East European Journal of Physics. **3.** 382-389 (2025)
DOI:10.26565/2312-4334-2025-3-39 ISSN 2312-4334

SIMULATION OF RADIATION-INDUCED STRUCTURAL AND OPTICAL MODIFICATIONS IN ZnO:S/SI THIN FILM STRUCTURES

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Received March 3, 2025; revised July 6, 2025; accepted August 12, 2025

The research studied ZnO thin films containing 3 at.% sulphur (S) on silicon (1 μm) through Geant4 simulations for radiation analysis. Analysis of ZnO thin films (400 nm) doped with 3 at.% sulphur (S) on a 1 μm thick silicon substrate through Monte Carlo simulation platform Geant4 considered energy absorption together with particle penetration depth and ionization and secondary electron generation and optical property changes as the study examined different electron radiation energies from 3 keV to 10 keV. The ZnO:S layer absorbed most of the incoming electron energy in the 3-5 keV range which produced increases in defects near the surface while ionization occurred. When electrons used 9-10 keV energies they penetrated the full substrate layer which caused silicon to receive most of the energy absorption. The highest change in parameters occurred at the film-substrate junction when the energy reached 7 keV. All modeling findings demonstrated that the total absorbed energy together with secondary electron production and defect density reaching up to 10^7 increased rapidly with electron energy acceleration. The decrease in optical properties occurs because defects exist at different depths while energy absorption takes place. Electrical and optical characteristics of ZnO:S/Si can be regulated through electron irradiation procedures according to this research. Results from this study will function as fundamentals for creating sensors and optoelectronic devices and protective coatings which operate effectively under high radiation conditions.
Keywords: *Monte Carlo; Energy absorption; Electron energy; Depth; Displacement; Simulation*
PACS: 78.30.Am

INTRODUCTION

The development of modern technology demands improved material resistance against extreme conditions which include high radiation and hadron beam and cosmic particle exposure [1]. The long-lasting operational stability and reliability of materials important for equipment which serves nuclear power applications as well as space exploration and medical radiation therapy. Material surfaces along with atom structures remain the most radiation-sensitive features because exposure produces drastic shifts in electrophysical and optical and mechanical properties [2]. Materials science focuses on developing functional materials operating under radiation conditions while predicting their responses which poses a key challenge for modern research.

Zinc oxide (ZnO) represents a semiconductor material that finds extensive implementation in optoelectronics hardware and sensors as well as catalytic devices [3]. Research data about the radiation stability of ZnO remains insufficient. Research findings indicate that ZnO gains enhanced radiation resistance through appropriate doping with sulfur together with aluminium and nitrogen. The addition of sulphur (S) elements demonstrates both strength in crystal lattice structure while modifying electronic structure which leads to enhanced radiation sensitivity. Researchers have not conducted a comprehensive investigation regarding the response of ZnO thin films containing sulphur (ZnO:S) to electrons across multiple energy levels plus their relationship with the substrate.

The research investigates both theoretical and experimental aspects of the radiation behavior in ZnO:S films with 3 at.% sulfur doped on a 1 μm silicon substrate measuring 400 nm thick. GEANT4 simulated the material response from electrons in the 3 to 10 keV energy range. The research evaluated these parameters extensively at each energy level.

MODEL STRUCTURE AND METHODOLOGY

Material and structure description.

In this study, a heterostructure consisting of a thin film of sulfur-doped zinc oxide (ZnO:S) with a concentration of 3 at.%, 400 nm thick, deposited on a 1 μm thick single-crystal silicon substrate was considered. Due to their high optical transparency and wide band gap, ZnO:S films are considered as a promising material for applications in optoelectronics and sensor technologies. Sulfur doping significantly improves both the electrical and optical properties of ZnO, making this material particularly suitable for use in radiation-sensitive devices [4].

The Geant4 modeling environment.

