

Comparative Radiation Tolerance of Lead and Antimony based Perovskites under Proton Irradiation for Photovoltaic Applications

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ABSTRACT

All-inorganic metal halide (IMH) perovskites have been the subject of intensive experimental and theoretical research in the recent past for their superior thermal and chemical stability, along with high radiation tolerance relative to their organic-inorganic counterparts. IMH perovskites' high radiation tolerance and defect-resistance make them promising candidates for photovoltaic applications in high radiation environments, such as those of outer space.

Currently, among inorganic metal halide perovskites, caesium-lead halides such as CsPbI_3 and CsPbBr_3 see the widest use and research attention. Their main drawback is toxicity, stemming from the lead they contain. Hence, research is now being done into lead-substituted IMH perovskites, but lead is a key component that contributes to the radiation tolerance of IMH perovskites. In this study, we have employed molecular dynamics and Monte Carlo simulations to compare the radiation damage induced by H^+ ions in lead-based and antimony-based (lead-substituted) perovskites, aiming to elucidate the differences in radiation tolerance between the two materials.

The results show that mid-energy protons (50-100 keV) produce the greatest displacement damage and directly impact absorber-critical depths. Iodine loss is the dominant structural degradation pathway in both materials. Although $\text{Cs}_3\text{Sb}_2\text{I}_9$ demonstrates slightly less B-site displacement at low energies, both compositions exhibit high halide susceptibility, since iodine loss is the dominant pathway for structural degradation, indicating that halide stabilization is essential for improving the endurance of perovskite solar cells.

INTRODUCTION:

All-inorganic metal halide perovskites with the molecular structure ABX_3 have emerged as promising candidates for modern-day and next-generation photovoltaic applications due to their high carrier mobility, long diffusion lengths, and high thermal and chemical stability. These characteristics make them well-suited for numerous applications including optoelectronics, terrestrial photovoltaics and even for

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extreme environments like the solar energy systems deployed in space (Bouhmouche et al., 2023; Tu et al., 2021). At present, the most commonly used and researched class of IMH perovskites is caesium-lead halides, which show superior structural robustness under high temperature, moisture and radiation, unlike their widely used counterparts: hybrid organic-inorganic perovskites, which exhibit poor environmental stability due to the volatile nature of their organic cations (Hoefler et al., 2017; Oyewande & Akinpelu, 2018a).

Among these materials, CsPbI_3 has drawn considerable research interest owing to its optoelectronic properties - direct bandgap (~ 1.73 eV) and a high absorption coefficient, allowing efficient solar energy conversion (Oyewande & Akinpelu, 2018a). Nonetheless, the presence of lead in its structure has raised environmental concerns due to its toxicity. As a result, researchers have directed efforts towards finding lead-free perovskite, an alternative, while preserving the desirable properties of IMH perovskites, and reducing the negative ecological impact of the presence of lead. To achieve this goal, a variety of perovskites with B-site cations including tin (Sn), germanium (Ge), bismuth (Bi), and antimony (Sb) have been investigated as possible substitutes for lead-based systems. Of these, the antimony-based perovskite $\text{Cs}_3\text{Sb}_2\text{I}_9$ looks particularly promising due its air stability, low toxicity, and tunable electronic structure (Hoefler et al., 2017).

The deployment of perovskite-based solar cells in high-radiation environments gives rise to new challenges. Displacement damage under proton irradiation could cause performance deterioration in photovoltaics. Proton interactions essentially cause nuclear stopping at low-to-medium energies, creating lattice vacancies and interstitials that disrupt the charge transportation pathways. Monte Carlo simulation software like the Stopping and Range of Ions in Matter (SRIM) and its counterpart, Transport of Ions in Matter (TRIM) are widely used to model these effects by estimating defect generation rates and ion penetration profiles in solid targets (James Ziegler - SRIM & TRIM, n.d.; Martinie et al., 2014; Ziegler et al., 2010).

Lead halide perovskites are generally understood to exhibit defect tolerance, attributed to antibonding coupling between Pb 6s and halide p orbitals at the valence band edge, which confines most native point defects to shallow rather than deep, recombination-active trap states (Yin, Shi & Yan, 2014). CsPbI_3 , sharing this Pb-halide bonding framework, is expected to benefit from a similar mechanism, though this has not been directly confirmed for the all-inorganic composition. Substituting lead with a cation such as antimony would likely alter this behavior, given differences in atomic mass, lattice structure, and bonding character. How such compositional changes affect damage mechanisms under proton exposure therefore remains an important open question.

This study investigates the comparative radiation tolerance of lead-based and antimony-based inorganic perovskites, CsPbI_3 and $\text{Cs}_3\text{Sb}_2\text{I}_9$, under varied proton energies, ranging from 20 keV to 500 keV using molecular dynamics and Monte Carlo simulations. It focuses on the quantification of lattice vacancies to identify vulnerabilities at the elemental level. By analyzing the vacancy profiles and elemental displacement contributions, this work aims to show the effects of two different cations (lead and

antimony) on the degradation of perovskites to help judge the substitutability of lead. The findings of this project will also provide insights into the dominant degradation pathways that govern radiation damage in IMH perovskites.

METHODS

In this section, we explain the methods and techniques employed to run the simulations for this research. Details of the theoretical background for the calculations and simulation algorithms embedded in the TRIM and SRIM packages are discussed in the papers by Ziegler and Biersack (Ziegler et al., 2010).

