Quantitative design of perovskite X-ray flat-panel detectors enabled by numerical parameter optimization

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Abstract

Metal halide perovskites have emerged as promising candidates for direct X-ray detection owing to their strong attenuation, excellent charge transport, and low-temperature processability. High X-ray absorption efficiency requires perovskite with large thicknesses, while increased thickness simultaneously raises the probability of charge carriers being trapped by defects, leading to an inherent trade-off. Achieving an optimal balance therefore requires careful optimization of key parameters such as absorber thickness and operating electric field. However, recent studies have not systematically optimized these detection parameters. Here, we establish a simulation framework based on cascaded linear system theory to systematically optimize the performance of MAPbI3-based X-ray detectors. The model quantifies the trade-off between X-ray absorption and charge collection, identifying an optimal thickness of 460 μm and an electric-field range that maximizes sensitivity while preserving spatial resolution. Guided by the simulation, we fabricate pixelated detectors integrated with thin-film transistor backplanes. The optimized detector exhibits a high sensitivity of 6588 μC · Gyair-1 · cm-2 and a spatial resolution of 3.23 lp/mm at a 200 μm pixel size, in good agreement with theoretical predictions. Furthermore, the detector demonstrates high-quality two-dimensional and three-dimensional imaging capabilities, highlighting its potential for advanced medical and industrial X-ray imaging applications.

Full Text

Preamble

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Abstract

Metal halide perovskites have emerged as promising candidates for direct X-ray detection owing to their strong attenuation, excellent charge transport, and low-temperature processability.

High X-ray absorption efficiency requires perovskite with large thicknesses, while increased thickness simultaneously raises the probability of charge carriers being

trapped by defects, leading to an inherent trade-off. Achieving an optimal balance therefore requires careful optimization of key parameters such as absorber thickness and operating electric field. However, recent studies have not systematically optimized these detection parameters. Here, we establish a simulation framework based on cascaded linear system theory to systematically optimize the performance of MAPbI3- based X-ray detectors. The model quantifies the trade-off between X-ray absorption and charge collection, identifying an optimal thickness of 460 μm and an electric-field range that maximizes sensitivity while preserving spatial resolution. Guided by the simulation, we fabricate pixelated detectors integrated with thin-film transistor backplanes. The optimized detector exhibits a high sensitivity of 6588 μC · Gyair -1 · cm-2 and a spatial resolution of 3.23 lp/mm at a 200 μm pixel size, in good agreement with theoretical predictions. Furthermore, the detector demonstrates high-quality two-dimensional and three-dimensional imaging capabilities, highlighting its potential for advanced medical and industrial X-ray imaging applications.

Keywords Perovskite, Numerical optimization, X-ray flat-panel detector, Spatial resolution

1 Introduction

Metal halide perovskites have recently garnered significant attention for X-ray detection due to their high attenuation coefficient, low trap density, and excellent charge transport properties[1-3].

In addition, perovskites can be processed at low temperatures using scalable methods[4]. Recent efforts have moved beyond single-pixel devices toward integration with pixelated readout backplanes, including thin-film transistor (TFT) and complementary metal-oxide-semiconductor (CMOS) arrays[5-7]. This progress enables flat-panel detector (FPD) with high sensitivity and spatial resolution[8]. However, reported device parameters vary widely across the literature. Key parameters, including material thickness and operating electric field, are often chosen empirically (Figure 1 [Figure 1: see original paper]). This arbitrary parameter selection limits the possibility of achieving the best detector performance and underscores the urgent need for an application-scenario-based standardized framework[9-19].

From a fundamental perspective, X-ray absorption and charge collection in perovskite detectors are governed by competing physical mechanisms[20, 21]. According to the Beer-Lambert law, increasing the perovskite thickness enhances X-ray absorption and thus increases the number of generated charge carriers[21]. As described by the Hecht equation, thicker layers require stronger electric fields to ensure efficient carrier collection and to suppress bulk recombination and trapping[22]. Moreover, excessive thickness induces lateral carrier diffusion, leading to increased inter-pixel crosstalk and spatial blurring[23, 24]. Consequently, achieving optimal detection and imaging performance requires a systematic and quantitative optimization of key device parameters.