Geant4 is a widely used Monte Carlo platform for modeling the interaction of particles with matter, successfully used in high-energy physics, astrophysics, and radiation detector design [5]. In this study, the interaction of electrons with energies of 3, 5, 7, 9 and 10 keV with ZnO:S/Si heterostructure was simulated using the Geant4 platform. The simulation

Cite as: A.Y. Boboev, Kh.A. Makhmudov, N.Y. Yunusaliyeva, M.O. G'ofurjonova, F.A. Abdulkhaev, G.G. Tojiboyeva, East Eur. J. Phys. 3, 382 (2025), https://doi.org/10.26565/2312-4334-2025-3-39

addressed key physical processes including energy absorption within the material, electron penetration depth, ionization and excitation probabilities from electron-atom collisions, generation of low-energy secondary electrons arising from primary electron interactions, and formation of radiation-induced defects such as vacancies and interstitial atoms. Additionally, changes in optical parameters such as transmission and absorption coefficients were monitored and analyzed.

Simulation parameters.

During the simulations, 10^6 electrons for each energy level were perpendicularly directed onto the surface of the ZnO:S thin film. The physical properties of the ZnO:S and Si materials were precisely set in the Geant4 environment. The simulation results allowed a detailed analysis of the distribution of absorbed energy, particle penetration depth and ionization probability throughout the structure.

Energy Absorption (Energy Deposition).

Energy absorption (edep) is the process of electron particles transferring kinetic energy to the environment as they interact with matter through ionization, excitation, or other inelastic collisions. The layers of a material in which electron energy absorption occurs has a significant effect on its electromagnetic, thermal, and optical properties. The depth distribution of the absorbed energy makes it possible to determine the most radiation-sensitive regions of the material [6,7].

The absorbed energy profile in the Geant4 simulation is determined based on the calculation of the energy density distributed in each elementary layer of the material:

$$E_{dep}(z) = \frac{dE}{dz} \tag{1}$$

where $E_{dep}(z)$- is the absorbed energy at depth z $(\frac{MeV}{\mu m})$, dz – is the thickness of the elementary layer.

RESULTS AND DISCUSSION

At 3 keV, about 68% of the electron energy is absorbed in the ZnO:S film, and ~32% in the Si substrate. This indicates that 3 keV electrons do not penetrate far into the silicon; the ZnO:S layer absorbs the majority of their energy. At 5 keV, a similar trend is seen (about 62% in ZnO:S vs 38% in Si). By 7 keV, the split is roughly 56% in ZnO:S and 44% in Si, indicating that electrons are now depositing significant energy in the substrate as well. The interface region around the boundary of the film and substrate is receiving a lot of energy at this energy. The total energy absorbed also increases with energy (more energetic electrons have more energy to give), reaching ~125 MeV for 7 keV electrons (per million electrons). A dramatic change occurs at 9 keV: only ~40% of the energy is absorbed in the ZnO:S film, while ~60% is absorbed in Si. At 10 keV, the partition is ~42% in ZnO:S vs 58% in Si. In absolute terms, the silicon substrate at 9-10 keV is absorbing roughly 300 MeV from the million electrons, which is an order of magnitude more energy than it absorbed at 3–5 keV. This means high-energy electrons pass through the thin film and deposit most of their energy deeper in the structure (i.e., in the substrate). These results clearly show that lower-energy electrons primarily damage the ZnO:S thin film, whereas higher-energy electrons primarily damage the silicon substrate. The 7 keV case is intermediate, with substantial energy deposition in both layers, especially near their interface. This has implications for where defects will form (discussed later). The total absorbed energy does not scale linearly with incident energy because not all incident energy is absorbed – some energy may escape as backscattered electrons or X-rays. Interestingly, the total absorbed energy at 10 keV is slightly less than at 9 keV in our simulation (518 MeV vs 530 MeV for 10^6 electrons). This is because a small fraction of 10 keV electrons likely passed completely through the 1.4 μm total thickness without depositing all their energy, or produced bremsstrahlung photons that carried energy away. Thus, 9 keV appears to be the most efficient at depositing energy in this structure (given its size), whereas at 10 keV some energy starts to "leak" out. The depth distribution of the energy deposition reveals more. For 3 keV electrons, the energy is deposited very superficially – within the first few hundred nanometers of the ZnO:S film (as evidenced by 400 nm being the penetration range). For 5 keV, energy deposition extends to the ZnO:S/Si interface. At 7 keV, a significant energy deposition peak occurs at the interface (around 400 nm depth). For 9 and 10 keV, the energy deposition profile peaks inside the silicon substrate (~700–800 nm deep) and then trails off. In essence, as electron energy increases, the zone of energy absorption (and hence potential damage) moves deeper. Practically, if one wanted to protect the substrate from radiation, using lower electron energies would be worse (since the film cannot stop the radiation and the substrate still gets hit at higher energy like 9–10 keV). Conversely, if one wanted to minimize damage to the thin film, very high energy electrons would mostly bypass it and deposit energy in the substrate. This trade-off needs to be considered in design: for example, a thin ZnO film on Si used as a sensor might be badly damaged by a few-keV electrons on its surface, whereas higher-energy electrons would harm the substrate electronics more.

