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Research Article

Effect of Irradiation on Nanoisland Formation and Structural Evolution of Bi_2Te_3 Thermoelectric Materials

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Abstract

Thermoelectric materials, particularly those derived from Bi_2Te_3, have received significant interest because of their capacity to directly transform thermal energy into electrical power, thereby making them suitable for energy conversion applications. This research centered on the surface morphology of Bi_2Te_3 crystals, specifically examining the (0001) surfaces both prior to and following irradiation, employing Atomic Force Microscopy (AFM) for analysis. The formation of nanoislands and their fractal nature were studied, which helped to understand their nucleation and growth through Ostwald ripening (OS), a process where smaller islands combine to form larger ones. This research also examined radiation affecting the structure and thermoelectric properties of materials made from Bi_2Te_3. The fractal characteristics of these nanostructures lead to the appearance of nanoislands of different sizes. The present investigation centered on the fractal characteristics inherent in nano-objects, thereby facilitating the emergence of multi-scale nanoislands. This research investigated the fractal features of nano-objects, which are instrumental in the generation of nanoislands across a spectrum of length scales. Consequently, the fractal morphology exhibited by nanoscale formations gives rise to nanoislands that encompass diverse size regimes.

Keywords: thermoelectric material, energy conversion, Bi_2Te_3, nanoislands, AFM, XRD

1. Introduction

Thermoelectric materials can convert heat directly and reversibly into electrical energy [1]. Because of these properties, along with their small size and reliable performance, they are very useful in environmentally friendly and energy-efficient technologies [2], [3]. Bi_2Te_3 is known to be one of the most effective materials at room temperature, which is due to its layered crystal structure that has different properties in different directions. This structure promotes superior electrical conductivity alongside diminished thermal conductivity [4]. Enhancing the thermoelectric efficiency coefficient (ZT) frequently necessitates optimizing phonon scattering while preserving relatively high carrier mobility [5], [6]. The incorporation of nanoscale characteristics, including nanoislands, holes, and grain boundaries, proves beneficial. These features can be generated via environmental influences like radiation or through meticulously controlled synthesis methods. Nanoscale surface structures primarily form through nucleation, growth, coupling, and Ostwald ripening. Radiation exposure has been reported to cause defects, change the surface structure, and increase atomic mobility [7], [8]. This study aims to investigate the surface properties and structural changes of irradiated Bi_2Te_3 crystals, focusing on the formation of nanoislands and their relationship with diffusion-driven processes.

2. Materials and Methods

2.1. Sample Preparation

Bi_2Te_3 crystals were synthesized using a standard method. These were then cleaved along the (0001) plane to create both pure and atomically smooth surfaces. Many studies on the structural integrity of Bi_2Te_3 demonstrate that the creation of these high-quality crystal surfaces is critical for the accurate separation of surface effects resulting from irradiation [9], [10].

2.2. Irradiation Conditions

The samples were exposed to a total radiation exposure of 30 Mrad (MegaRad). The chosen dose was based on earlier experiments that illustrated controlled irradiation could successfully induce point defects. This method improves atomic movement and surface modifications in tellurium compounds [11]. The irradiation parameters were carefully adjusted to generate significant structural changes while yet maintaining the crystal structure.

2.3. AFM Analysis

Atomic force microscopy (AFM), specifically in tapping mode, was employed to examine surface morphology across scan areas spanning from 1 to 5 μm^2. To ensure accurate topographical measurements, standard silicon probes, which possess a typical spring constant of approximately 40 N/m, were utilized in combination with a high-resolution commercial AFM instrument. AFM is a common tool for studying nanoscale surface phenomena, such as Ostwald ripening and coalescence, which were the main focus of this research [11], [12]. In addition, to accurately measure the size of the created nanoislands, height profiles were obtained from the AFM images using specialized image processing software.