Such optimization must be tailored to the X-ray energy spectrum and the intrinsic carrier transport properties of the perovskite. A comprehensive framework that jointly considers X-ray absorption, charge generation, transport, and collection is therefore essential to maximize sensitivity while preserving spatial resolution.

In this work, we establish a quantitative simulation framework based on cascaded linear system theory to optimize perovskite X-ray FPDs from both detection and imaging perspectives. The framework enables the calculation of average sensitivity and modulation transfer function (MTF) under polyenergetic X-ray spectra, providing a physically consistent basis for performance evaluation. Using this approach, we systematically optimized key device parameters for MAPbI3 X-ray detectors. Guided by the simulation results, we designed and fabricated corresponding FPDs.

Experimental results obtained under a series of different thicknesses and electric fields were in good agreement with the predictions. Finally, the optimized detector achieves a sensitivity of 6588 μC · Gyair -1 · cm-2 as well as a spatial resolution of 3.23 lp/mm at 200 μm pixel size in standard testing, approaching its theoretical limit. Furthermore, the detector enables high-quality two-dimensional and three-dimensional imaging, demonstrating its strong potential for advanced X-ray imaging applications.

Figure 1. Simulated Optimization Space of Perovskite X-ray Detectors: Correlating Thickness, Electric Field intensity, and X-ray Energy.

2.1 Materials

All the chemicals were used as received without any further purification. Lead iodide (PbI2 $\geq$ 99.999%) and Methylammonium iodide (MAI $\geq$ 99.9%) were purchased from Advanced Election Technology Co., Ltd. Polyacrylonitrile (PAN) was purchased from Shanghai Macklin Biochemical Technology Co., Anhydrous γ-butyrolactone (GBL $\geq$ 99.9%) were purchased from Chron Chemicals.

N, N-dimethylformamide (DMF $\geq$ 99.8%), N-Methyl pyrrolidone (NMP) and Chlorobenzene were purchased from Sigma-Aldrich. Tin Oxide (SnO2) and Nickel oxide (NiOx) were purchased from Xi' an Yuri Solar Co., Ltd. Biphenyl tetracarboxylic acid dianhydride (BPDA $\geq$ 99%) and p- phenylenediamine (PD $\geq$ 99%) were purchased from Shanghai Aladdin Biochemical Technology Co., Ltd.

2.1.1 Suspension preparation and device fabrication

2074.55 mg of lead PbI2, 715.37 mg of MAI, a 1 cm magnetic stir bar, and 1 mL of γ- butyrolactone were transferred to a 10 mL polyethylene (PE) tube. The mixture was stirred at 85℃ and 1200 rpm for 8 hours to obtain a flowable suspension. Subsequently, 30 mg of polyacrylonitrile (PAN) was added to this unstable suspension and stirred for 30 minutes. The substrate was pretreated

by spin-coating with a nickel oxide (NiOx) solution, followed by annealing at 100℃ for 30 min.

Subsequently, a solution of polyimide (PI) was spin-coated and annealed again at 100℃ for 30 min to achieve a mirror-like reflective surface. The stabilized suspension was then doctor-bladed onto the substrate and heated first at 80℃ for 2 hours, followed by heating at 100℃ for 8 hours, to yield the film. After spin-coating the tin oxide solution on the film, followed by annealing at 100℃ for 30 min. Finally, the film was spin-coating with the tin oxide (SnO2) solution, followed by annealing at 100℃ for 30 min. Gold (Au) electrodes were prepared by thermal evaporation.

2.1.2 Pixelated substrate

The pixelated substrate for evaluating the electrical uniformity of perovskite-based X-ray detectors is configured as a 3 × 3 array. The top row features single pixels of varying dimensions, while the bottom row consists of corresponding pixel arrays. From left to right, the pixel distribution in each column is: Column 1: one 200 μm pixel (top) and nine 200 μm pixels (bottom); Column 2: one 80 μm pixel (top) and nine 80 μm pixels (bottom); Column 3: one 60 μm pixel (top) and nine 60 μm pixels (bottom); Column 4: one 40 μm pixel (top) and nine 40 μm pixels (bottom); Column 5: one 30 μm pixel (top) and nine 30 μm pixels (bottom). The active pixel regions are patterned with indium tin oxide (ITO), while the surrounding passivation regions are coated with silicon nitride (Si3N4). Each pixel and pixel array is electrically connected to a large ITO contact pad at the substrate edge via an ITO interconnect passivated with Si3N4.