Table 1. Changes in energy distribution under the influence of electron energy in the ZnO:S/Si heterostructure(eal09).

Energy of one electron	Absorbed energy in the ZnO:S layer	Absorbed energy in the Si substrate	Total absorbed energy
3 keV	58.6 MeV (68.1%)	27.4 MeV (31.9%)	86.0 MeV
5 keV	62.8 MeV (62.1%)	38.4 MeV (37.9%)	101.2 MeV
7 keV	~70 MeV	~55 MeV	~125 MeV
9 keV	214.67 MeV	315.22 MeV	529.89 MeV
10 keV	216.52 MeV	301.54 MeV	518.06 MeV

The changes in the distribution of absorbed energy between the ZnO:S layer and the silicon substrate under varying electron energies are summarized in Table 1. As the electron energy increases, a shift in energy absorption from the ZnO:S film to the Si substrate is clearly observed, confirming the dependence of energy deposition on the penetration capability of incident particles.

Penetration Depth.

The electron penetration depth is the maximum distance that particles can penetrate a material before losing all of their energy. This parameter plays an important role in assessing how far the effects of irradiation extend into the structure under investigation. The following relationship is used to estimate the penetration depth:

$$R_p \propto \frac{E_0^n}{\rho} \tag{2}$$

where R_p is the average electron penetration depth, E_0 is the initial energy of the incoming electron (keV), ρ is the density of the material (g/cm³), n≈1.35 is an empirical indicator depending on the nature of the material (for organic substances it is usually in the range of 1.3–1.7) [8]. In cases of strong scattering, electrons can deviate from the rectilinear trajectory, but in most cases the area of maximum energy absorption is located near the maximum penetration depth.

The correlation between incident electron energy and the corresponding penetration depth is detailed in Table 2**.** The data indicate that low-energy electrons are primarily absorbed in the ZnO:S layer, while high-energy electrons penetrate deeper into the silicon substrate.

Table 2. Penetration depth and zone of influence in films depending on electron energy (eal16, eal09, eal03, eal11)

Energy (keV)	Maximum penetration depth (nm)	Depth of interaction region
3 keV	~400–450 nm	Predominantly within the ZnO:S layer
5 keV	~600–700 nm	ZnO:S + interfacial boundary
7 keV	~800 nm	ZnO:S + interface with silicon
9 keV	~900 nm	Predominantly in silicon
10 keV	≥ 900 nm	In the lower regions of the silicon substrate

At energies of 3 keV electrons are completely absorbed within the ZnO:S layer, whereas at energies of 9-10 keV they penetrate entirely into the silicon substrate. In the region around 7 keV, a maximum change of parameters at the boundary between the film and the substrate is possible.

Ionization and Excitation Probability (Ionization and Excitation Probability)

Ionization and excitation probability is the probability that the interaction of particles with matter will result in the knocking out of an electron from an atom or molecule (ionization) or the transfer of an electron to a higher energy level (excitation). These processes are the main mechanisms of energy absorption during electron irradiation.