SRIM's stopping-and-range tables were first used to run Monte Carlo simulations of 10,000 protons incident at normal incidence (0 degree) on each of the two target materials, CsPbI_3 and lead-substituted $\text{Cs}_3\text{Sb}_2\text{I}_9$. These simulations provided the projected range of ion energies. A line graph representing this data is attached below:

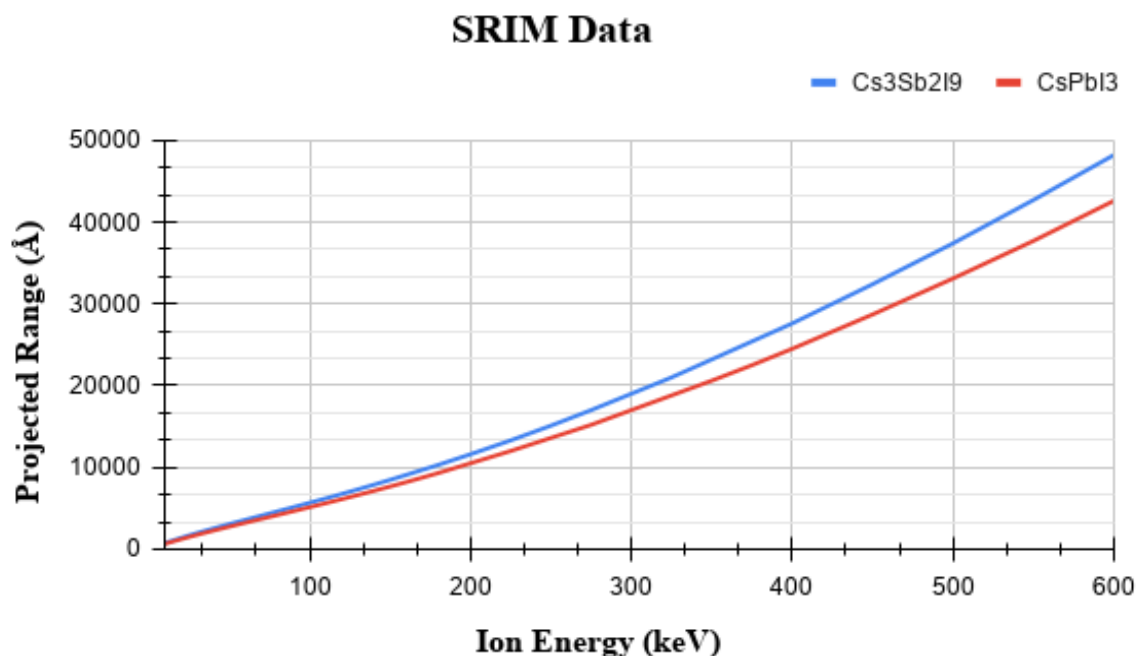


Figure 1: Projected ranges of 10,000 protons in CsPbI_3 and $\text{Cs}_3\text{Sb}_2\text{I}_9$ at different ion energies

This range data was then used to determine the target thickness needed to fully contain all 10,000 simulated ions, that is, a thickness large enough that no ions exit through the back of the target, which is a necessary step before running the complete damage-cascade simulation in TRIM. Based on this, a target (wafer) thickness of 10,000 Å (1,000 nm) was selected for the full TRIM simulation.

TRIM was then set-up to run Monte Carlo simulations for the detailed calculation of full damage cascades for both materials. For both SRIM and TRIM, the lead perovskite was built from their composites in the stoichiometric ratio 1:1:3 for Cs, Pb and I, respectively. And, the antimony perovskite (lead-substituted) was built using Cs, Sb and I, replacing lead with antimony, in the stoichiometric ratio 3:2:9. The density of the perovskite materials calculated by SRIM/TRIM itself was not used for the simulations because the program code assumes that targets are homogenous and amorphous at atomic levels while experimental densities can vary due to factors like porosity, crystal defects, surface conditions etc. Since calculated density values do not account for the aforementioned factors, experimental values for perovskite materials' densities are to be used. To the best of our knowledge, density values for both CsPbI_3 and $\text{Cs}_3\text{Sb}_2\text{I}_9$ currently available in the literature are computational ones and vary in different places. To that end, we obtained estimates for experimental densities by using a 5/3 basis correction as Oyewande and Akinpelu did in their work (Oyewande & Akinpelu, 2018a).

Five different proton energy levels (20 keV, 50 keV, 100 keV, 200 keV and 500 keV) were used to run the simulations. Higher ion energies, typically in MeVs are used for studying bulk material damage, but significantly higher target thickness would be required to experiment with those energy levels. Hence, the proton energies were selected in consideration of our chosen target width. Five simulations were run for each of the target materials, one corresponding to each of the chosen proton energy levels. Each simulation produced tabular results, listing respectively the vacancies produced in the atoms of each of the three elements composing the wafer. These vacancy values were given at 100 different depths, starting from 100.1 Angstroms, incrementing by 100 Angstroms each time, and reaching 10000 Angstroms at the last value.

RESULTS

Simulated vacancies represent uncoordinated “dangling bonds” and structural voids in the crystal lattice. These physical vacancies break the coordinate bonds of the lattice introducing localized energy levels within the material's electronic bandgap. These newly-formed trap states act as recombination centers that reduce carrier lifetime, which ultimately manifests a macroscopic drop in open-circuit voltage V_{OC} , J_{SC} , and fill factor.

Graphical Analysis

Following are the results for our Monte Carlo simulations, plotted as line-symbol graphs. Vacancies produced per angstrom per ion (vacancies/(Å·ion)) are plotted on the Y-axis with target depth in Angstroms (Å) on the X-axis. The geometric shapes represent vacancies produced in certain compositional elements of the target material at corresponding depths. The curves' correspondence to elements can be identified through the key in the upper right-hand corner of each graph. Total vacancies in each material are also shown by the highest curve in each graph.