2.1.3 TFT backplane

The TFT backplane (overall dimensions: 30 × 30 mm, active area dimensions: 12.8 × 12.8 mm) was supplied by LinkZill Technology Company Limited. The active area comprises 64 × 64 pixels with a pixel pitch of 200 μm. The individual pixel capacitance is 1.6 pF. The pixel electrodes are patterned with indium tin oxide (ITO), while the surrounding passivation regions are coated with silicon nitride (Si3N4). Outside the active area are the gate line and read line interconnects. The readout integrated circuits (ROICs) were also provided by LinkZill Technology Company Limited.

The ROICs employed feature a 64-channel/16-bit analog front end.

2.1.4 X-ray characterization and imaging

X-ray detector performance measurement: X-ray imaging was performed using a commercially available X-ray tube (IXS080BP056P228 80 kV 56 W) as the X-ray source. X-ray photons were generated at an accelerating voltage of 50 kV and a working current of 0.2-0.7 mA. The distance between the X-ray tube

and detector was varied from 80 cm. 1 mm thick copper absorber was used to adjust the radiation dose rate. The X-ray dose rate was calibrated using an ion chamber dosimeter (MagicMax from IBA DOSIMETRY). A Keithley 6571B Source Meter was used to apply the bias voltage and record the response current. The X-ray dose rate was calibrated with an ion chamber dosimeter (MagicMax from IBA DOSIMETRY). Use this set of equipment for the performance characterization of X-ray FPD. The slanted-edge method specified in ISO 12233 was performed to measure the MTF curve of X-ray FPDs. A 3 mm thick rectangular lead plate was used as the edge and put longitudinal to the X-ray FPD with a 5° angle. Furthermore, it incorporates a micro-focus X-ray source (L9181-02, HAMAMATSU, Japan). It consists of a horizontal linear platform with a stroke of 200.0 mm, featuring a rotating axis, and a vertical linear platform with a stroke of 40.0 mm. Use this device for MTF and Coaxial cable testing. The CT imaging uses a medical-grade G-

2.1.5 Material characterization

Powder X-ray diffraction (XRD) measurements were performed using a Rigaku MiniFlex 600 diffractometer. Field-emission scanning electron microscopy (SEM) was conducted using a Zeiss Sigma-300. For the $\mu\tau$, I-V, I-t measurements, the Keithley 6571B Source Meter was used to apply the bias voltage and record the response current. A 365 nm LED light (model M365L, Zolix, Beijing) was used as the excitation source for $\mu\tau$ measurement. The power is controlled by the Thorlabs DC2100 high-power LED driver.

2.2 Methods

A comprehensive numerical model was developed based on cascaded linear system theory, extending the formalism pioneered by Rabbani and Cunningham et al. for multistage imaging systems[25-27]. This framework enables a systematic analysis of signal and noise propagation in perovskite detectors, incorporating the interplay between material properties and operational conditions[28]. The model quantitatively describes the dependence of sensitivity and charge collection efficiency on perovskite thickness, electric field strength, and incident X-ray energy (50- 90 keV), with explicit consideration of $\mu\tau$. Spatial-frequency-dependent performance metrics were derived, identifying a well-defined optimal parameter space (Figure 1) that maximizes sensitivity while minimizing recombination losses.

A pixelated perovskite-based X-ray imaging detector is modeled here. As shown in Figure 5a [Figure 5: see original paper], one side is the common electrode (top electrode) covering the whole detector and the electrode (bottom electrode) on the other side is segmented as square pixel of size $d' \times d'$. Additional parameters used in the simulation are shown in Table 1 .