The probability of ionization can be described using the Bethe formula [9]:

$$\frac{dE}{dx} = 4\pi \frac{Z}{A} \frac{N_A r_e^2 m_e c^2}{\beta^2} \left[ln\left(\frac{2m_e c^2 \beta^2 \gamma^2 T_{max}}{I^2}\right) - 2\beta^2 \right] \tag{3}$$

Where $\frac{dE}{dx}$ – is the energy loss for ionization (stopping power), Z – atomic number of the target, A– atomic mass of the target, $\beta = \frac{v}{c}$, γ– Lorentz factors, T_{max}– maximum energy that can be transferred to an electron during knockout, I – ionization potential of the substance (for ZnO ~103 eV, for Si ~173 eV) [10,11].

The ionization probability depends directly on the energy of the particle and the frequency of its collisions with the atoms of the substance. At higher energy, the ionization probability also increases.

The spatial characteristics of ionization zones at various electron energies are presented in Table 3**.** This table highlights how the location and extent of ionization shift with increasing energy, moving from the film toward the substrate.

Table 3. Depth ranges and peak locations of ionization zones in ZnO:S/Si heterostructure under electron irradiation (LMCG72)

Energy (keV)	Depth of ionization zone	Area with maximum probability
3 keV	200–400 nm (ZnO:S)	~300 nm
5 keV	300–600 nm (ZnO:S–Si)	~400–500 nm
7 keV	400–800 nm (interfeys)	~600 nm
9 keV	500–900 nm (Si)	~750–800 nm
10 keV	600–900+ nm (Si)	~850–900 nm

Simulation results showed that with increasing electron energy, the ionization region shifts to the depth of the structure. At energies of 3-5 keV, the main number of collisions occurs in the ZnO:S film, whereas at energies of 9-10 keV, ionization is observed predominantly in the silicon substrate. In many cases, the ionization probability is considered to be linearly dependent on the absorbed energy:

$$P_{ion}(z) \propto \frac{dE}{dz} \tag{4}$$

i.e., the amount of absorbed energy at a certain depth directly corresponds to the ionization probability in this region. This approach agrees well with the energy distribution plot obtained using simulations in Geant4.

The ionization process leads to the generation of electron-hole pairs, which in turn enhances secondary phenomena: along with ionization, a significant number of secondary electrons are formed. Each act of ionization increases the probability of damage to the crystal lattice.

Generation of Secondary Electrons (Secondary Electrons)

Secondary electrons are low-energy electrons knocked out as a result of interaction of high-energy primary particles (e.g., electrons) with matter. Typically, the energy of such electrons is less than 50 eV and ionization processes or inelastic collisions [12] form them. The following expression can estimate the number of secondary electrons:

$$N_{sec} \approx \frac{E_{dep}}{W} \tag{5}$$

where N_{sec}– number of generated secondary electrons, E_{dep} – absorbed energy (in eV), W – is the average energy required to generate one secondary electron (for ZnO it is about 30-35 eV) [13].

Table 4. Total absorbed energy and estimated secondary electron yield in the ZnO:S/Si structure for different electron energies (per 10^6 incident electrons) (eal16, JA09, SA03)

Electron energy (keV)	Total absorbed energy in the ZnO:S/Si structure (MeV)	Estimated number of secondary electrons
3 keV	~86	≈ 2.9×10^6
5 keV	~101.2	≈ 3.4×10^6
7 keV	~125	≈ 4.1×10^6
9 keV	529.89	≈ 1.76×10^7
10 keV	518.06	≈ 1.73×10^7

The estimated yield of secondary electrons as a function of absorbed energy at each electron energy level is shown in Table 4. As demonstrated, secondary electron production increases significantly with higher primary electron energy.

