East European Journal of Physics. 2. 361-367 (2026)
DOI:10.26565/2312-4334-2026-2-38 ISSN 2312-4334

MODELING THE EFFECT OF Co-ION IMPLANTATION ON ZnO, Mg-DOPED ZnO THIN FILMS USING MONTE CARLO SRIM

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Received February 28, 2026; revised May 6, 2026; accepted May 20, 2026

The interaction behavior of 1.25 MeV Co ions with Si, ZnO, and Mg-doped ZnO (ZnO:Mg) targets has been systematically analyzed using the latest SRIM 2013 simulations. The findings show that atomic displacements, the production of vacancies and energy loss are greatly influenced by the composition and structural density of the target. The results reveal that the highest number of atomic displacements is observed in crystalline Si, followed by ZnO, whereas Mg-doped ZnO exhibits the lowest displacement level. On the other hand, ZnO exhibits moderate defect generation, as its high atomic density and bonding energy make it harder for the lattice to become disordered. Moreover, the presence of Mg in the ZnO matrix slightly reduces overall damage, indicating that the lattice is more stable and tolerant to radiation. These results indicate that Mg doping improves the structural robustness of ZnO against high-energy Co-ion bombardment, thereby making ZnO:Mg films more appropriate for radiation-resistant optoelectronic and sensing applications.
Keywords: *Stopping power; ZnO; Mg-doped ZnO; SRIM; Ion implantation; Vacancy; Defect; Radiation damage; Monte Carlo simulation*
PACS: 61.72.U

INTRODUCTION

In recent years, ion implantation techniques have become one of the most widely used methods for manipulating the physical, structural, and electronic properties of semiconductor materials. The ability to precisely control the energy, flux, and type of ions allows researchers to modify the properties of materials at the atomic level. This is especially important for creating materials that will operate in high-radiation environments or under extreme conditions. Among the various ions studied for this purpose, cobalt (Co) stands out due to its medium atomic mass, its ability to interact strongly with electronic and nuclear systems, and its ability to simultaneously induce magnetic and structural changes in oxide-based semiconductors [1].

Zinc oxide (ZnO) is a group II–VI compound with a wide band gap ($E_g \approx 3.3$ eV). Due to its unique properties such as high optical transparency, piezoelectric properties, and chemical stability, it is used as a key material in the development of optoelectronic devices [2], gas sensors [3], ultraviolet photodetectors [4], and transparent conductive films. However, ZnO can change its crystal structure and form defects when exposed to high-energy particles or radiation [5]. The defects formed by such radiation, for example, oxygen vacancies, zinc interstitial atoms, or complex defect clusters, can significantly change electrical and optical conductivity, carrier mobility, and even the type of conductivity [6]. Therefore, improving the radiation resistance and defect stability of ZnO materials is one of the most important issues in modern semiconductor physics today.

One of the most effective ways to improve the radiation resistance of ZnO is to introduce other elements instead of cations (doping), and magnesium (Mg) atoms are especially widely used in this process. The incorporation of Mg^{2+} cations into the Zn^{2+} sublattice leads to a noticeable widening of the band gap energy [7], accompanied by an improvement in the crystalline rigidity and enhancement of the overall lattice stability of the ZnO matrix [8].Therefore, ZnO doped with Mg (ZnO:Mg) is considered a promising material for optoelectronic and sensor systems that operate stably under radiation and high-temperature conditions. However, the interaction process of high-energy ions with pure and doped ZnO systems has not been sufficiently studied. To understand this process in depth, an analysis of the atomic-level interaction mechanisms between ions and solids is required. When Co ions with an energy of 1.25 MeV pass through a solid, they lose their energy mainly through two main processes: electron stopping (inelastic collisions with electrons of target atoms) and nuclear stopping (elastic collisions with atomic nuclei) [9]. The ratio of these two mechanisms determines the depth of ion penetration (ion range) and the nature and spatial distribution of structural damage. The degree of energy scattering and the processes of atom recoil are determined by the mass and charge of the ion, as well as the density, atomic mass and binding energy of the target material. These parameters reflect changes in the material's properties under radiation and determine its operational stability. To accurately describe and predict these interaction processes, Monte Carlo-type