Table 1. Input Parameters of MAPbI3 Parameter type Density Electron-hole pair ionization energy (W) Average atomic number (Zeff) Average atomic mass

(Mat) Pixel size Circuit noise Numerical value 4.15 g cm-3 200 μm 2000 e- Material parameters System parameters The probability density function of an X-ray photon with energy E at a given X-ray spectrum is calculated by pE(E)= where Φ(E) is the incident X-ray fluence with unit of photons per unit area per unit energy. A total X-ray photons per unit area can be calculated as $ $0= $\int$ Where Emax, Emin are the minimum and maximum energy of the spectrum. According to Beer- Lambert law, X-ray is attenuated exponentially by the absorber. The probability density for an X- ray photon that interact at a distance x form the top electrode of the detector is α(E)e-α(E)x px(E, x)= { , 0 $\leq$ x $\leq$ L 0, elsewhere L is the thickness of the detector. η is the X-ray quantum efficiency and given by η(E)=1-e-α(E)L Normalized values are used in this paper for simplified calculation, where normalized distance is x = x′/L, normalized pixel size is d = d′/L and normalized spatial frequency is f = f′L.

Sensitivity of X-ray detector Sensitivity is an important parameter for direct conversion material-based X-ray detector. It reflects the charge generated by semiconductor per unit area (cm2) per unit dose (Gy or R). The sensitivity is related to W and charge collection efficiency (CCE, ηcc) of semiconductor. An X-ray photon with energy E and totally absorbed by the semiconductor will create N = E/W electron hole (e-h) pairs. If the CCE is a hundred percent, which means all generated charges are collect by electrode, the maximum sensitivity of the detector is given by[29]:

S0(E)= [5.45$×$1013e Where αair is energy absorption coefficient of air, ρair is density of air, αen is the energy absorption coefficient of the semiconductor.

Assume that the top electrode is negatively biased, the CCE of the detector can be derived from Hecht equation and is given by[30]: ηcc=le [1+ η(Δ/le-1) le-e-Δ)] +lh [1- Where le,h = μe,hτe,h F/L (μe,h is the carrier mobility, τe,h is the carrier lifetime and F is the electron field) is the normalized electron and hole schubweg and Δ = 1/αL is normalized attenuation depth.

Hence, the CCE and absorption limited X-ray sensitivity of the detector is:

S(E)=η(E)ηcc(E)S0(E) For a polyenergetic X-ray beam, the sensitivity of the detector is:

E=$\int$ η(E)ηcc(E)S0(E) pE(E)dE

2.2.2 Modulation transfer function

The presampling MTF is designed by aperture function, range of primary photoelectrons, and charge trapping. Hence, the presampling MTF can be expressed as:

MTF(E, f)=Ta(E, f)×Tpe(E, f)×Ttr(E, f) Where Ta(E, f) is the MTF relate to the aperture function of the pixel electrodes (bottom electrode), Tpe(E, f) is the MTF for the range of primary photoelectrons, Ttr(E, f) is the MTF cause by charge trapping. For FPD with square pixel (dimension d), the Ta(f) is:

Ta(f)=|sinc(df)|= | sin(πdf) An X-ray photon creates thousands of electrons and generates charge cloud inside the semiconductor. The shape of the charge cloud is close to a sphere and its size affects spatial resolution. The Tpe(f) is associated with the function of the range of the primary photoelectron, which Tpe(f)= exp(-π 2σ 2f 2) Where σ is a parameter relates with the maximum range of the primary photoelectron Rmax. The expression of Rmax is given by Kanaya and Okayama, which is:

Rmax=2.761$×10−6×$ MatE0 Where Mat is the atomic mass, ρ is density, Z is the atomic number and E0 is the energy of primary photoelectron. Que and Rowlands gave a relationship between σ and Rmax, as σ Rmax/2.5[31].

