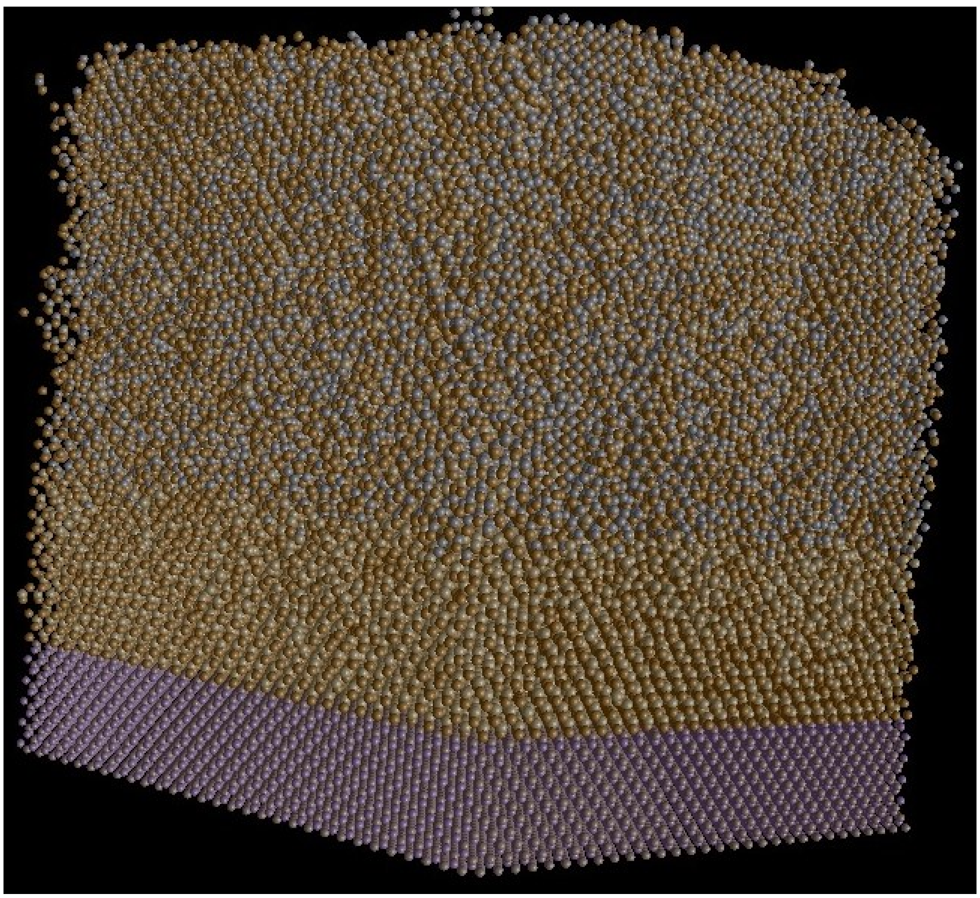

Fig. 1: Atomistic growth of CdTe followed by MCT on GaAs substrate