Cite as: A.Y. Boboev, N.Y. Yunusaliyev, B.M. Ergashev, G.G. Tojiboyev, S.R. Kadirov, M.M. Arabboeva, East Eur. J. Phys. 2, 361 (2026), https://doi.org/10.26565/2312-4334-2026-2-38
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computational models, in particular the Stopping and Range of Ions in Matter (SRIM) software package, are widely used [10]. SRIM simulations enable accurate calculations of parameters such as ion trajectories, stopping powers, recoil distributions, ion ranges, and defect formation rates. This allows for microscopic analysis of energy distribution processes and lattice failure mechanisms. While experimental measurements are often performed under complex and constrained conditions, SRIM-based calculations provide a fully theoretical, yet informative method for comparing different material systems.

In this work, the interaction of Co ions with 1.25 MeV energy with silicon (Si), pure ZnO, and Mg-doped ZnO (ZnO:Mg) thin films was modeled using Monte Carlo SRIM-2013 simulations. The selection of these materials enables a comparative analysis of the radiation response of semiconductors with different atomic masses and structural characteristics. The research primarily focuses on evaluating the mechanisms of energy loss, the behavior of stopping power, and the tendencies of damage formation. Particular attention was given to analyzing how incorporating Mg into the ZnO lattice alters energy-dissipation pathways and structural response mechanisms under cobalt-ion irradiation. These findings serve as an important theoretical basis for designing radiation-resistant variants of oxide semiconductors.

THEORETICAL DETAILS

Simulation tools are essential to modern materials science and semiconductor physics for understanding ion interactions with solid targets. Through these computational approaches, scientists can at least partly represent the atomic-scale phenomena that are otherwise difficult to observe in the laboratory. One of the most popular and trusted Monte Carlo–based programs is SRIM (Stopping and Range of Ions in Matter). SRIM programs enable the determination of ionic trajectories, energy-loss mechanisms, and defect formation within complex multilayer structures [11]. The SRIM code provides a self-consistent framework for estimating the energy loss and scattering of Co ions as they pass through the Si, ZnO, and ZnO:Mg thin films. The present study, using SRIM 2013, simulated the implantation of 1.25 MeV Co ions into the three systems mentioned above to analyze their stopping power, penetration depth, and structural damage characteristics. The program simulates the trajectory of each ion as a sequence of discrete elastic and inelastic collisions with the target atoms, represented by a statistical Monte Carlo algorithm. Kinetic energy loss occurs with every collision and is shared between the two processes: nuclear stopping (elastic scattering) and electronic stopping (inelastic ion–electron interactions). The ions slowly lose their energy as they pass through the target material, where their paths are also slightly altered by small-angle scattering events. The total energy loss per unit distance (stopping power or –dE/dx) is a crucial metric that indicates the extent to which a material either absorbs or dissipates the energy of the ion [12,13]. At high energies in this scenario, electronic stopping power is the primary factor, as the incident ions dissipate their kinetic energy primarily through ionization and excitation of target atoms. This kind of interaction that leads to the path of the Co ions in Si and ZnO lattices. As energy loss continues, nuclear stopping becomes increasingly dominant at lower energies, especially in the end-of-range (EOR) region, where ions move slowly, and interactions lead to large atomic displacements and the creation of vacancies [14]. The simulations play a crucial role in anticipating material responses during and after irradiation, especially in semiconductor production, where ion implantation is a common practice for doping and modifying interfaces. The precision of SRIM in calculating stopping powers, recoil distributions, and ionization profiles makes it an essential tool for microelectronics, thin-film technology, and radiation protection research. Besides SRIM, there are other computational packages like TRIM, TRIDYN, and SDTrimSP that also employ Monte Carlo algorithms to simulate dynamic ion–solid interactions; nevertheless, SRIM remains the most convenient and widely compared to other methods owing to its well-validated physics models and user-friendly interface [15]. Theoretically, SRIM simulations are consistent with analytical models, such as the Bethe–Bloch equation, which quantifies the electronic energy loss of fast-moving charged particles in solids. Although Bethe–Bloch provides a continuous slowing-down approximation, SRIM not only goes beyond it but also accounts for stochastic (random) collision processes associated with angular scattering, secondary atom recoils, and defect cascades. This mixed theory-numerical method provides a clear view of both the spatial and energetic distributions of ion-induced damage. In the current situation, SRIM simulations are in accord with the following atomic density and structural stiffness; therefore, the total damage energy, vacancy concentration, and atomic displacements have been systematically decreased from Si to ZnO to ZnO:Mg. The propagation of electronic stopping at the initial stage of penetration and the rise in the nuclear-collision contribution near the EOR are the reasons behind the characteristic Bragg-like energy-deposition profiles for each material. Knowledge of these phenomena is important for guiding the development of radiation-resistant semiconductors and for altering material properties through compositional engineering. So, the SRIM-based Monte Carlo framework not only provides a clear method but also a robust one for visualizing and quantifying the energy loss of different materials due to Co ions and the resulting structural changes. The results of such computational experiments are useful not only for explaining radiation-matter interactions but also for producing advanced oxide semiconductors with improved resilience and greater control over defect architecture.