The MTF due to charge carrier trapping has been studied by Kabir and Kasap and is given by[23]: where Ttr(f)= G(f) G(f)= (le+lh)(ω cossech ω-e- Δ ω coth ω -Δ-1 e- η$ $2(1-le Δ⁄)(1+le Δ⁄)(Δ-2-$ $2) ω cossech ω-e ηΔ(1-le Δ)(⁄ leω coth ω-le -2-$ $2) lh ω cosech ω-e- Δ ω coth ω +lh -2-$ $2 ηΔ(1+lh Δ)(lh le(e- ηΔ(1- ω = 2πf, and G(0)= (le+lh)(1-e- Δ-Δ-1e- η(1-le Δ⁄)(1+lh Δ⁄) le(le-e le-lee ηΔ(1-le Δ⁄) lh(lhe Δ-lhe- lh+e- ηΔ(1+lh Δ⁄) For a polyenergetic X-ray beam, the MTF of the detector is:

MTF(f)=∫ MTF(E, f) pE(E)dE le(e- ηΔ(1-le Δ⁄)

3.1 Systematic Performance Quantification and Parameter Optimization

Based on the established theoretical framework, we proceeded to systematically quantify the detector performance metrics under a wide range of operational parameters. In the simulation, $\mu\tau$ for the MAPbI3 layer was parameterized at 1 × 10-3 cm2 • V-1. It ensuring sufficient charge collection efficiency while preventing severe lateral charge diffusion that would degrade spatial resolution (other simulation parameters can be found in Table 1.). As shown in Figure 2b [Figure 2: see original paper], the MAPbI3-based flat-panel detector exhibits remarkable bias stability with decreasing applied voltage. At a thickness of 400 μm, the sensitivity exhibits only a marginal decrease from 812.8 μC • Gyair -1 • cm-2 at 10 V/μm to 801.9 μC • Gyair -1 • cm-2 at 0.1 V/μm, corresponding to a reduction of approximately 1.34%. A more substantial decline in sensitivity is observed only when the electric field is reduced to 0.01 V/μm, with the value falling to 712.0 μC • Gyair -1 • cm-2.

Figure 2. Systematic simulation of the performance and imaging characteristics of a MAPbI3- based X-ray detector. (a) X-ray flat-panel detector model. (b) Sensitivity of MAPbI3 as a function of thickness under different electric fields. (c) Normalized two-dimensional heatmap illustrating the relationship among thickness, carrier diffusion length, and sensitivity of MAPbI3 at 50 kV. (d) Optimal operational window of electric field determined based on the optimized carrier diffusion length. (e)The optimal MTF determined from the optimized carrier diffusion length. (f) Influence of the $\mu\tau$ product of MAPbI3 on the system' s MTF.

Building upon the electrical characterization, the interplay among perovskite thickness, carrier diffusion length ($\mu\tau$F) and sensitivity was quantitatively analyzed. By identifying the combinations corresponding to 90% of the maximum sensitivity, an optimal parameter space was delineated. The simulation results indicate that a thickness of 460 μm and $\mu\tau$F of 4.45 cm collectively yield a peak sensitivity of 801.3 μC · Gyair -1 · cm-2 (Figure 2c). It is generally considered that charge collection is nearly complete when $\mu\tau$F $>$ 10d (d represents the thickness of the photosensitive layer). Thus, by fixing $\mu\tau$F = 10d, the suitable electric field range is determined to be 4.8 V/mm to 460 V/mm. As shown in Figure 2d, corresponding to a $\mu\tau$ product range of 10-2 to 10-4 cm2 · V-1. This operational window aligns well with the sensitivity trends observed in Figure 2b, confirming the consistency and robustness of the proposed design strategy. Such a field range ensures efficient charge extraction while minimizing dark current, making it suitable for low-noise and high-dynamic-range X-ray imaging applications. Furthermore, under these optimized conditions, the detector simultaneously achieves an excellent spatial resolution, theoretically characterized by 4.1 lp/mm at MTF = 0.2, as shown in Figure 2f.