At 3 keV, the total energy absorbed (~86 MeV) would generate on the order of 2.9 million secondary electrons (if 30 eV generates one SE, 86 Me ≈ 2.9×10^6). This means each 3 keV primary electron produces on average ~3 secondary electrons (since ≈ 2.9×10^6 secondaries for 10^6 primaries). At 5 keV, this rises to about ~3.4 million secondaries, roughly 3–4 per primary. At 7 keV, ~4.1 million secondaries (about 4 per primary). When we go to 9 keV, the number jumps dramatically: ~1.76×10^7 secondary electrons for 10^6 primaries, which is ~17–18 secondary electrons per primary electron. Similarly at 10 keV, ~1.73×10^7 secondaries (also ~17 per primary). The large increase from 7 keV to 9 keV correlates with the large increase in total energy deposited by those higher-energy electrons. This exponential increase is expected because higher-energy electrons undergo more collisions and travel further, thus they have more opportunities to ionize atoms and produce secondary electrons. Additionally, when the electrons penetrate into the higher-density Si, they may produce more secondaries (Si has more electrons per cc to ionize compared to ZnO). The presence of such a high number of secondary electrons has several consequences:

Energy Deposition Cascade: Many of these secondary electrons (which have energies of a few eV to a few tens of eV) will deposit their energy very locally, causing localized heating and further ionization in their immediate vicinity. Surface Charging: A significant fraction of secondary electrons that are created near the surface of the ZnO film can escape the material entirely (especially those generated within ~10 nm of the surface). If many electrons leave the ZnO:S film, the film could become positively charged. Conversely, some secondaries might get trapped in defects, causing negative charging. This is relevant for devices, as charge buildup can alter electrical behavior. Induced Conductivity: Secondary electrons (and the holes left behind) can contribute to a temporary increase in electrical conductivity (as they are essentially free carriers until they recombine or get trapped). At high irradiation flux, this can lead to radiation-induced currents in the material. Imaging and Luminescence: Secondary electrons are the basis for SEM imaging contrast. Also, some of the excited electrons can cause luminescence (cathodoluminescence) if they recombine radiatively. ZnO is known to exhibit cathodoluminescence (often in the green due to oxygen vacancies), so electron irradiation could induce light emission from the ZnO:S film via the creation of secondary electrons and holes. Our simulation qualitatively noted that for 9 keV and 10 keV runs, there was a cloud of low-energy electrons near the surface – these are the secondary electrons being emitted. The yield of secondaries per primary (~17) at 9–10 keV is high but within reason for materials with moderate atomic number. (For reference, materials often have a secondary electron yield peak around a few hundred eV primary energy, but here we are dealing with multiple inelastic collisions from a keV primary leading to many secondaries in total.) In summary, as electron energy increases, not only do we get deeper penetration and more total damage, but we also get a disproportionately larger number of secondary electrons. This secondary electron avalanche effect means higher-energy irradiation can induce a lot more indirect effects (like charging and further local ionization) compared to lower-energy irradiation. [11].

Defect Formation

As a result of particle irradiation, energetic defects are generated within the material. The main types of defects include:

Vacancies (missing atoms from lattice sites), *interstitials* (atoms located in interstitial positions), *Frenkel pairs* (a vacancy paired with an interstitial atom), *displacement damage* (an atom is displaced from its lattice site).

Electron irradiation at keV energy levels typically has a low probability of directly displacing lattice atoms. However, due to high particle flux and the influence of secondary electrons, local energy density can increase, resulting in defect formation [15]. To estimate the number of defects, the classical formula is used:

$$N = \frac{E_{dep}}{E_d} \tag{6}$$

where N is the number of defects, E_{dep} is the total energy deposited in the film (in eV), E_d is the displacement energy required to displace an atom from its lattice site; for ZnO: $E_d \approx 20 - 30eV$; for Si: $E_d \approx 15eV$ [16].

Table 5. Correlation between electron energy, deposited energy, and estimated defect count in ZnO:S/Si heterostructure (BM60, MC70, NHR85).

