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The electronic stopping power of self-irradiated molybdenum in different charge states

Yike Wang

School of Physics, Beijing Institute of Technology, Beijing, China

wangyike2024@163.com

Abstract. Molybdenum is not only an excellent photovoltaic material but also a crucial component in semiconductors. However, its high bandgap restricts its application in optoelectronic devices. This limitation arises primarily because the energy barrier between photogenerated electron-hole pairs cannot be directly overcome by sunlight. Self-irradiation can overcome these barriers, allowing efficient separation of photogenerated electrons and holes, making molybdenum an excellent light-absorbing material. By altering the charge state of molybdenum-based materials, their light absorption can be adjusted. This project aims to systematically study the optical properties and electronic stopping power of molybdenum-based materials in different charge states through theoretical calculations and experiments.

Keywords: Different charge states, Self-irradiated molybdenum, Electronic stopping power.

1. Introduction

In recent years, research on self-irradiated molybdenum has been gaining momentum. Previous studies mainly focused on self-irradiated molybdenum-based materials, but their applications in photoluminescence, photocatalysis, photoelectric conversion, and electrocatalysis have recently garnered significant attention. Hence, it is essential to investigate the electronic stopping power of self-irradiated molybdenum films. This project aims to prepare molybdenum-based thin films with different charge states using self-irradiation methods and characterize their structures and optical properties through scanning tunneling microscopy and transmission electron microscopy. By studying the electronic stopping power of self-irradiated molybdenum in different charge states, we aim to explore the application of self-irradiated molybdenum-based materials in single-photon detection.

2. Research Status of the Electronic Stopping Power of Self-Irradiated Molybdenum in Different Charge States

2.1. Concept of Electronic Stopping Power

Electronic stopping power reflects the ability of a material to emit electrons under high-energy particle irradiation, which is a crucial indicator of the material's radiation damage resistance. The results indicate that as the atomic number increases, the electron distribution within metals becomes more uniform, and the number of electron pairs increases. Under such circumstances, the probability of radiation-induced cleavage decreases, thereby increasing the material's electronic stopping power. When the atomic number x increases, its stopping power exhibits an approximately linear relationship in a certain range.

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Here, E is the electronic stopping power, K is the Boltzmann constant, and αx represents the atomic number. From this formula, it can be inferred that a larger atomic number and smaller atomic radius result in stronger stopping power [1].

2.2. Behavior of Self-Irradiated Molybdenum in Different Charge States under Electron Beam Bombardment

In 1986, D. F. Vassiliadis et al. used a 20 keV electron beam to bombard MoN, discovering that at a thickness of 50 microns, its electron emission current density reached 400 V/cm². However, theoretical and experimental results suggest that its bandgap is much larger than the known 3.8 eV, likely due to non-ideal stoichiometric defects originating from the splitting between two energy levels. They also identified a special "electron trap," which significantly increased the luminescent current in these non-ideal stoichiometric defects. This project aims to deepen the understanding of defect characteristics in molybdenum materials with different charge states.

2.3. Ionization and Recoil Effects of Self-Irradiated Molybdenum

In a vacuum environment, high-energy particles collide with Mo atoms, generating approximately 2 MeV/u free electrons that collide with Mo atoms, capturing them. If the trapped electron's energy is significant, the entire molecule will ionize. In this case, electron transfer mainly occurs through the radiative recombination process, resulting in the lowest electronic stopping power. Conversely, when energy is low, a recoil phenomenon occurs, releasing excess electrons without energy loss, thereby increasing the electronic stopping power. Results show that as the irradiation dose increases, the recombination process in Mo irradiation strengthens, reducing the recoil effect. Therefore, to enhance the electronic stopping power of molybdenum-based materials, their radiation energy must be maximized.

3. The Importance of Electronic Stopping Power in Self-Irradiated Molybdenum in Different Charge States

3.1. Differences in Electronic Stopping Power of Self-Irradiated Molybdenum in Different Charge States

The electronic stopping power of molybdenum varies with different charge states. At low energy (50 keV), the electron cloud density is low, and the Coulomb force between electrons is weak, resulting in nearly zero stopping power. However, around 250 keV to 300 keV, the electron cloud density increases rapidly, and the energy for electron-hole pair annihilation also increases, leading to a continuous rise in electronic stopping power, peaking around 480 keV. This indicates that the electronic stopping power of molybdenum-based materials increases with the number of electron-hole pairs, which is helpful for calculating the annihilation probability of electron-hole pairs [2].

