Comparative study of thermal mismatch effects in CdTe/Si, CdTe/Ge, and CdTe/GaAs composite structures

R.N. Jacobs,[1,4] L.A. Almeida,[1] J. Markunas,[1] J. Pellegrino,[1] M. Groenert,[1]
M. Jaime-Vasquez,[1] N. Mahadik,[2] C. Andrews,[2] S.B. Qadri,[2] T. Lee,[3] and M. Kim.[3]

1- U.S. Army RDECOM, CERDEC Night Vision and Electronic Sensors Directorate, Fort Belvoir, VA 22060.
2- U. S. Naval Research Laboratory, Washington, DC 20375.
3- Department of Electrical Engineering, University of Texas, Dallas, TX 75083.
4- Email: info@nvl.army.mil

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Abstract

The rising interest in low-cost, large-area substrates for high performance HgCdTe infrared detectors has fueled research efforts in heteroepitaxial structures including CdTe/Si(211), CdTe/Ge(211), and CdTe/GaAs(211)B. The enormous lattice-mismatch inherent in these systems ranges from -14.6 to -19.3%, and is responsible for large dislocation densities and other defects which may limit detector performance. Though greater differences exist with regards to thermal mismatch (13.8 to -92%), the effects have not been well documented. Here, we investigate the relative contributions of lattice and thermal mismatch on CdTe film characteristics including dislocation density and residual stress. Based on x-ray techniques we consistently measure a tensile residual stress for CdTe/Si, but observe compressive residual stresses for CdTe/Ge and CdTe/GaAs. Consistent with theoretically predicted stress levels, the experimental data implies the dominance of thermal mismatch in the residual film stress characteristics. These findings may hold significance for the design and fabrication of large-format HgCdTe infrared focal plane arrays.

INTRODUCTION

CdTe/Si composite substrates potentially provide a low-cost, large-area alternative to CdZnTe for high performance HgCdTe based short and mid-wavelength infrared detectors. However similar successes have not yet been realized for long-wavelength ($\geq$ 9.5 μm) IR detection. This is largely due to the enormous lattice mismatch which is responsible for structural defects that reduce device performance.[1-3] On the other hand, materials issues including thermal expansion mismatch could also have an impact on dislocation densities or other important defects in CdTe/Si composite substrates. At present, little work has been performed to directly examine the impact of thermal mismatch effects in this epitaxial system.

CdTe buffered Ge(211) and GaAs(211)B composite substrates have also been examined. Table I provides a comparison of these substrate materials for HgCdTe heteropitaxy. Recent data suggests these substrates can be used for HgCdTe IR detectors with quality similar to that obtained using Si.[4-5] In fact Ge could be a better option due to better lattice and thermal expansion (α) matching and compatibility with Si processing equipment. An almost equally better lattice and thermal expansion match (to CdTe buffer layers) can be achieved through use of GaAs substrates. Furthermore, GaAs provides a potential benefit due to its zinc-blend structure and thus naturally polar (211) surface, on which achieving uniform B-phase CdTe(211) may be more straightforward.

TABLE I
SELECTED SUBSTRATES FOR HgCdTe/CdTe EPITAXY

Subst.	Cost ($/cm^2)	Max avail. size (cm^2)	Structure	Lattice Param. (Å)	Misfit (w/ CdTe)	α(10^{-6}/C)	α-mismatch (w/CdTe)
CdZnTe	~200	~50	ZB	6.48	-	5.0	-
Si	~1	~700	Diamond	5.43	-19.3%	2.6	-92.3%
Ge	~8	~180	Diamond	5.66	-14.6%	5.8	13.8%
GaAs	~5	~180	ZB	5.65	-14.6%	5.8	13.8%

Here, we investigate the effects of thermal expansion in MBE grown CdTe/Si(211), CdTe/Ge(211), and CdTe/GaAs(211)B heteroepitaxial structures. Based on known material properties, residual thin film stresses were predicted with a focus on the individual contributions from lattice and thermal-mismatch. We perform experimental measurements of residual film stress based on x-ray diffraction and profilometry techniques. Out-of-plane thermal expansion coefficients are obtained via temperature dependent lattice parameter measurements. We also characterize thermally cycled substrates using defect decoration Etch Pit density (EPD), x-ray, Nomarski and transmission electron microscopy (TEM).