The aforementioned prospects render SRIM a necessary tool in present-day materials research, as it connects theoretical models, experimental verification, and technological applications in ion-beam engineering.

RESULTS AND DISCUSSION

The implant simulation of 1.25 MeV cobalt (Co) ions was performed using the SRIM 2013 code for three different target materials: silicon (Si), zinc oxide (ZnO), and magnesium-doped zinc oxide (ZnO:Mg). The physical parameters used

in the study were based on experimentally reported values and verified literature data [16-18]. The simulation geometry created a Co ion beam of uniform density that was incident normally on the planar target layers, as depicted in Figure 1.

The density of crystalline silicon was set at 2.321 g/cm^{-3} and that of pure ZnO was fixed at 4.074 g/cm^{-3}. The density of Mg-doped ZnO layer was decreased to 3.972 g/cm^{-3}, which was equivalent to atomic ratios of Zn (44.3 %), O (51.7 %), and Mg (4.0 %). The displacement energies were determined according to the elemental composition: 15 eV for Si, and 25 eV (Zn) and 28 eV (O) for the ZnO-based systems. The surface and lattice binding energies were also modified according to the stronger ionic covalent bonding nature of the Zn-O and Zn-Mg lattices.

Table 1. Chemical formula of the samples.

Material	Chemical Formula
Silicon Substrate	Si
Zinc oxide	ZnO
Magnesium-doped zinc oxide	ZnO:Mg

RESULTS AND DISCUSSION

The different target layers and recoiled atoms are visualized through these graphs (Figure 1). The sketched trajectories indicate the energy consumption, scattering, and material transformation that happened during ion penetration. Silicon (Fig. 1a) allowed Co ions to form the longest and most extensive tracks, as they penetrated deep into the substrate and straggled widely laterally. This behavior is due to Silicon's relatively low atomic mass and density (2.321 g/cm^{-3}), which results in lower resistance to incident ions. The spatial distribution of ion trajectories is thick and elongated, showing that ions still have a considerable fraction of their kinetic energy before considerable deceleration takes place. The large scattering angle distribution indicates that elastic nuclear collisions significantly contribute to energy dissipation close to the end of the range, resulting in higher defect concentration and displacement density within the silicon matrix. According to SRIM-derived data, the mean projected range of Co ions in silicon reached approximately 1.8 μm, confirming that Si possesses the deepest penetration path and the largest longitudinal straggling among the studied materials. This greater ion range correlates with the low stopping power of Si, allowing Co ions to retain high kinetic energy over longer distances before substantial deceleration. Consequently, silicon exhibits the most extended collision cascades and the largest damage region within its lattice.