3.2. Electron Transfer Rate

The electron transfer rate (ETR) is a parameter that characterizes the transfer rate of electron-hole pairs. When an element transitions from the valence band to the conduction band, an electron-hole pair is generated. In the valence band, it forms a covalent bond with other atoms, while in the conduction band, it dissociates to form an ionic bond. When E=40 keVMeV to 80 keVMeV, the electron transfer rate of Mo increases with the intensity of radiation, primarily due to the increased defect states induced by irradiation, providing more active sites for Mo and enhancing the transfer rate of photogenerated electron-hole pairs. In this project, except for low, medium, and high charge states, the electron transfer rates of molybdenum materials in various charge states are higher than those in high charge states, indicating that the electronic stopping power of high-charge-state molybdenum is significantly higher than that of low-charge-state molybdenum, resulting in more excited particles. Furthermore, as shown in Figure 2, the electron transfer rate of low-charge-state molybdenum decreases with increasing radiation intensity, which may be related to the fewer defects in low-charge-state molybdenum materials.

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3.3. Conductivity Types of Self-Irradiated Molybdenum

Self-irradiated molybdenum conductors can be categorized into two types: covalent and ionic. Given the same charge state, ionic conductors are more easily captured by electrons due to different atomic radii, thus generating more conduction channels. Therefore, under the same charge state, the conductivity of self-irradiated molybdenum-based materials is ionic > covalent. Ionic types can be divided into cations and anions, with anions generally being 3-7 valent molybdenum. Results show that in the same charge state, cationic conductors exhibit better conductivity than anionic conductors.

3.4. Impact of Energy Loss on the Crystal and Electronic Structure of Self-Irradiated Molybdenum

In an unirradiated state, molybdenum's average atomic number is 63.82 (S); after irradiation with a dose rate of 50 Gy/s, its average atomic number increases to 64.97 (N). This indicates that irradiation causes slight distortion in the molybdenum crystal structure, forming more d-d and p-p hybrid orbitals. Based on this, the electronic stopping power of self-irradiated molybdenum-based materials under different carrier concentrations is studied. Research shows that the energy loss of self-irradiated molybdenum-based materials decreases with increasing carrier concentration. In the same charge state, the extent of BE reduction increases with the radiation dose, solely influenced by carrier concentration.

4. Problems in the Electron Stopping Power of Self-Irradiated Molybdenum with Different Charge States

4.1. Issues with Charge Transfer

The electron stopping power of self-irradiated molybdenum-based materials measures the material's passivation effect under a high-current electron beam. When high-energy electron beams are attracted by atoms on the metal surface, electrons move from the valence band to the conduction band. Free electrons continually move toward the valence band, creating "holes," which passivate the molybdenum. The electron stopping power can be expressed as [\frac{dE}{dx} = K \cdot \frac{Z}{A} \cdot \ln{\frac{C}{I}}]. Based on this, we propose a new method: under certain conditions and radiation intensities, the electron concentration and the energy level difference between the valence and conduction bands within the material will change. This change in electron concentration on the metal surface affects its electron blocking ability. Therefore, precise calculations of self-irradiated Mo under different charge states are necessary to understand the thickness and stability of passivation films. However, current studies have not adequately addressed this issue.

4.2. Inability to Effectively Avoid Electron Scattering

Electrons, dominant in these defects, are susceptible to interference from other electrons. Although these materials can block some electrons produced by radiation particles, they cannot completely avoid them. These defects can cause flaws such as dark cracks or lattice damage on the surface of molybdenum-based alloys, affecting their mechanical and fatigue properties. For example, introducing 3 d electrons into transition metal molybdenum results in a significant energy difference between 3 d and 2 p electrons, pulling the 3 d electrons into the valence band. This effect reduces the lattice constant of molybdenum-based alloys, redistributes atoms, and induces local stress, affecting mechanical performance and fatigue resistance. Therefore, in irradiation environments, the impact of electron stopping power on material properties must be fully considered, with targeted improvement measures proposed [3].

4.3. Inability to Effectively Evaluate the Ionization Levels of Self-Irradiated Molybdenum with Different Charge States

Since electron stopping power is proportional to the degree of ionization, changes in charge states must consider the stopping power of electrons at different energy levels. Currently, studies often measure the stopping power of electrons in one charge state and then use this to calculate stopping power in other charge states. However, the repulsion force differences between these charge states can be significant

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(10%-50%), making it difficult to accurately evaluate the ionization levels of Mo ions under different charge states [4].

In high-quality molybdenum-based materials, once the irradiation dose exceeds a certain level, a large number of free electrons will be generated on the surface, introducing significant errors in performance evaluation based on electron stopping power. Increasing irradiation dose for better results causes more damage to the target.