SUMMARY OF RESULTS

Table II shows a summary of CdTe growth characteristics for various samples. The best crystalline quality CdTe buffer layers have been obtained on Si(211)

TABLE II
FILM CHARACTERISTICS FOR SELECTED SAMPLES

Sample ID	Subst.	Growth Temp. (°C)	Annealing Temp (°C)	h_{CdTe} (μm)	RC-FWHM (arc-sec)	EPD (x10^6 cm^{-2})
C4077	Si	290	460	11.7	75	6.60
C5019	Si	290	N/A	7.84	140	-
C6037	Si	290	465	9.04	93	-
C6039	Si	290	465	11.7	83	-
C6040	Si	290	465	13.4	85	-
C6043	Si	290	465	16.0	78	-
C6045	Si	290	465	13.5	77	-
C6048	Si	290	N/A	7.4	147	12.7
C6051	Si	290	465	12.3	90	-
C6054	Si	290	465	13.0	89	-
C6058	Si	290	465	13.0	90	-
C6062	Si	290	465	11.7	117	-
C6063	Si	290	465	12.3	111	-
C7004	Si	290	N/A	8.8	190	29.2
C5024	Ge	260	N/A	7.4	180	32.3
C6046	Ge	250	N/A	7.4	129	12.8
C6056	Ge	250	450	9.4	124	22.6
C6059	Ge	250	430	11.9	114	23.8
C7006	Ge	250	N/A	8.6	202	31.7
C6060	GaAs	300	450	8.2	190	>50
C6064	GaAs	310	N/A	8.8	167	17.0
C7005	GaAs	310	N/A	9.2	190	25.0

substrates annealed at optimized temperatures. For annealed layers, state of the art values of the x-ray rocking curve-full width at half maximum (RC-FWHM) and etch pit density (EPD) are <100 arc-sec, and ~5 x 10^6 /cm^{-2}, respectively. Full optimization of our CdTe/Ge and CdTe/GaAs structures will require further fine-tuning of growth parameters. Note however that CdTe/Ge films of quality similar to CdTe/Si (RC-FWHM and EPD) have been obtained for un-annealed layers (samples C6048 and C6046). Given the large differences in thermal expansion coefficient α, for Ge and Si (see Table I), the data implies no measurable contribution of α-mismatch effects in crystallinity and dislocation density. Whether or not such a conclusion is premature, other potential effects of α-mismatch are worth investigating.

THEORETICAL RESIDUAL FILM STRESS

To predict the residual film stress for these epitaxial systems, we have employed a generalized approach[3] in which the lattice and thermal mismatch components are separated. The misfit stress is derived from a thickness dependent strain, such that initial (at the start of growth) and residual stresses $\sigma_{r\text{-}misf}$, can be calculated. The thermal component σ_α, is calculated from the difference in thermal expansion coefficients as the composite substrate is cooled from the growth temperature. The expressions include;

$$\sigma_{residual} = \sigma_{r-misf} + \sigma_\alpha \quad (1)$$

$$\sigma_{r-misf} = \frac{E\varepsilon_{misf}(h)}{1-\nu} \quad (2)$$

$$\sigma_\alpha = \frac{(\alpha_s - \alpha_f)(T - T_g)E_f}{1-\nu_f} \quad (3)$$

where:

$\sigma_{residual}$ = residual film stress
$\sigma_{r\text{-}misf}$ = residual misfit stress
σ_α = residual thermal stress
E = elastic modulus (averaged)
E_f = film elastic modulus
h = film thickness
ν = Poisson's ratio (averaged)
ν_f = Poisson's ratio (film)
T_g =Growth Temperature

A more detailed treatment is provided in the conference proceedings. The results of these calculations show that for all three epitaxial systems, the initial misfit stress (~10^5 MPa) is reduced to levels well below the thermal mismatch stress at the end of growth. Thus, thermal mismatch dominates the residual stress characteristics and positive values of $\sigma_{residual}$ are predicted for CdTe/Ge and CdTe/GaAs, while negative values are predicted for CdTe/Si.

EXPERIMENTAL RESIDUAL STRESS

Residual stress has been experimentally determined from radius of curvature measurements based on x-ray and profilometry techniques. Due to strain-induced bowing, Bragg peak positions will differ slightly at different points on the film surface. The angular positions of peak intensity determined during RC-FWHM mapping of the CdTe layer was used to generate a surface profile from which a radius of curvature is extracted. The change in radius, ΔR (before and after CdTe deposition) can then be used to measure the residual film stress from the Stoney formula,[6]

$$\sigma_{residual} = \frac{E_s h_s^2}{6\Delta R(1-\nu_s)h_f} \quad (4)$$

where h_f and h_s are the film and substrate thickness, respectively. In addition to x-ray techniques, profilometry was used to obtain radius of curvature and associated film stress for several samples. Figure 1 shows the residual film stress for samples listed in Table II, as determined by x-ray and profilometry techniques. The predicted residual stress for un-annealed samples (based on equations 1-3) is also plotted for comparison. The experimental and predicted data are in agreement in that the overall residual stress is tensile for CdTe/Si, but compressive for CdTe/Ge and CdTe/GaAs. The tensile stress measured for CdTe/Si is best explained by the positive $\Delta\sigma_\alpha$ exerted on the film during cool down. The opposite residual stresses observed here supports earlier assertions[3] that thermal mismatch (not lattice misfit) is in fact, the dominant stress mechanism after growth. Error bars associated with x-ray data are due to specified tolerances for substrate thickness (+/- 25 μm), while those associated with profilometry data are based on instrumental sensitivity. The limitations in measurement accuracy may make it impractical to compare absolute values of the stress levels