2.4. XRD Measurements

X-ray diffraction (XRD) analyses were conducted employing a diffractometer utilizing CuKα radiation (λ~1.5418 Å). To facilitate the detection of minor alterations in the crystal structure, diffraction patterns were gathered across a 2θ range extending from 50 to 800 [13], [14], incorporating an extended integration period and a minimal step size. The generated patterns were subsequently studied to ascertain the modifications in peak width (indicative of microleaflet or crystallite dimensions), position (reflective of variations in lattice parameters), and intensity (related to structural irregularities) produced by the irradiation-induced structural transformations.

3. Results and Discussion

3.1. AFM Surface Morphology Before and After Irradiation

On the surface of pure Bi_2Te_3, uniform terraces typical of layered crystals were observed. After irradiation, numerous nanoislands appeared on the surface, along with pore-like features and curved edge defects. The island dimensions were verified using a height profiling approach and were found to be approximately 20 nm wide and 35 nm high. The development of these islands is a hallmark of increased atomic mobility and nucleation activity caused by radiation. Ostwald ripening (OS) is characterized by growth mechanisms where smaller, more abundant structures dissolve and reconnect to larger, energetically more favorable islands. Even without direct physical contact, small clusters coalesce through surface diffusion in this process. Upon contact, larger islands (those with a diameter greater than 20 nm) coalesce, exchanging mass through the junction region. It has been shown that misoriented islands form transient internal grain boundaries before dissolving through mass diffusion (Figure 1).

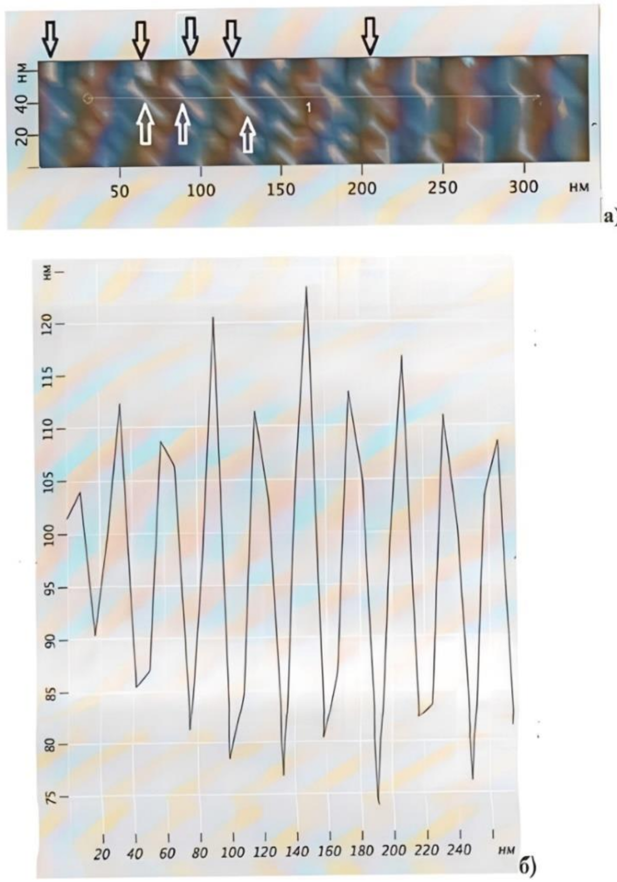

Figure 1. AFM image and height profilogram of irradiated Bi_2Te_3 surface depicting nanoislands and 2D surface defects.

3.2. 3D AFM Topography Analysis

In the 3D AFM map, a significant surface rearrangement consistent with increased Te and Bi atom diffusion is observed on the (0001) surface. The increased roughness seen after irradiation, which is caused by flaws, supports the creation of active nanostructures (Figure 2).