Following the optimization of the operational parameters, we further evaluated the imaging performance of the MAPbI3 detector by examining the influence of $\mu\tau$ on the MTF. While previous analyses assumed high-quality material properties, practical devices may exhibit defects that degrade charge transport, significantly reducing $\mu\tau$ and impairing detection performance. As depicted in Figure 2f, a decline in $\mu\tau$ leads to reduced spatial resolution. For instance, when $\mu\tau$ decreases from 10-2 cm2 · V-1 to 10-5 cm2 · V-1 the spatial resolution at MTF = 0.2 drops from 4.1 lp/mm down to 2.3 lp/mm. The degradation in resolution arises from the reduced $\mu\tau$, which impairs charge collection efficiency. For individual pixels, this diminishes the signal-to-noise ratio (SNR) and consequently degrades contrast. For multiple pixels, the lateral diffusion of charge enhances inter-pixel crosstalk across the detector array consequently degrading the spatial resolution. These results highlight the imperative for precise control over material uniformity and defect suppression during fabrication to achieve consistent and high-performance imaging devices.

3.3 Material Structural Characterization

Under the guidance of the simulation results, we proceeded to fabricate MAPbI3 thick films.

The structural and morphological properties of the synthesized samples were systematically characterized. As shown in Figure 3 Figure 3: see original paper, the XRD pattern of the as-prepared MAPbI3 film agrees well with the standard reference pattern, confirming the successful formation of the perovskite phase without detectable impurities. The XRD curve of a polyimide-modified MAPbI3 interlayer, introduced to mitigate thermal stress, also exhibits high consistency with the standard, indicating good compatibility and structural stability. Figure 3b presents a surface SEM image of the MAPbI3 film, showing densely

packed and large-grained morphology. Statistical analysis of grain sizes (Figure 3c) reveals an average grain size of 32.07 μm. Such large grains are beneficial for reducing grain boundary defects, thereby enhancing charge carrier mobility and lifetime-critical factors for achieving high sensitivity in X-ray detection. Figures 3(d-g) display cross-sectional SEM images of MAPbI3 films with thicknesses of 405 μm, 460 μm, 505 μm, and 548 μm, respectively. These samples were prepared to experimentally explore the thickness-dependent performance predicted by the simulation. A film with a thickness close to the theoretically optimized value of 460 μm was selected for subsequent device fabrication and performance evaluation.

Figure 3. Structural and morphological characterization of MAPbI3 thick films. (a) Comparison of XRD patterns between standard MAPbI3 and the synthesized PI-MAPbI3 and MAPbI3. (b) Surface SEM image of the MAPbI3 film. (c) Grain size distribution histogram of the MAPbI3 perovskite. (d-g) Cross-sectional SEM images of MAPbI3 films with thicknesses of 405 μm, 460 μm, 505 μm, and 548 μm, respectively.

3.4 Experimental Validation and Charge Transport Analysis

The product of charge carrier mobility (μ) and lifetime (τ) serves as a key figure of merit for evaluating charge transport characteristics in semiconductor materials. Figure 4a [Figure 4: see original paper] presents the $\mu\tau$ values measured under positive and negative bias conditions reflecting the electron and hole transport properties respectively. These parameters are directly correlated with those used in our simulations. The $\mu\tau$ product was extracted by fitting the photoconductive response of uniform Au/perovskite/ITO thick films using a modified Hecht equation: 1- exp (- Where I0 is the saturated photocurrent, L is the perovskite thick film thickness, V is the applied bias, τ is the carrier lifetime, μ is carrier mobility. The resulting $\mu\tau$ values were determined to be 1.65 × 10-3 cm2 • V-1 for holes and 1.33 × 10-3 cm2 • V-1 for electrons. The high $\mu\tau$ values can be attributed to the large grain size observed in the perovskite films, which effectively reduces grain boundary density and associated defect trapping sites[32]. These experimentally derived $\mu\tau$ values were directly used as key input parameters in our numerical device model, ensuring a physically realistic foundation for the subsequent simulation of detector performance.

Figure 4. Performance characterization of MAPbI3 thick-film X-ray detectors (460 μm) at 50keV. (a) Bias-dependent photocurrent of the perovskite film. The solid line represents the fitting result using the Hecht equation. (b) Current density under X-ray illumination (dose rate: 113.4 μGyair • s-1) and in the dark. (c) X-ray response under various dose rates. (d) X-ray response under different electric fields. (e) Sensitivity of detectors with different thicknesses as a function of X-ray dose rate. (f) Dark current density of original single-pixel and array devices (up) and dark current density after pre-treated (down).