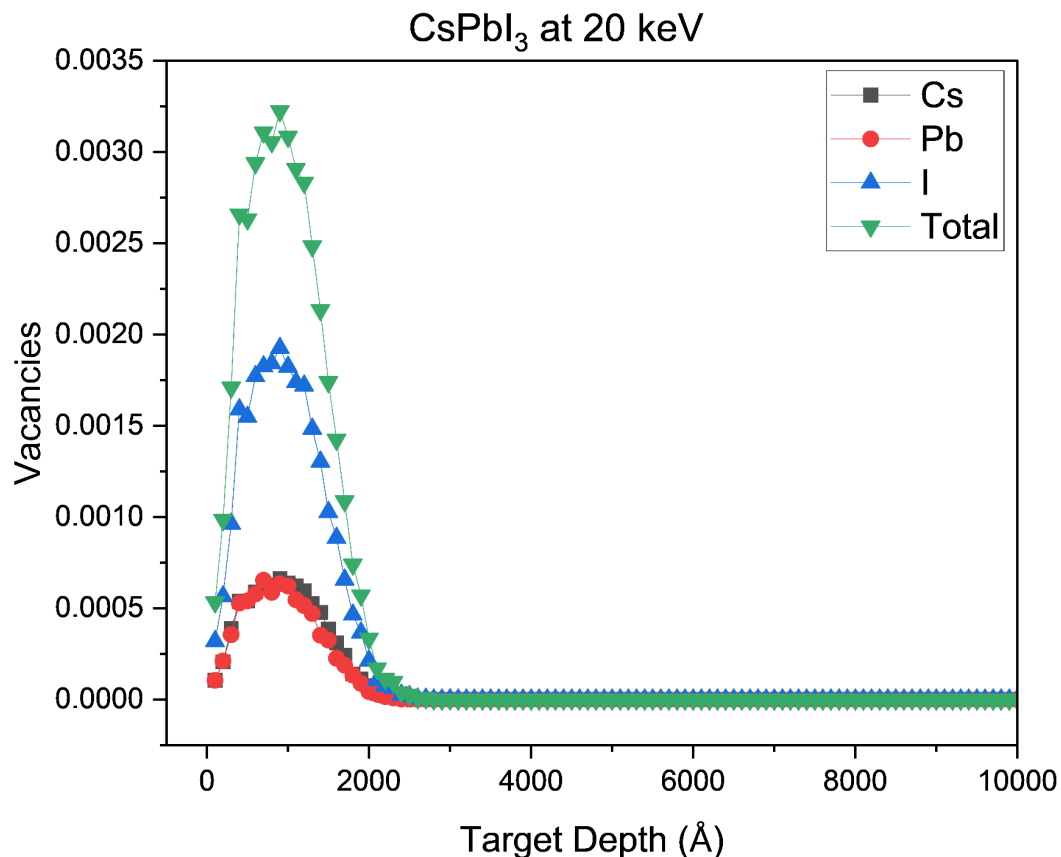


Figure 2: SRIM/TRIM-calculated vacancy distributions for CsPbI₃ under 20 keV proton irradiation

According to Figure 2, at 20 keV, vacancy formation peaks around a depth of ~ 900.01 Å below the surface of the CsPbI₃ perovskite. At this depth, vacancy formation is at its highest at ~ 0.00322 vacancies/(Å·ion) - transferring maximum kinetic energy to lattice atoms, which produces the vacancy spike. The drop in total vacancies is rapid after the peak as protons now slow down and lose energy, reaching a lowest point of 0.000001 at ~ 2800 Å. Beyond this point, bombarded protons hit the lattice atoms with less energy than that required for vacancy production, and stop penetrating further in depth. Hence, the graph becomes horizontal.

Iodide ions are lighter and more weakly bound than lead and caesium ions in the lattice, so they have lower displacement energy values. Hence, they are the most dominantly displaced specie. At peak vacancy production, ~ 0.00192 out of a total of 0.00322 vacancies/(Å·ion) stem from iodine atoms. Lead ions are heavy and strongly bonded, while those of caesium are lighter but still more strongly bonded than iodine, so they require much more energy to get displaced.