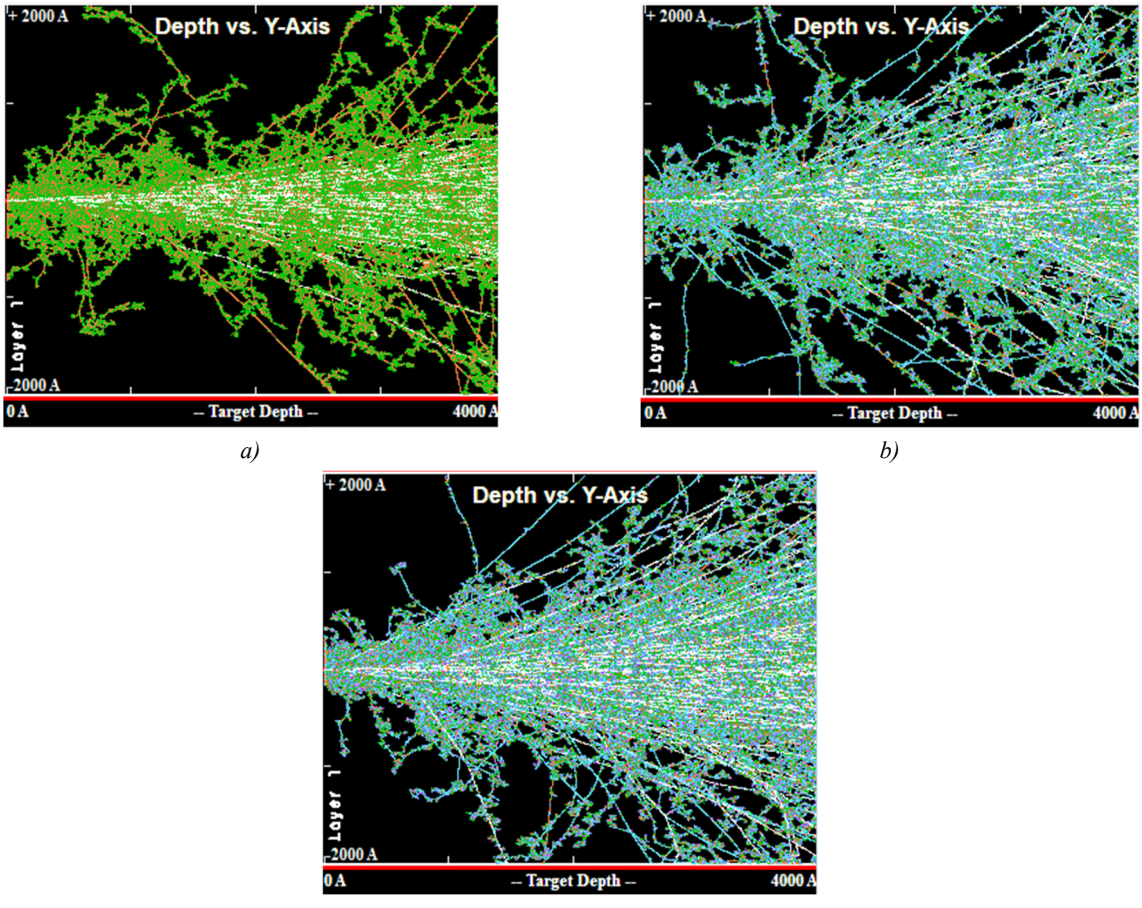

Figure 1. SRIM-simulated ion trajectories of 1.25 MeV Co ions in (a) ZnO, (b) ZnO:S, and (c) ZnO:S/Si targets showing the longitudinal distribution and scattering profiles of implanted ions through the target depth.

On the other hand, for ZnO (Fig. 1b), the ion trajectories are shorter and more compact compared to those in Si. The atomic arrangement is denser (4.074 g/cm^{-3}), and the ionic bonding is stronger (Zn–O bonding), which together restrict penetration depth and scattering amplitude. Most Co ions are stopped within a projected range of around 1.2 μm (or ≈ 276 nm in thin-film geometry), where the energy loss mainly occurs through the transition from electronic to nuclear stopping. The higher atomic masses of Zn and O atoms leads to reduced recoil mobility, thus confining the cascade within a very small volume. Hence the ZnO structure undergoes moderate atomic displacements and there is a distinct central collision zone that is followed by rapid energy attenuation. This behavior demonstrates that ZnO's stronger ionic–covalent bonding provides greater resistance to structural disorder than in silicon, leading to reduced defect density and shallower ion paths. The average displacement energy values of Zn = 25 eV and O = 28 eV ensure that most recoil events are localized near the end-of-range (EOR) region [19,20].