Figure 4b displays the current density of the MAPbI3 thick-film detector under X-ray illumination and in the dark. The electrical resistivity of the film is 9.52 $\times$ 108 $\Omega \cdot$ cm. This relatively high resistivity contributes to the suppression of dark current, which is beneficial for enhancing the X-ray detection limit by improving the signal-to-noise ratio[33]. The response of the device to X- ray exposure at varying dose rates was characterized by adjusting the X-ray tube current (Figure 4c).

As expected, the generated photocurrent density exhibits a linear relationship with the X-ray dose rate. The bias-dependent response was also recorded (Figure 4d). The device shows significant bias- dependent sensitivity, with measured values of 639, 2553, 3870, 4636, 5513, and 6588μC$\cdot$Gyair 1$\cdot$cm-2 at electric fields of 2.5, 10, 20, 30, 50, and 100 V mm-1, respectively. This trend is well justified by the enhanced collection efficiency of non-equilibrium charge carriers under stronger electric fields, leading to higher sensitivity. The sensitivity obtained from the experiment is higher than the simulated value, which is attributed to the photoconductive gain. In this mechanism, the prolonged transit time of trapped carriers allows a single incident photon to induce multiple charge circulations in the external circuit thereby amplifying the output signal.

Furthermore, the sensitivity of detectors with different photosensitive-layer thicknesses (270, 400, 460, 510 and 550 μm) was evaluated across a range of X-ray dose rates, as summarized in Figure 4e. The sensitivity initially rises with increasing thickness but plateaus beyond around 500 μm. The trend that aligns well with our simulations and reflects the inherent trade-off where enhanced X-ray absorption in thicker films is counterbalanced by greater charge recombination losses[34].

The pixel-level uniformity of the perovskite thick films was systematically characterized using pixelated substrates with feature sizes ranging from 30 $\times$ 30 μm2 to 200 $\times$ 200 μm2. Both single- pixel and pixel array configurations were fabricated. As shown in the upper panel of Figure 4f, the normalized dark current density of the as-prepared films exhibited a significant decrease with increasing pixel size. This behavior is attributed to the agglomeration of nickel oxide particles in the precursor dispersion, which hindered the formation of a uniform PI interlayer during spin- coating and resulted in the formation of pinholes or voids. In larger pixel areas, these defects led to ineffective electrical connections, thereby reducing the signal amplitude. In contrast, smaller pixels were either completely disconnected or less affected by localized defects, though a higher proportion of non-functional or low-response pixels was observed.

To address this issue, the nickel oxide aqueous colloidal dispersion was re-optimized and subjected to thorough ultrasonic treatment prior to deposition. This process effectively suppressed particle agglomeration and significantly improved the uniformity of the PI layer, eliminating large- area pinhole defects[35, 36]. As demonstrated in the lower panel of Figure 4f, the treated films exhibited highly uniform and stable responses across all pixel sizes. This improvement in film homogeneity provides a solid foundation for the further development of

large-area perovskite-based X-ray imaging.

3.5 Imaging Performance

The $MAPbI_3$ thick film was integrated with an TFT (Figure 5a). The detector panel measures 30 × 30 mm2 with an active area of 12.8 × 12.8 mm2, a pixel size of 200 μm, and a resolution of 64 × 64 pixels. ITO serves as the bottom electrode connected to the TFT source, while SiNx passivates the non-active regions. A common gold top electrode is connected to external bias pads, with bias adjustable from 0 to 15 V. Signals are read out at 60 frames per second in a line-by-line fashion.

The MTF measurement was performed using the micro-focus X-ray source operating at a tube voltage of 50 kV. The distance from the X-ray focal point to the tungsten plate was 130 mm and that from the tungsten plate to the surface of the detector was 20 mm. The spatial resolution was quantified using the slanted-edge method. The MAPbI3-based X-ray flat-panel detector achieved a resolution of 3.23 lp/mm at MTF = 0.2 (Figure 5c), which is slightly lower than the simulated prediction. This discrepancy can be attributed to the reduction in $\mu\tau$ caused by interfacial defects and stress introduction during the actual integration process[37-39]. Although the measured MTF decreased due to the lower $\mu\tau$, it still falls within the MTF range predicted by the simulation for different $\mu\tau$ values.