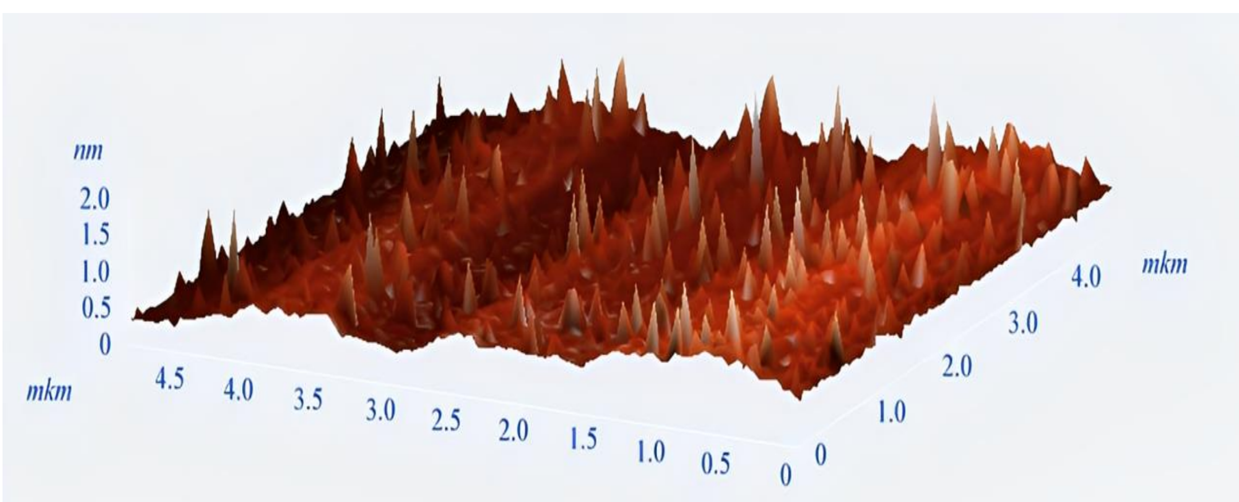

Figure 2. The 3D AFM topography of the irradiated Bi_2Te_3 surface exhibiting nanoscale roughness and the distribution of islands.

Figure 3 presents a more detailed three-dimensional AFM reconstruction of the irradiated Bi_2Te_3 surface, offering further insights into nanoscale height fluctuations and the arrangement of surface characteristics. The scan data reveals a diverse surface, marked by the presence of nanopeaks and clusters. This surface shows considerable roughness and the development of islands of different sizes. Bright yellow and white areas, indicative of high atomic deposition sites, suggest enhanced surface diffusion and clustering of Bi/Te atoms in areas with a high density of defects. Consequently, these observations provide additional support for a radiation induced, diffusion-driven Ostwald ripening process.