In ZnO:Mg (Fig. 1c), the Co ion paths are more uniformly scattered and their concentrations are lower at the end-of-range area. The presence of Mg atoms influences the lattice structure and decreases the average electron density slightly, this in turn leads to the reduction of both electronic and nuclear stopping probabilities. The resultant scattering pattern is therefore smoother and more uniform. The film doped with elements exhibits a lesser number of extended collision chains and lower lateral dispersion which signifies that the structural tolerance to energetic ion impact has been improved. The mean projected range for ZnO:Mg was estimated at 1.0–1.1 μm, indicating the shortest ion penetration depth among all materials studied. This reduction in range corresponds to an increase in the effective stopping power and lattice stability. Magnesium atoms, having a lighter atomic mass (24 amu), act as local energy buffers that moderate recoil cascades and mitigate defect accumulation, leading to enhanced radiation tolerance. ZnO:Mg is less affected by recoils and has a smaller energy dissipation profile when compared to pure ZnO, which means its lattice has a greater ability to relax and less damage to accumulate. All in all, the longitudinal trajectory maps in this work provide strong, unambiguous evidence that the penetration depth and scattering intensity take the order Si > ZnO > ZnO:Mg. The Si target not only suffers the most but also the disorder and range are the most extreme, while the introduction of Mg into the ZnO lattice leads to a more durable and less radiation-sensitive structure. These results agree with the assertion that modifying the composition—most notably, the addition of Mg—has a beneficial effect in the reduction of radiation-induced defects, thus making ZnO:Mg a more reliable material for semiconductor and thin-film applications where ion irradiation is involved. SRIM presents its calculations of total displacements, vacancies, and replacement collisions induced by 1.25 MeV Co ions in Si, ZnO, and ZnO:Mg targets. The simulated data shed light on the defect-formation tendencies of each material in a comparative manner [21]. The displacement and vacancy curves show how well each target resists atomic disorder under high-energy Co-ion bombardment (Figure 2).

In the case of silicon (Si), the total number of atomic displacements reaches its maximum, approximately 3090 displacements per ion, indicating that Si is the most susceptible to radiation-induced damage. This immense defect creation is ascribed to Silicon's low atomic mass and weak bonding forces which together allow for the easier transfer of kinetic energy from the impinging Co ions to the lattice atoms. Consequently, nuclear collisions and electronic energy losses greatly facilitate the creation of vacancies and interstitial defects. The high vacancy number (∼3016/ion) and large replacement collision rate (74/ion) show that there is a lot of atomic mixing and cascade overlapping going on in the crystal lattice.

For zinc oxide (ZnO), the total number of atomic displacements is slightly lower, reaching approximately 3038 displacements per ion, indicating a comparable but slightly reduced level of damage relative to Si. This means that ZnO, although less damaged than Si by metal ion bombardment, nevertheless absorbs a whole lot of ion energy due to its higher density and mass (Zn = 65, O = 16) but its more rigid ionic–covalent bonds do not allow atom to migrate. Thus, zinc oxide's effective stopping power not only limits atomic displacements but also confines recoil cascades to compact near-surface regions, minimizing large-scale rearrangements. This confirms that ZnO exhibits moderate structural damage and enhanced defect localization under energetic Co ion exposure. The Zn and O sublattices tend to prevent not only the formation of large-scale atomic rearrangements but also the creation of deep collision cascades. Therefore, most of the recoil events take place near the end-of-range region, resulting in the formation of compact and shallow damage zones instead of deep ones In Mg-doped ZnO (ZnO:Mg), the total number of atomic displacements decreases further to approximately 2879 displacements per ion, demonstrating that Mg incorporation effectively suppresses radiation-induced defect formation. This decrease indicates that the incorporation of Mg atoms effectively suppresses lattice damage and mitigates the extent of defect cascade formation within the ZnO matrix [22]. The lighter Mg atoms are like local "energy buffers" that have the effect of softening the incoming energy and, at the same time, reducing the defect accumulation. The vacancy concentration (∼2654/ion) still stays lower than that of pure ZnO and Si, thus the radiation tolerance is notably superior. The comparison among all the three targets gives a clear indication of one important fact, that is, the efficiency of ion-induced disorder has been systematically reduced according to the trend Si > ZnO > ZnO:Mg. This diminishing pattern is connected to the three factors of atomic bonding, density, and displacement energy among the materials [23]. Silicon, owing to its relatively low atomic mass, low density, and covalent bonding structure, is more susceptible to recoil displacement, whereas the ionic–covalent Zn–O framework exhibits greater resistance to such displacement. The better part is that the doping with Mg creates an even more stable situation with regard to the mentioned factors by increasing the overall scattering cross-section and, thus, slowing down the escape movement from the lattice. To conclude, the SRIM simulations reveal that Co ion implantation leads to the highest level of lattice defects in Si and moderate damage in ZnO, while the lowest defect density is observed in ZnO:Mg.