Nevertheless, its performance remains superior to previously reported printed MAPbI3 detectors (3.1 lp/mm for 70 μm pixel) and soft-sintered MAPbI3 detectors (3.3 lp/mm for 50 μm pixel)[13, 17]. Furthermore, the stitched image of the line-pair card is presented in Figure 5e, where line pairs with a spatial resolution of 3.15 lp/mm remain clearly distinguishable. We also performed imaging demonstrations on a scalpel tip, an access control card, and a circuit board (Figure 5d), where the outlines and internal structures of the objects were clearly resolved.

Figure 5. X-ray imaging performance of the fabricated detectors. (a) The structure of the perovskite-based flat-panel detector. (b) Optical image of the MAPbI3 detector integrated on a TFT backplane. (c) Measured spatial resolution; the inset shows the corresponding edge spread function. (d) X-ray images of various test objects: a scalpel tip, an access control card, and a circuit board. (e) The X-ray image of the line pair card. (f) Computed tomography imaging of a walnut: photograph of the sample (top), the reconstructed cross-sectional image (middle) and three-dimensional image (bottom).

Computed tomography (CT) measurements were conducted using a medical-grade G-242 X- ray source with a tube voltage of 50 kV. The walnut was fixed on the rotation axis, with the X-ray focal spot-to-detector distance set to 100 mm and the sample-to-detector distance set to 150 mm.

Projections over 360° were acquired by rotating the walnut around the central

axis with a 2° step interval. The projections were then stitched and reconstructed into a 3D volume using a reconstruction algorithm. Density-weighted correction was applied, allowing internal features such as the walnut shell, kernel, and air gaps to be clearly visualized in the cross-sectional image (Figure 5f). These results demonstrate that this study successfully addressed the challenge of random thickness variation, achieving excellent image quality in both 2D and 3D X-ray imaging. The developed detector exhibits strong potential for medical imaging applications.

4 Conclusion

In summary, we established a comprehensive theoretical framework for optimizing MAPbI3 thick-film X-ray detectors through systematic numerical modeling and experimental validation. The cascaded linear system model successfully identified optimal operational parameters, achieving excellent agreement between predicted and measured performance. The fabricated detectors demonstrated remarkable charge transport properties ($\mu\tau$ = 1.65 × 10-3 cm2 • V-1), high sensitivity (up to 6588 μC • Gyair -1 • cm-2), and superior spatial resolution (3.23 lp/mm for 200 μm pixel). Furthermore, the achieved performance, while exceptional, indicates room for further improvement as it does not yet reach the fundamental theoretical limit, primarily due to non-ideal interfacial charge extraction and bulk traps which curtail the ultimate charge-collection efficiency. Through optimized processing, we resolved critical challenges in film uniformity and thickness control, enabling high-quality 2D and 3D X-ray imaging. These results validate the robustness of our design strategy and demonstrate the strong potential of perovskite-based detectors for medical imaging applications, particularly in high-resolution diagnostic scenarios.

Author contributions Yu-Hao Zhang and Zi-Meng Li contributed equally to this work. All authors contributed to the study conception and design. Conceptualization was performed by Yu-Hao Zhang, and Zi-Meng Li.

Material preparation and data collection were performed by Yu-Hao Zhang, Xin Zhang, and Xu- Long Pang. Data validation was performed by Yu-Hao Zhang, Zi-Meng Li, Xin Zhang, and Xu- Long Pang. Funding acquisition was performed by Meng-Ling Xia, Yong-Shuai Ge, and Hao-Di Wu. Writing was performed by Yu-Hao Zhang, and Hao-Di Wu. The first draft of the manuscript was written by Yu-Hao Zhang, and all authors commented on previous versions of the manuscript.

All authors read and approved the final manuscript.

Conflict of Interest The authors declare no conflict of interest.

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