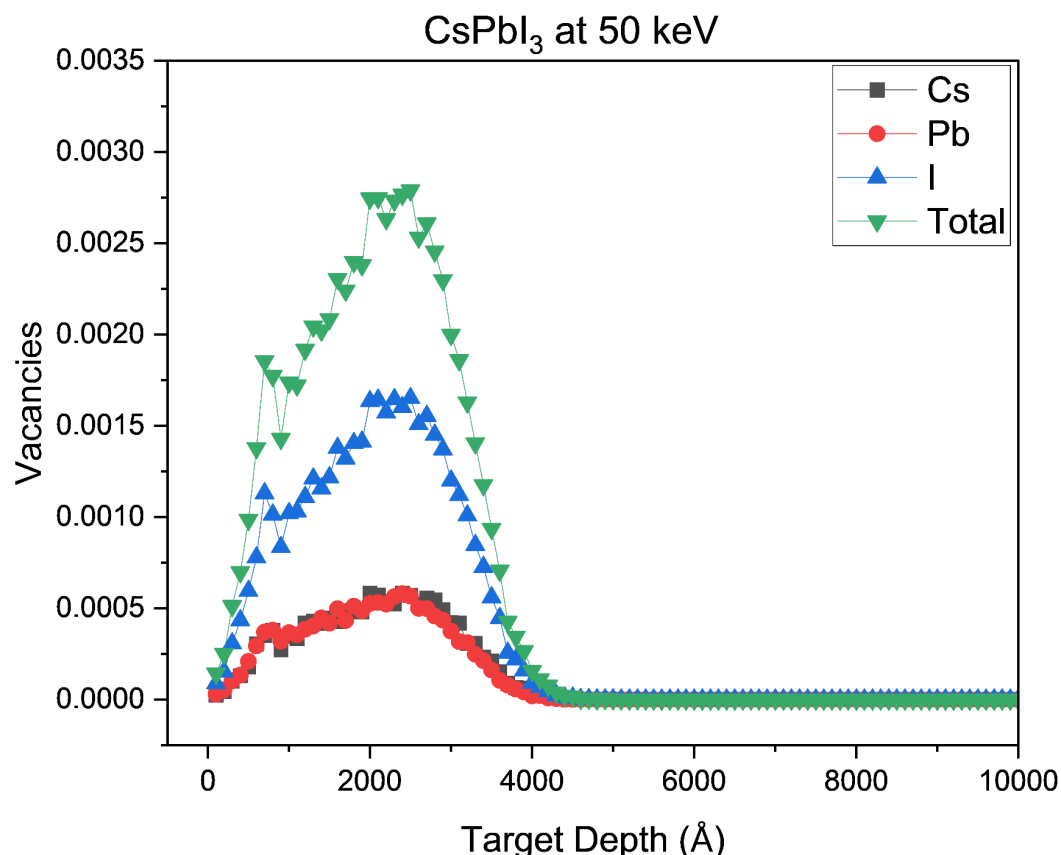


Figure 3: SRIM/TRIM-calculated vacancy distributions for CsPbI₃ under 50 keV proton irradiation

As shown by Figure 3, at 50 keV, CsPbI₃ exhibits increased lattice disorder than it did at 20 keV, with total vacancy peak shifting to ~ 0.00279 vacancies/(Å·ion) at a depth of ~ 2500.01 Å. This now nears the range of perovskites' functional absorber region which is estimated to be around (300 nanometer - 1 micrometer). The functional absorber region is the active light-harvesting layer in a perovskite solar cell, so vacancies in this region can potentially lead to greater macroscopic performance loss.

Iodine still dominates the vacancy curve, contributing with ~ 0.00160 out of the total ~ 0.00279 vacancies/(Å·ion) at the peak - making up 57.3% of the total vacancies.

However, lead and caesium displacement now occurs over a larger range of depth compared to 20 keV. Most damage remains confined to upper regions of the absorber layer. At this energy, protons still lose most momentum via nuclear stopping in the near-surface region, but they have enough range to penetrate deeper, and enough velocity to reach the higher displacement thresholds for lead and caesium.

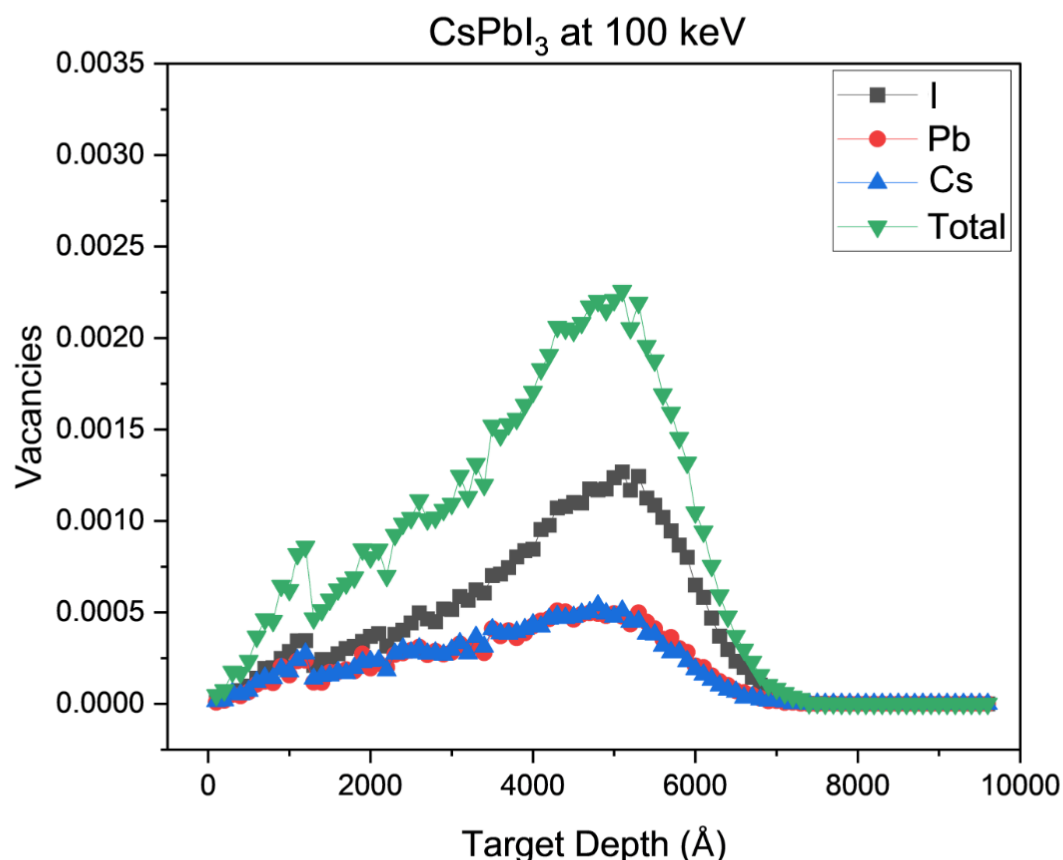


Figure 4: SRIM/TRIM-calculated vacancy distributions for CsPbI₃ under 100 keV proton irradiation

As can be seen in Figure 4, at 100 keV, peak vacancy generation shifts deeper to around 3000-6000 Å, a crucial range for the functional absorber region of the perovskites. Total damage is significantly higher than that in 50 keV in Figure 3. since there is more nuclear stopping alongside a more energetic cascade. The peak vacancy production in this case reaches ~0.00226 vacancies/(Å·ion) at a depth of ~5100.01 Å, which is the highest recorded for CsPbI₃ in this study.

Iodine still dominates the damage due to its bonds' relative weakness compared to lead and caesium. Since the energy is now high enough to displace heavier ions effectively, caesium and lead displacement becomes relatively more prominent.