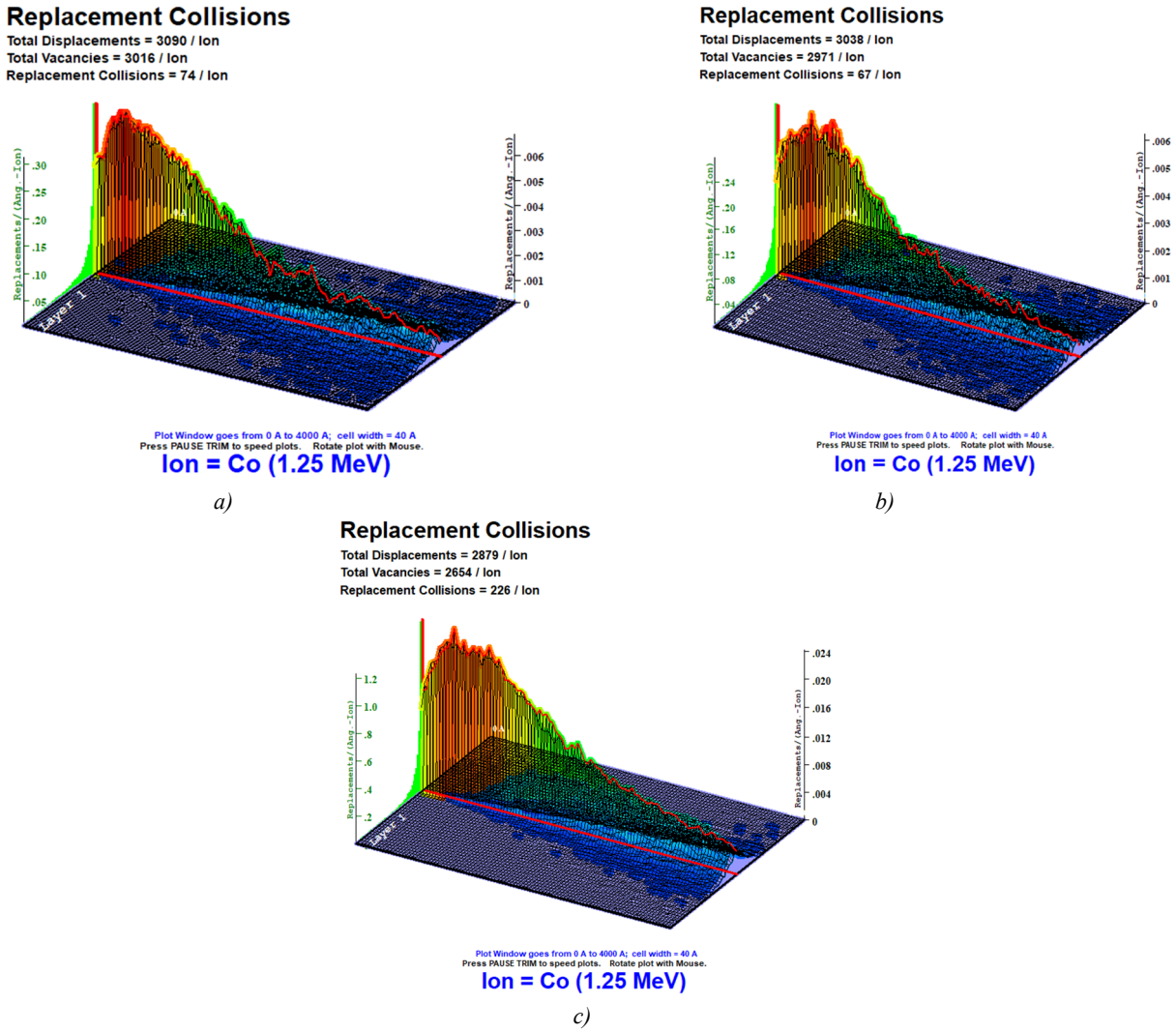

Figure 2. SRIM-simulated total displacements, vacancies, and replacement collisions produced by 1.25 MeV Co ion implantation in (a) Si, (b) ZnO, and (c) ZnO:Mg targets

The drop in total displacements and replacement collisions in Mg-doped ZnO demonstrates its great potential as a radiation-hardened oxide semiconductor for advanced optoelectronic and sensor applications that must operate in ionizing environments.

CONCLUSIONS

The Monte Carlo-based SRIM-2013 simulation was used to analyze the stopping behavior, energy dissipation, and defect formation processes of 1.25 MeV Co ions in Si, ZnO, and ZnO:Mg targets. The following main conclusions were drawn from the calculation results:

1. The ion penetration depth showed a strong dependence on the material composition, and the average projection range values were ≈ 1.8 μm for Si, ≈ 1.2 μm for ZnO, and ≈ 1.0–1.1 μm for ZnO:Mg.

2. The SRIM results show that the total number of atomic displacements is highest in Si (~3.09×10^3 displacements per ion), slightly lower in ZnO (~3.04×10^3 displacements per ion), and lowest in ZnO:Mg (~2.88×10^3 displacements per ion). This confirms that Mg incorporation into the ZnO lattice suppresses defect formation and enhances the radiation tolerance of ZnO:Mg.

3. The introduction of Mg^{2+} ions into the Zn^{2+} lattice changed the atomic mass and potential field, increased the lattice stability and smoothed the energy distribution. This significantly improved the radiation resistance of ZnO:Mg and reduced the depth distribution of defects.

4. The stopping power (–dE/dx) dominated at high energies in the electron stopping stage, and nuclear scattering mechanisms played a dominant role in the EOR (End-of-Range) region. Therefore, the energy distribution formed a Bragg-type profile for each material.