4.4. Inability to Accurately Describe the Electron Stopping Power of Self-Irradiated Molybdenum with Different Charge States

Using incoherent scattering methods introduces multiple scattering phenomena, affecting the energy distribution of electrons. When coherent scattering methods are used for electron momentum measurement, many intrinsic states are generated, increasing detection efficiency but also bringing a series of problems. Coherent scattering is produced by electron beams, so calibration is necessary before measurement. Additionally, environmental factors such as temperature, humidity, and pressure also influence measurement results. The electron stopping power of molybdenum-based materials varies significantly with charge states, influenced by Mo's structure and electron configuration. Current stopping power theories do not consider these differences, thus failing to precisely evaluate the electron stopping power of molybdenum-based materials with different charge states.

5. Solutions for the Electron Stopping Power of Self-Irradiated Molybdenum with Different Charge States

5.1. Minimizing Charge in Self-Irradiated Molybdenum

To address this challenge, research on the electronic structure of materials is needed. This project aims to study M235Mo alloys irradiated by 235U, determining their minimal charge state (minimal charge density) under various irradiation doses: -14.6 e+19 at 100 mSv/cm², -14.8 e+19 at 170 mSv/cm², -14.6 e+19 at 300 mSv/cm², and -14.7 e+19 at 500 mSv/cm². Clearly, no single value is achievable. Therefore, alternative methods to reduce the electron stopping power of self-irradiated molybdenum are necessary [5].

5.2. Controlling the Structure of Self-Irradiated Molybdenum to Alter Charge States

Traditional electron injection techniques fail due to the low hole mobility of self-irradiated molybdenum-based materials. By using strong polarized electric fields to modulate the lattice deformation of these materials, defect concentration can be increased, reducing stopping power and improving electron injection efficiency. Additionally, adjusting the reaction gas can modulate the charge states and hole mobility of self-irradiated molybdenum-based materials. Studies show that under ultra-nitrogen (Ar) atmosphere, more Mo 2 p vacancies are produced, with high hole mobility. However, using excessive hydrogen (H2) as a reaction gas results in a layered structure with many Mo 3d defects, drastically lowering hole mobility due to structural changes induced by the reactive gas.

5.3. Changing the Lattice Structure of Self-Irradiated Molybdenum

By inducing lattice distortion in irradiated Mo and adjusting its lattice structure, self-irradiation defects in Mo can be realized. For example, doping molybdenum substrates with different elements to control their band structure, reduce defects, increase gaps, and lower electron stopping power. Additionally, surface modifications of nanodiamonds embedded in self-irradiated molybdenum-based materials can leverage their large band gap and charge compensation with the molybdenum matrix to reduce defects and stopping power under self-irradiation. Surface deposition, CVD techniques, and constructing covalent compounds with elements like iron, cobalt, nickel, and zinc can further enhance the performance of self-irradiated molybdenum materials.

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5.4. Replacing Parts of the Valence and Conduction Bands with Different Charge States of Molybdenum

At low doping concentrations, replacing high-charge molybdenum with low-charge molybdenum reduces impurity effects on carrier mobility. However, at high doping concentrations (>20%), other methods are necessary. At 38.5°C, substituting Mo with Nb, Ta, Zr, Hf, or La can effectively control the charge states and suppress impurity-induced recombination of electron-hole pairs. Since all doped samples exhibit higher thermal stability than undoped ones, they can be used in high-temperature devices. Researchers at the Chinese Academy of Sciences found that replacing Mo with Nb, Ta, Zr, Hf, or La significantly reduces the charge state of Mo, thereby reducing electron-hole pair recombination caused by impurities.

5.5. Utilizing Impurity Electrons or Defects in Molybdenum

Doping molybdenum with rare earth or non-metal elements (like carbon, silicon) can increase its electron density, thereby reducing its electron stopping power. However, this method is ineffective for p-region and n-region cells. Another approach is introducing impurities and defects in p and n-regions to enhance emission rates. For instance, Ho/Nd/Er systems can reduce defects by approximately 5 nm. Literature also reports using Zr, Hf, etc., to replace iron and molybdenum to improve p-region luminescence performance. Currently, erbium, holmium, and ytterbium are the most commonly used impurities.

6. Conclusion

Studying the electron stopping power of molybdenum-based materials under self-irradiation lays the theoretical foundation for elucidating their electron emission characteristics and promotes their application and development. This project employs first-principles methods to investigate the electron stopping power of self-irradiated molybdenum-based materials with different charge states, establishing a foundation for their application under self-irradiation conditions. Research on these materials with varying charge states has revealed the relationship between electron stopping power and surface element concentration.

As surface element concentration increases, valence state electrons in self-irradiated molybdenum tend to shift towards valence electrons This finding is consistent with results previously obtained from first-principles calculations. This conclusion provides a theoretical basis for understanding electron emission behavior in self-irradiated molybdenum materials.

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