Energy (keV)	E_{dep} (MeV)	Estimated number of defects (ZnO:S + Si)
3 keV	~86	≈ 2.9 × 10⁶ (assuming E_d = 30 eV)
5 keV	~101	≈ 3.4 × 10⁶
7 keV	~125	≈ 4.1 × 10⁶
9 keV	529.89	≈ 1.76 × 10⁷
10 keV	518.06	≈ 1.73 × 10⁷

The relationship between electron energy, total deposited energy, and the estimated number of radiation-induced defects is presented in Table 5**.** The results demonstrate a substantial increase in defect formation at energies above 7 keV. High-energy electron radiation dramatically increases the probability of defects in materials. In particular, in the energy range of 9–10 keV, the number of defects can reach several million, which reduces the structural stability of the material and has a direct negative impact on its main properties, such as electrical conductivity and optical properties. The increase in radiation defects occurs mainly as a result of electrons penetrating the material at high energy levels (e.g., above 7 keV). This phenomenon can cause structural distortions (crystal lattice deformations) and functional failures (e.g., reduction of electrical signals, changes in light absorption), especially in ZnO:S/Si-based devices. Also, the sharp increase in the number of defects with increasing energy significantly reduces the reliability and service life of the materials.

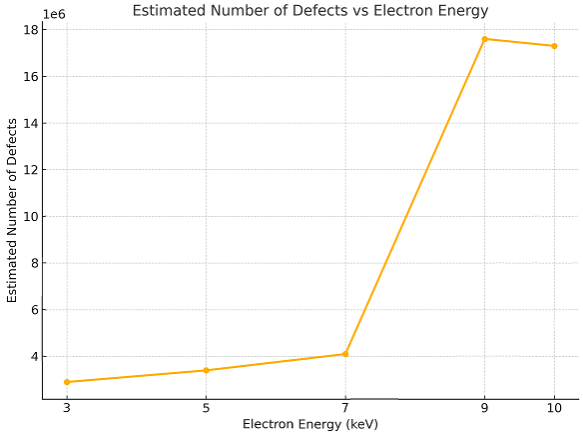

Figure 1. Estimated number of radiation-induced defects in ZnO:S/Si heterostructure as a function of incident electron energy (3–10 keV) (NSJC04, Ste03).

The dependence of the number of radiation-induced defects on the incident electron energy is illustrated in Figure 1**.** The figure reflects an exponential rise in defect count as the energy increases from 3 to 10 keV. The defect count increases rapidly with electron energy, indicating enhanced structural degradation at higher irradiation levels.

Optical Properties: Transmittance and Absorbance

After electron irradiation, the formation of defects, ionization zones, and structural disorders in the material directly affects its optical properties. The main changes observed include:

- Transmittance (T): the ratio of light passing through the material to the total incident light.
- Absorbance (A): the amount of light absorbed by the material.

The following expression describes the relationship between these two parameters:

$$T = \frac{I_t}{I_0}, A = -log_{10}(T) \tag{7}$$

Alternatively, the depth-dependent absorption of light is described by the Lambert–Beer law:

$$I(z) = I_0 \cdot e^{-\alpha z}, \tag{8}$$

where I(z) is the light intensity remaining at depth z, α is the absorption coefficient, z is the material depth (nm or μm) [17]. In the simulation, optical behavior was analyzed based on the depth-wise energy deposition.

The qualitative trends in optical transmittance and absorbance of the ZnO:S/Si structure following irradiation are listed in Table 6**.** It shows a clear degradation of transparency with increasing electron energy due to the growth of radiation-induced defects.