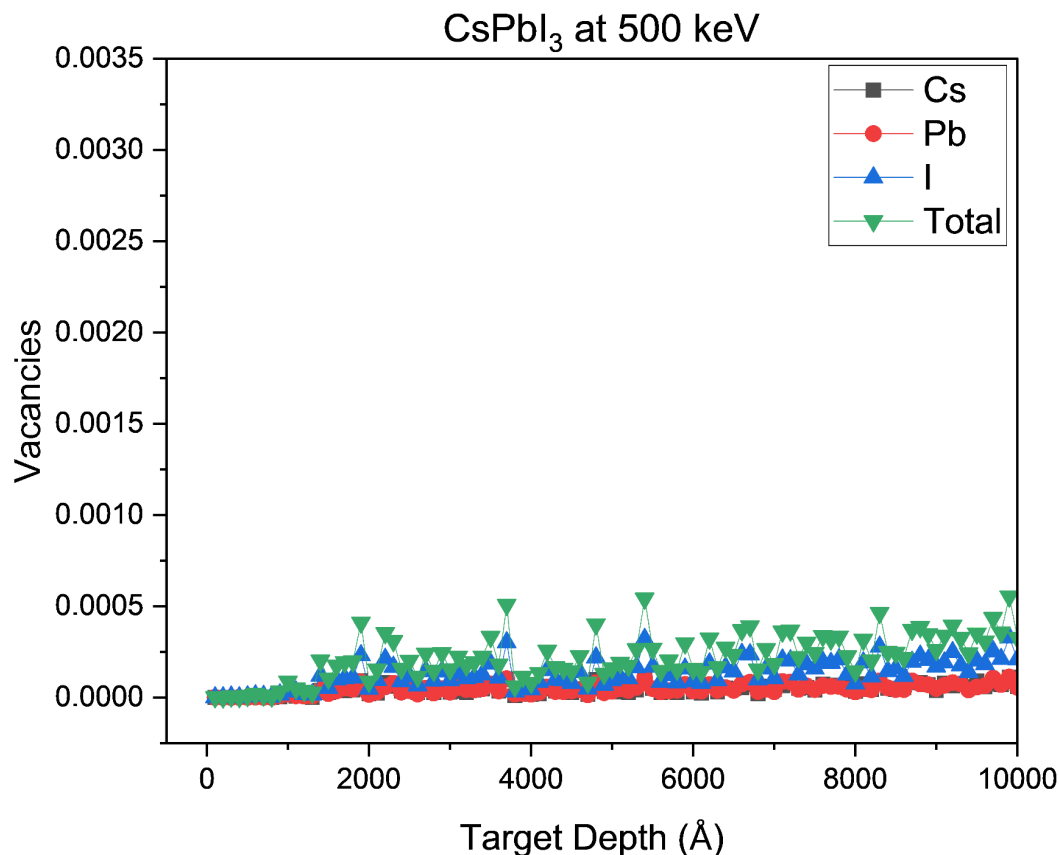


Figure 5: SRIM/TRIM-calculated vacancy distributions for CsPbI₃ under 500 keV proton irradiation

At 500 keV in Figure 5, vacancy concentrations are much lower despite higher energy. Damage is distributed very deep with low amplitude, with the curve being nearly flat with only small fluctuations. Maximum recorded total vacancies ~ 0.000543 vacancies/(Å $\cdot$ ion) occur at 5400.01 Å. Lead, caesium and iodine all now have very similar displacement behavior, and there is no definite trend in vacancy production.

At this high energy, the dominant energy loss mechanism changes from nuclear stopping to electronic stopping. The protons pass through too fast to transfer momentum effectively and they lose energy mostly to electrons instead of nuclei, causing very few vacancies to occur.