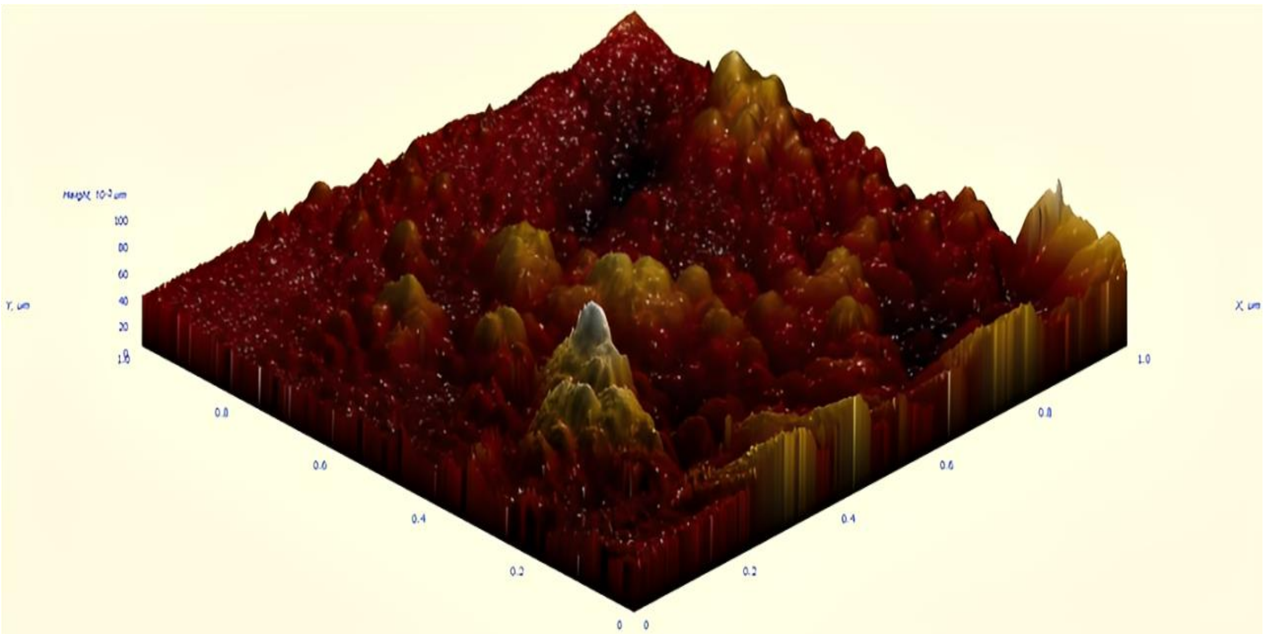

Figure 3. 3D AFM topography of the irradiated Bi_2Te_3 (0001) surface, exhibiting significant nanoscale roughness and height fluctuations linked to nanoisland formation after a 30 Mrad irradiation dosage.

3.3. XRD Analysis

According to XRD analysis, irradiated Bi_2Te_3+Te material exhibits significant structural changes after irradiation. Peak broadening was considered a characteristic of high concentration defects and microstress formation. Partial disorder and lattice disruption within the crystal structure can cause a proportional decrease in peak intensity. Small differences in peak positions indicate slight changes in interlayer distance due to radiation damage. All these effects point to a higher concentration of radiation-induced defects such as dislocation of clusters, gaps, interstitial atoms, and displacement defects (Figure 4).