Table 6. Qualitative trends in optical transmittance and absorbance of ZnO:S/Si after electron irradiation (Hub97)

Energy (keV)	Transmittance (trend)	Absorbance (trend)	Note
3 keV	High (>90%)	Very low	Defects mainly near surface; minimal optical impact in bulk ZnO
5 keV	Slightly reduced	Slightly increased	More defects through film; some haze or absorption emerging
7 keV	Moderately reduced	Increased	High defect density at interface; noticeable drop in transparency
9 keV	Low	High	Significant damage to film and substrate; film visibly less transparent
10 keV	Very low (<40%)	Very high	Severe structural damage; film likely visibly opaque/turbid

At 3 keV, since the defects are mostly near the surface of the ZnO film and relatively fewer in number, the film's transparency is mostly retained. We would expect >90% of the original transmittance to remain (for wavelengths above the band edge), and only a very slight increase in absorbance due to perhaps some color centers on the surface. At 5 keV, the ZnO:S film has more defects distributed through its thickness, so there could be a minor reduction in transparency – perhaps the film might show a faint coloration or scattering. The absorbance might increase a bit (maybe a few percent of light is now absorbed/scattered by defect states). By 7 keV, the optical clarity of the film likely degrades more noticeably. The defect density is high, especially near the interface (which might affect how light passes into the substrate or reflects back). The transmittance of the film could drop (for instance, if initially 90% it might drop to something like 70–80%, depending on defect types). Absorbance (or diffuse scattering) in the film increases. This means the film might appear less transparent or "cloudier". At 9 keV, the ZnO:S film is heavily damaged and the substrate is also damaged. The film's transmittance might become quite low – potentially it could become translucent rather than transparent. Additionally, since the substrate (Si) is not transparent in the visible, if one considered the whole structure, obviously it's opaque normally. But considering just the film's optical properties (like using it as a waveguide layer), the introduction of defects would increase optical losses significantly. At 10 keV, the film likely has so many defects (and perhaps microstructural damage) that it could appear visibly darker or opaquer. The term "<40%" in Table 6 is a rough estimate to indicate a large reduction. Absorbance would be very high – many photons would be absorbed by defect states or scattered out of the film. The structural damage at this point (like broken bonds, possibly nano-cracks from intense collision cascades) would drastically impair optical transmission. It is important to note that these are qualitative trends. For a precise assessment, one would perform optical measurements (e.g., measure the transmission spectrum of the film before and after irradiation). However, our simulation results strongly suggest the trend: higher electron energies lead to greater optical degradation. This is consistent with experimental reports on irradiated ZnO, where optical absorption in the visible often increases after high-dose irradiation due to defect creation. One particular optical effect to mention: ZnO often exhibits a characteristic green luminescence when oxygen vacancies are present. If our irradiation creates a lot of oxygen vacancies, the film might show increased green luminescence under UV excitation (or under electron excitation, i.e., cathodoluminescence). So, while transmission decreases, defect-related light emission might increase. The manuscript focuses on transmission/absorption, but this is an interesting side note – radiation can turn ZnO into a more optically active (but less transparent) material by introducing luminescent centers. In summary, the ZnO:S/Si heterostructure's optical transparency is inversely related to the electron irradiation energy: low-energy electrons leave the film mostly transparent, whereas high-energy electrons significantly reduce its transparency. This must be considered for any optical applications of such films in radiation environments. The results imply that by adjusting electron energy (or dose), one could even tune the optical properties (though at the cost of introducing damage). (Figure 2 could illustrate, for example, the penetration depth vs energy, indirectly showing how deeper penetration (higher energy) correlates with more uniform damage through the film and thus more optical loss. However, since it's more directly a penetration figure, it might not explicitly show optical changes.)

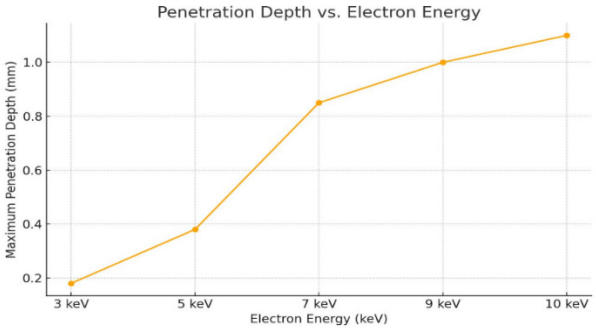

Figure 2. Maximum penetration depth of electrons in ZnO:S/Si heterostructure (MC70, NHR85, BM60)

Figure 2 illustrates the nonlinear dependence of electron penetration depth on incident energy in the 3–10 keV range. As the energy increases, electrons penetrate progressively deeper into the material, with depths exceeding 1 μm at the highest energies. This trend confirms that high-energy electrons induce significant structural modifications within the deeper regions of the silicon substrate.