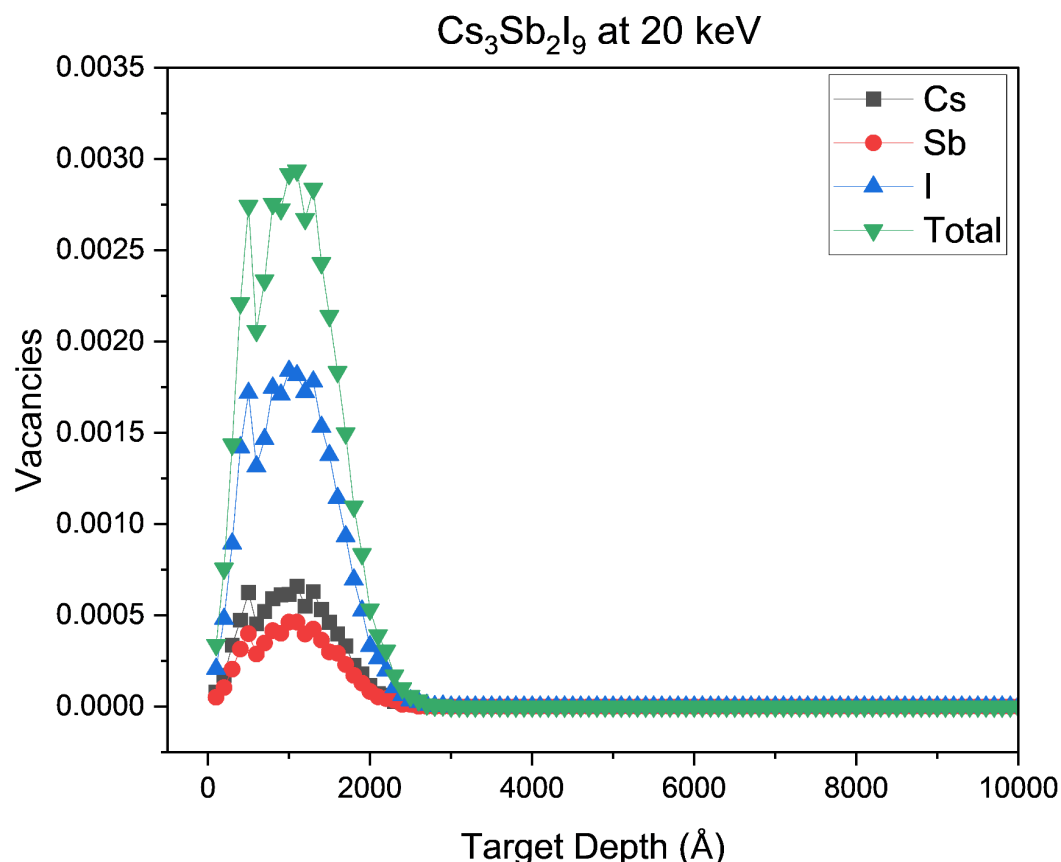


Figure 6: SRIM/TRIM-calculated vacancy distributions for $\text{Cs}_3\text{Pb}_2\text{I}_9$ under 20 keV proton irradiation

In Figure 6, vacancy production in $\text{Cs}_3\text{Pb}_2\text{I}_9$ peaks at ~ 0.00294 vacancies/ $(\text{\AA} \cdot \text{ion})$ at a depth of ~ 1100.01 $\text{\AA}$ from the surface. Iodine produces the largest vacancy concentration, followed by caesium. Antimony shows the smallest displacement contribution at this energy. The total vacancy curve closely follows the iodine curve, indicating halide-dominated damage as was the case in CsPbI_3 . Vacancy counts fall off rapidly beyond the peak reaching a minimum of ~ 0.000007 vacancies/ $(\text{\AA} \cdot \text{ion})$ at a depth of 2900.01 $\text{\AA}$.

At 20 keV the protons stop in the near-surface region and deposit most momentum there, with nuclear stopping being the dominant mechanism. Iodine atoms, with lower displacement thresholds and weaker binding, are preferentially displaced. Antimony resists displacement more strongly at low ion energy; its contribution to damage is small compared with iodine and caesium. It is worth noting that compared to lead vacancies CsPbI_3 in Figure 2, antimony has relatively less displacements.

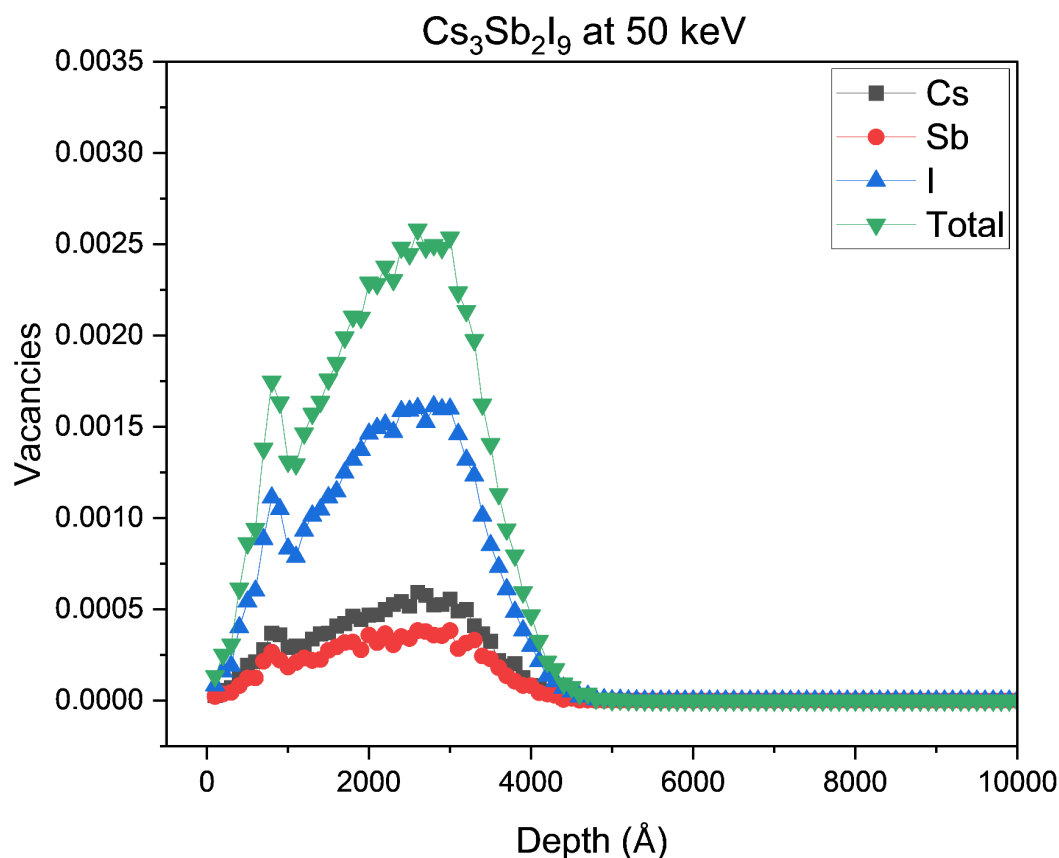


Figure 7: SRIM/TRIM-calculated vacancy distributions for $\text{Cs}_3\text{Pb}_2\text{I}_9$ under 50 keV proton irradiation

In Figure 7, the vacancy peak for $\text{Cs}_3\text{Pb}_2\text{I}_9$ is at ~ 0.00258 vacancies/(Å·ion) at a depth of ~ 2600.01 Å. Total vacancy amplitude increases compared with 20 keV in Figure 6; iodine still provides the largest share but caesium contribution also increases noticeably. Antimony displacement increases slightly but remains smaller than iodine and caesium. The damage profile broadens: higher vacancy production across a wider depth range.

