Multiscale Modelling of Curved Pixel Arrays

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I. INTRODUCTION

Large format infrared (IR) detector arrays that provide high image resolution over a wide field of view (WFOV), are of critical importance for both defense and civilian applications, for example surveillance, astronomy, and remote sensing. Reduction of pixel pitch has been aggressively pursued to increase the array format, and the pixel dimension is approaching a size comparable to the wavelength. While significant progress has been made to increase the resolution of IR focal plane arrays (FPA), a considerable effort is still required to design the optics needed to implement the camera. For applications where a WFOV is needed, the camera optics has to be designed to mitigate the optical aberrations that degrade illumination and resolution uniformity across the FPA. This is currently achieved by employing many optical elements to flatten the Petzval field curvature to match the footprint of the planar image sensor. As a result of the complex optics needed to achieve field flattening, and at the same time to minimize other aberrations, the size, weight, and cost of the entire camera increases considerably.

A potential solution to this problem is to curve the image sensor [1]. A curved pixel array would relax the design requirements of the optical system, reduce the number of optical elements, and provide additional degrees of freedom to the camera designer to further improve performance. Curving modern FPAs, that are composed of a pixel array realized using a suitable semiconductor material bonded to a silicon read-out circuit (ROIC), is a formidable task. This has been achieved for visible imagers entirely made of silicon, and more recently progress has been made toward curving FPAs for IR applications.

As a result of the non-uniform external strain field caused by the curvature, the electrical and optical characteristics of the arrays may exhibit spatial variation, with pixel-to-pixel variation in the most affected regions of the array. As a result, this work has focused on developing a multiscale simulation approach to predict the performance of both pixel detector and arrays under the effect of the strain induced by the curvature.

II. METHODOLOGY

The first step in predicting the pixel array performance is to perform finite element analysis (FEA) to estimate the strain induced in creating a curved FPA. The model dictates the displacement of the die surface directly, which forces the initially flat die into a spherical segment with a prescribed radius of curvature (ROC). The die is modeled as a 45 mm



Fig. 1: The four strains obtained by the FEA calculations of the $InAs_{0.91}Sb_{0.09}$ alloy curved to a 70 mm ROC

by 50 mm rectangular deformable part with a thickness of 100μ m. We consider pixel detectors that are realized with an absorber layers composed either of a bulk $InAs_{1-x}Sb_x$ alloy or a $InAs/InAs_{1-x}Sb_x$ strain layer superlattice (SLS) with a composition suitable for operation in the mid-wave IR (MWIR) spectral band.

Subsequently, we employ a density functional theory (DFT) approach to determine the band shifts in strained $InAs_{1-x}Sb_x$ alloys. This approach is limited by its high computational cost. Consequently, a machine learning-assisted methodology coupled with a limited number of computationally expensive, yet high-fidelity, DFT calculations [2] is used to predict the band shift resulting from an arbitrary strain configuration. The mobility of the strained bulk alloys is computed using a Monte-Carlo transport model and another model based on the non-equilibrium Green's functions (NEGF) formalism [3] is used to evaluate the transport properties of SLS-based absorber layers.

Once the transport characteristics of the strained materials have been determined, it is possible to evaluate the detector and array performance. For this task we employ a three-dimensional simulation approach based on drift-diffusion model, and compute the dark current and quantum efficiency (QE) variation as a function of the strain configuration and the modulation transfer function (MTF) of the array [4].



Fig. 2: Band gap variation compared to the unstrained material in different regions of the die under high curvature (70 mm ROC) for the $InAs_{0.91}Sb_{0.09}$ alloy.



Fig. 3: Calculated hole mobility in a $InAs/InAs_{1-x}Sb_x$ SLS with MWIR cut-off wavelength.

III. RESULTS

Figure 1 presents the four strain components obtained using the FEA calculations in the case of an $InAs_{0.91}Sb_{0.09}$ absorber layer. The strain values are used to design a suitable atomic supercell that is analyzed using DFT, and the variation of the energy gap is obtained. Figure 2 presents the calculated energy gap variation compared to the unstrained material in different regions of the die under high curvature (70 mm ROC) for the $InAs_{0.91}Sb_{0.09}$ alloy. The additional external spatially dependent strain induced by the curvature, and the relative energy gap variation, can be included in a NEGF simulation model to determine the carrier mobility. Figure 3 presents



Fig. 4: Calculated values of the product of the spatial frequency and pixel pitch corresponding to modulation transfer function of 50% including the presence of disorder (DO = 4%).

the calculated hole mobility in a $InAs/InAs_{1-x}Sb_x$ SLS with MWIR cut-off wavelength. It can be seen that the curvature induces strain leads to a change in hole mobility as large as a factor of two compared to the unstrained material. When either positive or negative strain is present, the mobility decreases. The largest reduction in mobility occurs when the strain is positive, and it is approximately half of the value for the noncurved SLS for a biaxial strain of $\varepsilon_{xx,yy} = 0.08\%$. From the knowledge of the transport parameters of bulk and SLS it is possible to quantify the performance of the single detector and the array. Of particular importance is the MTF, that provides an indication of resolution characteristics of the pixel array. Figure 4 presents the calculated values of the product of the spatial frequency and pixel pitch corresponding to modulation transfer function of 50%. It can be seen that in the case of bulk type absorber, even if the mobility changes as a result of strain, the MTF is not degraded. In the case of SLS absorbers, the mobility reduction due to the external strain in the direction of growth further increases the anisotropy of the material degrading the MTF. Additionally, the presence of disorder (DO = 4%) degrades the MTF further.

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