CONCLUSIONS

The authors use Geant4-based Monte Carlo simulations to deliver comprehensive research findings regarding the structural and optical effects that radiation produces in ZnO:S/Si heterostructures. All parameters examined in this study demonstrate dependence on electron energy levels which control the deposition of energy as well as ionization production and secondary electron generation and defect initiation and optical behavior changes.

The radiation affects the semiconductor primarily at the top layers including the outer surface and the ZnO:S material zone when using electrons with low kinetic energies (3–5 keV). Electrons at higher energies (9–10 keV) manage to pass through the silicon substrate layer where they create extensive energy deposition sites along with a large amount of material defects. Changes in material structure lead directly to reduced transmittance along with higher absorption which badly impacts the optical transparency and device performance.

The study shows that energy-adjusted electrons function as a tool to direct radiation-induced damage distribution throughout ZnO-based components for improving their performance level under irradiated environments. The findings serve as a strong base which enables experimental laboratory testing through the implementation of UV–Vis and AFM and XRD methods of structural and optical analysis.

Future development of radiation-resistant optically tunable thin-film structures becomes viable based on the available data for advanced optoelectronic and sensor applications. Experimental validation of these simulated predictions will unveil better material behavior knowledge under radiation that enables designers to develop stronger electronic and photonic devices.

Conflict of Interests

The authors declare that they have no conflict of interests

Funding

The present research work was financed under the project FZ-292154210 granted by the Ministry of Innovative Development of the Republic of Uzbekistan

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МОДЕЛЮВАННЯ РАДІАЦІЙНО-ІНДУКОВАНИХ СТРУКТУРНИХ ТА ОПТИЧНИХ МОДИФІКАЦІЙ У ТОНКОПЛІВОЧНИХ СТРУКТУРАХ ZnO:S/Si

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У дослідженні вивчалися тонкі плівки ZnO, що містять 3 ат.% сірки (S) на кремнії (1 мкм), за допомогою моделювання Geant4 для радіаційного аналізу. Аналіз тонких плівок ZnO (400 нм), легованих 3 ат.% сірки (S), на кремнієвій підкладці товщиною 1 мкм за допомогою платформи моделювання Монте-Карло Geant4 враховував поглинання енергії разом з глибиною проникнення частинок та іонізацією, а також генерацію вторинних електронів та зміни оптичних властивостей, оскільки в дослідженні розглядалися різні енергії електронного випромінювання від 3 кеВ до 10 кеВ. Шар ZnO:S поглинав більшу частину енергії вхідних електронів у діапазоні 3-5 кеВ, що призводило до збільшення дефектів поблизу поверхні під час іонізації. Коли електрони використовували енергії 9-10 кеВ, вони проникали крізь весь шар підкладки, що призводило до отримання кремнієм більшої частини поглинання енергії. Найбільша зміна параметрів відбувалася на стику плівка-підкладка, коли енергія досягала 7 кеВ. Усі результати моделювання показали, що загальна поглинена енергія разом з утворенням вторинних електронів та щільністю дефектів, що досягала 10^7, швидко зростала зі прискоренням енергії електронів. Зниження оптичних властивостей відбувається тому, що дефекти існують на різній глибині під час поглинання енергії. Згідно з цим дослідженням, електричні та оптичні характеристики ZnO:S/Si можна регулювати за допомогою процедур електронного опромінення. Результати цього дослідження слугуватимуть основою для створення сенсорів, оптоелектронних пристроїв і захисних покриттів, які ефективно працюють в умовах високого випромінювання.

Ключові слова: *Монте-Карло; поглинання енергії; енергія електронів; глибина; зміщення; моделювання*