Higher-energy protons penetrate deeper before stopping, so the damage region moves into the functional absorber layer, as it did in Figure 3. As well. Greater transferred energy increases vacancy production for heavier species (caesium and to a lesser extent than antimony). Iodine is still the weakest link, but the lattice begins to experience multi-species disruptions at mid-energies.

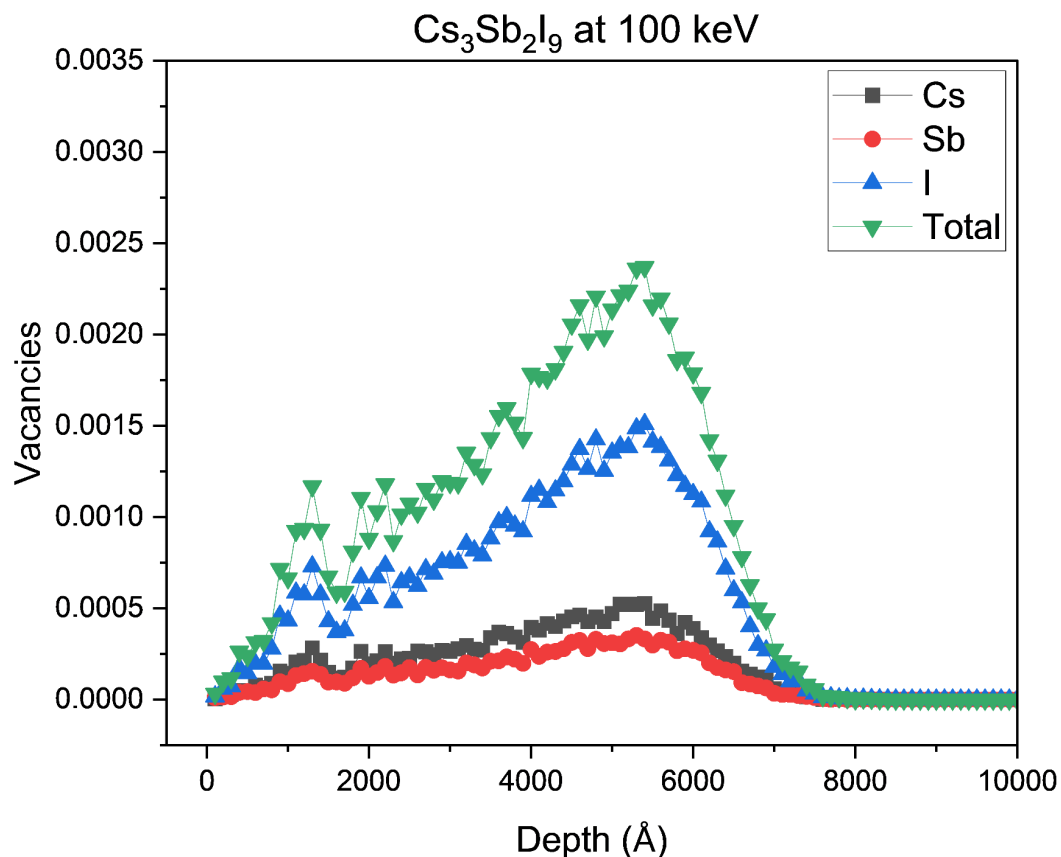


Figure 8: SRIM/TRIM-calculated vacancy distributions for $\text{Cs}_3\text{Pb}_2\text{I}_9$ under 100 keV proton irradiation

In Figure 8, Vacancy production peaks at ~ 0.00237 vacancies/ $(\text{\AA} \cdot \text{ion})$, at a greater depth of ~ 5400.01 than at lower energies. Iodine still produces the largest vacancy concentration. Caesium and antimony show increased displacement relative to at lower energies; antimony contributes more than at 20 and 50 keV but remains less than iodine and caesium. The damage profile is broad, with a pronounced maximum in the mid-depth region i.e the functional absorber layer region.