Thus, it was found that Mg-doped ZnO can be effectively used as the most stable and radiation-resistant oxide semiconductor against high-energy particles.

The results obtained serve as an important basis for improving the stability of optoelectronic and gas-sensing devices operating in ion-irradiation environments.

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МОДЕЛЮВАННЯ ВПЛИВУ Co-ІОННОЇ ІМПЛАНТАЦІЇ НА ТОНКІ ПЛІВКИ ZnO, ЛЕГОВАНІ Mg ЗА ДОПОМОГОЮ МОНТЕ-КАРЛО SRIM

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Поведінка взаємодії іонів Co з енергією 1,25 МеВ з мішенями ZnO (ZnO:Mg), легованими Si, ZnO та Mg, була систематично проаналізована за допомогою останньої версії симуляційного пакета SRIM 2013. Результати показують, що атомні зміщення, утворення вакансій та втрати енергії значною мірою залежать від складу та структурної щільності мішені. Результати показують, що найвища концентрація дефектів спостерігається в кристалічному Si через його нижчу порогову енергію зміщення та меншу атомну масу, що підвищує ймовірність зіткнень віддачі. З іншого боку, ZnO демонструє помірне утворення дефектів, оскільки його висока атомна щільність та енергія зв'язку ускладнюють упорядкування решітки. Крім того, присутність Mg у матриці ZnO дещо зменшує загальне пошкодження, що означає, що решітка стабільніша та стійкіша до впливу радіації. З цих результатів можна зробити висновок, що легування Mg дійсно покращує структурну стійкість ZnO до бомбардування високоенергетичними іонами Co і таким чином робить плівки ZnO:Mg більш придатними для радіаційно стійких оптоелектронних та сенсорних застосувань.

Ключові слова: *гальмівна здатність; ZnO; ZnO, легований Mg; SRIM; іонна імплантація; вакансія; дефект; радіаційне пошкодження; моделювання методом Монте-Карло*