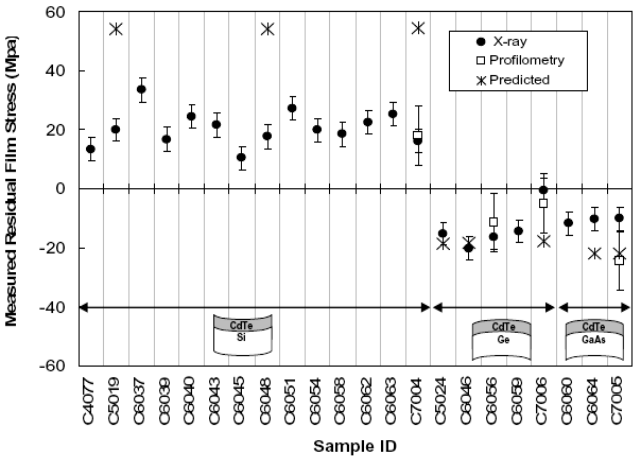

FIG 1. Residual film stress for CdTe/Si, CdTe/Ge, and CdTe/GaAs wafers (see equation 4) based on radius of curvature measurements by x-ray and profilometry techniques. Respective film characteristics were listed in Table II. Theoretically predicted values for un-annealed samples (based on equations 1-3) are also shown.

among the three epitaxial systems. On the other hand, the larger disparity between predicted and measured residual stress for CdTe/Si compared to CdTe/GaAs and CdTe/Ge, should not be overlooked. First, the fact that absolute values of the $\sigma_{residual}$ are fairly similar in all three systems, likely implies the layers are beyond elastic limits[7] and into the plastic flow regime. In that case the larger disparity in predicted and measured $\sigma_{residual}$ for CdTe/Si, implies greater plastic deformation in comparison to CdTe/Ge and CdTe/GaAs.

It should also be noted that the CdTe/Si samples shown in Figure 1 are for both optimized (annealed), and non-optimized growth runs. For example, x-ray RC-FWHM was 78 arc-sec for annealed sample C6043, and 147 arc-sec for non-annealed sample C6048. Such variations in epitaxial quality have not lead to significant differences in the observed film stress. This notion lends some credence to residual stress data obtained for CdTe/Ge and CdTe/GaAs, despite the samples being non-optimal.

THERMAL EXPANSION COEFFICIENT MEASUREMENT AND EFFECTS OF THERMAL CYCLING

We have also examined temperature dependent out-of-plane lattice parameter $a^{\perp}(T)$ via x-ray techniques, and studied effects of operational thermal cycling for selected samples. As the ambient temperature is increased. from room to 200 C, the overall change in film stress based on $a^{\perp}(T)$, are -24 MPa for CdTe/Si and ~2 MPa for CdTe/Ge. After cycling our samples between room and 77 K, we have not observed significant changes in dislocation density or x-ray RC-FWHM. Morphological changes in the films such as cracking were also not apparent. Cross-sectional TEM imaging and interface diffraction patterns failed to reveal microstructural differences between as-deposited and thermally cycled CdTe/Si samples.

CONCLUSIONS

The significance of thermal expansion matching in lattice mismatched composite structures including CdTe/Si, CdTe/Ge, and CdTe/GaAs, has been investigated from the standpoint of the structural properties. It does not appear that threading dislocation density and film crystallinity is strongly affected by α-mismatch. On the other hand, residual stress characteristics appear to be dominated by α-mismatch. Consistent with theory, tensile stresses were measured for CdTe/Si, while compressive stresses were measured for CdTe/Ge and CdTe/GaAs structures. We speculate that the larger disparity between predicted and measured stress data for CdTe/Si may indicate greater plastic deformation. For CdTe/Si and CdTe/Ge, temperature dependent out-of-plane-lattice measurements confirmed expected trends in the post-growth thermal mismatch strain.

Though our observations suggest greater plastic deformation in CdTe/Si composites, we have not yet observed evidence of thermal-cycling induced defects based on EPD, XRD, and TEM characterization. Nonetheless, we do not discount the possibility that subtle benefits may yet exist for Ge and GaAs over Si for CdTe buffers, and subsequent HgCdTe device layers.

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ACRONYMS

EPD: Etch Pit Density
RC-FWHM: rocking curve full width half max
XRD: X-ray Diffraction
N/A: No Annealing
TEM: Transmission electron microscopy