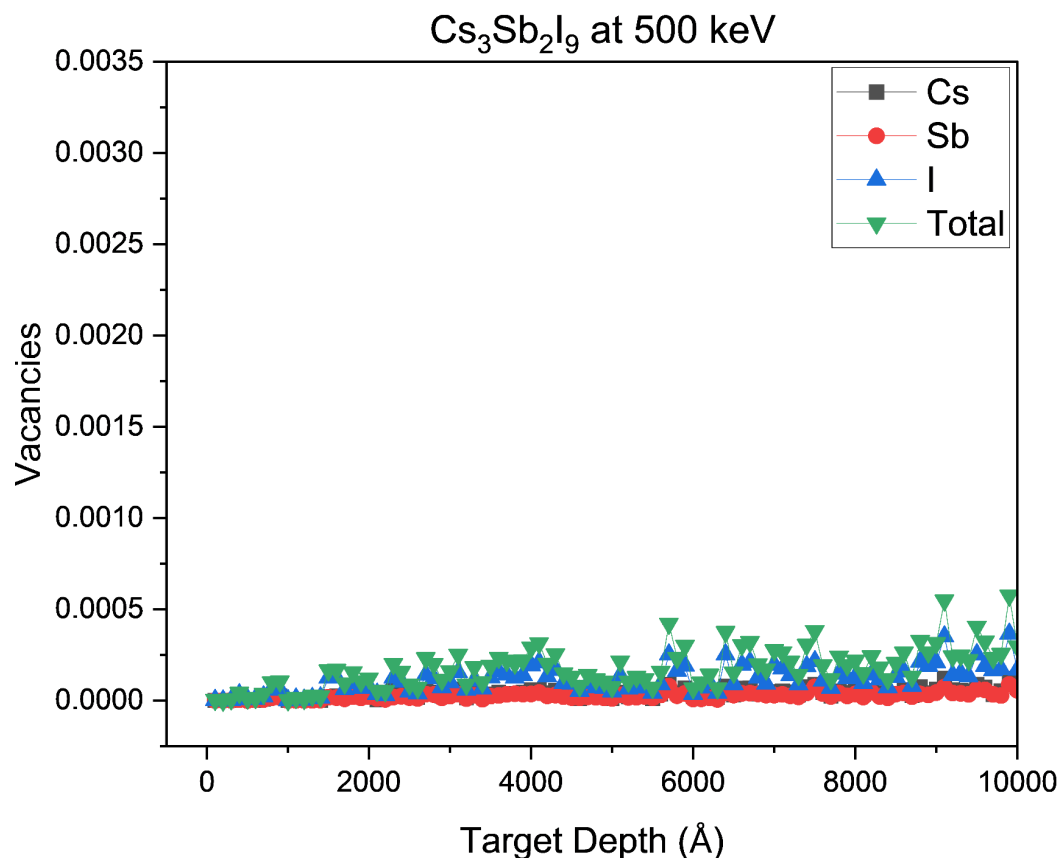


Figure 9: SRIM/TRIM-calculated vacancy distributions for $\text{Cs}_3\text{Sb}_2\text{I}_9$ under 20 keV proton irradiation

At 500 keV in Figure 9, vacancy concentrations for $\text{Cs}_3\text{Sb}_2\text{I}_9$ are low and broadly distributed across depth - the plot shows a low-amplitude, nearly flat background with small fluctuations. Iodine, caesium and antimony have comparable small displacement signals; there is no sharp peak as at mid energies.

At this point, energy loss shifts toward electronic stopping as it did in Figure 5. Protons traverse the lattice faster and transfer less momentum to nuclei, so nucleic displacements drop even though protons penetrate deeper. This is consistent with the typical nuclear-to-electronic stopping transition at high ion energies.

Implications and Comparative Summary

It is important to note that binary collision approximation simulations employed herein (e.g SRIM) predict spatial atomic displacement profiles and structural vulnerabilities. While these simulations do not directly solve the drift-diffusion equations for electrical device performance, they quantify the primary defect generation rate. These simulated vacancies serve as structural precursors to deep-level trap states,

which are well-documented experimentally to drive non-radiative Shockley-Read-Hall (SRH) recombination and subsequent photovoltaic loss.

Across both materials, vacancy production is strongly energy-dependent, except for the 500 keV cases, where the dominant energy transfer mechanism has transitioned from nuclear stopping to electronic stopping. Low-energy protons produce shallow, halide-dominated damage. Mid-energy protons (50-100 keV) produce the largest displacement damage with peaks moving into active absorber regions and causing multi-species lattice disorder. Both compositions show a critical vulnerability to halide displacement which remains the dominant source of structural degradation throughout the proton energy spectrum studied in this paper.

Despite there being significant vacancy production in both materials, CsPbI_3 generally displays higher vacancy production than $\text{Cs}_3\text{Sb}_2\text{I}_9$ across low to mid-energy proton exposure, meaning the lead-based lattice suffers more structural degradation through displacement damage. The antimony-based material retains its B-site stability more effectively at low and mid energies. These results imply a high degree of substitutability of lead. However, translating this simulated displacement damage into macroscopic photovoltaic degradation requires examining the electronic nature of these specific defect centers.

DISCUSSION

Although the aim of this paper was to investigate the comparative vacancy profiles of lead-based and lead-substituted inorganic metal-halide perovskites, an interesting finding is presented in this piece: iodine displacement dominates across all energies and both compositions, confirming that halide loss is the primary structural vulnerability in these perovskites. This finding aligns with known halide migration-driven degradation in terrestrial perovskites and highlights an even more urgent role for halide stabilization in high radiation environments. This, alongside the stronger B-site stability of antimony compared to lead suggests that improving radiation hardness in inorganic IMH perovskites, and subsequently photovoltaic devices, requires design strategies that prioritize halide binding strength and suppression of vacancy accumulation in the active absorber region.

While this computational framework established a structural vulnerability profile, the actual irreversible photovoltaic degradation depends on how these physical vacancies translate to electronic defect states. But in a real-world device, these radiation-induced point defects do indeed disrupt lattice symmetry, introducing mid-gap states. Hence, calculated increase or decrease in vacancy density can be correlated with performance loss to some degree, pertaining to the experimentally observed reduction in open-circuit voltage.

Since IMH perovskites have self-healing properties, a simulated vacancy-interstitial pair (Frenkel pair) might recombine and self-heal at room temperature. Our simulations calculate generated defects, but do not account for their potential reversibility. This can be misleading in terms of macroscopic material

damage because actual device degradation is governed by only the retained stable defects after ambient thermal annealing.

Furthermore, not all simulated vacancies essentially kill device performance. Some vacancies are benign. For example, iodine vacancies often create shallow states near the conduction/valence bands, which are relatively benign. Lead or organic cation vacancies, however, are more likely to create deep traps in the lattice. Therefore, we also need to consider the nature of specific vacancies in order to make any judgments regarding macroscopic degradation or device performance loss.

This study could potentially help us on a journey towards radiation-hardened perovskites for space photovoltaics if reproduced with higher energy values - those representative of radiation present in these extraterrestrial environments.

CONCLUSION

Monte Carlo radiation damage modeling demonstrates that both CsPbI_3 and $\text{Cs}_3\text{Sb}_2\text{I}_9$ remain vulnerable to halide vacancy formation under proton irradiation, with peak structural damage occurring at mid-range proton energies. Although $\text{Cs}_3\text{Sb}_2\text{I}_9$ suffers significant halide displacement, it shows modest advantages in B-site resilience. These results indicate that although lead-substitution alone cannot guarantee radiation-hardened performance and targeted halide stabilization is essential, antimony can be a good candidate to substitute the toxic lead in IMH perovskites.

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