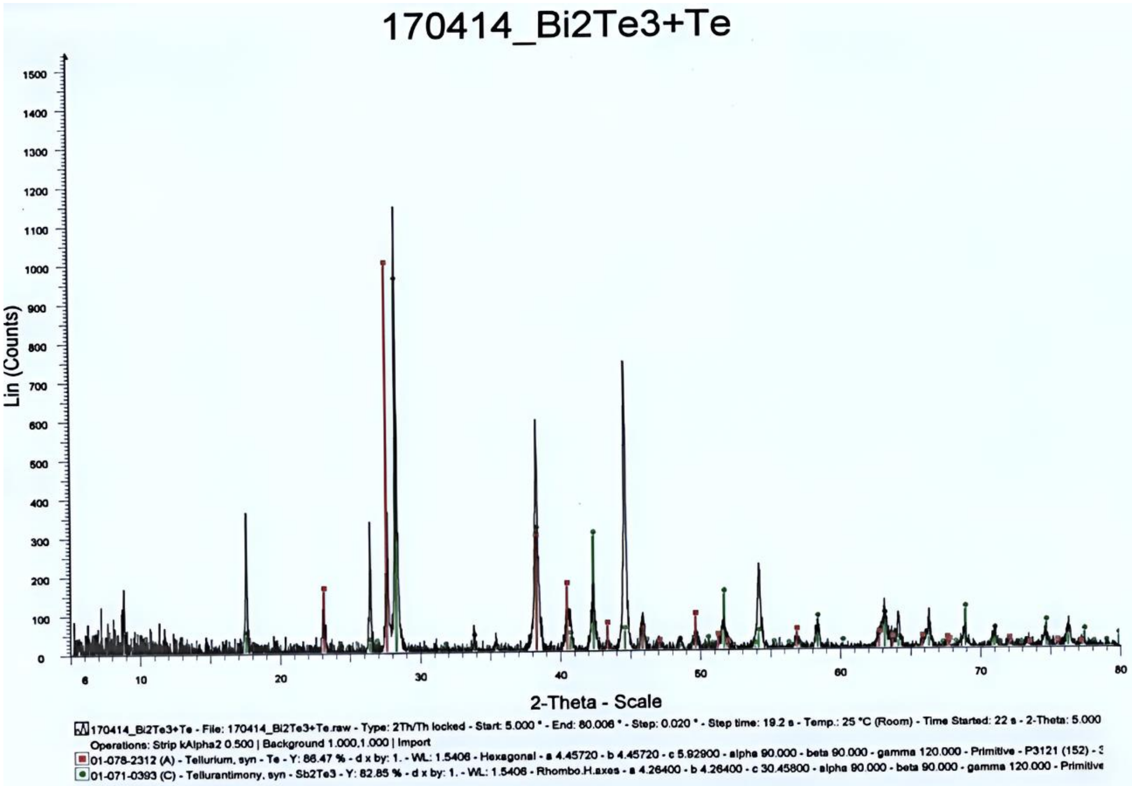

Figure 4. XRD pattern of Bi_2Te_3 + Te post-irradiation (30 Mrad).

3.4. Interpretation of Defect-Mediated Nanostructuring

Radiation-induced mechanisms interact in a complex manner to produce the observed nanoislands and diffraction changes. Multilayer structure and higher atomic mobility accelerate surface diffusion. High concentration of radiation-induced point defects promotes mass diffusion. Preferential nucleation occurs within pore domains or defect clusters. Interlayering of atoms into van der Waals vacancies of the layered structure leads to structural instability or the formation of nanostructures [15], [16]. When radiation-induced defects are present, atomic mobility increases, and island-like defect development is promoted. These generated nanoscale structures have been shown to significantly affect phonon scattering, which can decrease thermal conductivity and increase the thermoelectric ZT value. On the other hand, too many defects can restrict how well carriers move. This underscores the necessity to carefully adjust the parameters for controlled irradiation, to find a compromise between these contradictory effects.

4. Conclusion

Thermoelectric materials are environmentally friendly and offer potential solutions for energy and pollution challenges, though their thermoelectric conversion efficiency remains limited by material properties. Under the influence of radiation defects, nanostructures may either partially amorphize or stabilize due to the presence of numerous interfaces. The mechanisms of nanostructure formation on the Bi_2Te_3 (0001) surface during Ostwald ripening provide a model for studying self-organized nanostructure growth in layered materials. Studying interlayer systems helps us comprehend how moving atoms on a surface interacts with true structural flaws, such as vacancies and tiny pores.

Author Contributions

S. Nabieva conceived and designed the experiment. D. Rustamova reviewed and edited the manuscript.

Conflict of Interest

The authors declare no conflicts of interest.

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Abbreviations

Atomic Force Microscopy (AFM), X-ray Diffraction (XRD), Ostwald (OS), Bismuth Telluride (Bi_2Te_3).

References

[1] Rowe, D. M. (Ed.). (2005). *Thermoelectrics handbook: macro to nano*. CRC press.
[2] Liu, W., Yan, X., Chen, G., & Ren, Z. (2012). Recent advances in thermoelectric nanocomposites. *Nano Energy*, *1*(1), 42-56. https://doi.org/10.1016/j.nanoen.2011.10.001
[3] Zebarjadi, M., Esfarjani, K., Dresselhaus, M. S., Ren, Z. F., & Chen, G. (2012). Perspectives on thermoelectrics: from fundamentals to device applications. *Energy & Environmental Science*, *5*(1), 5147-5162. https://doi.org/10.1039/c1ee02497c
[4] Rowe, D. M. (Ed.). (2005). *Thermoelectrics handbook: macro to nano*. CRC press.
[5] He, J., & Tritt, T. M. (2017). Advances in thermoelectric materials research: Looking back and moving forward. *Science*, *357*(6358), eaak9997. https://doi.org/10.1126/science.aak9997
[6] Poudel, B., Hao, Q., Ma, Y., Lan, Y., Minnich, A., Yu, B., & Ren, Z. (2008). High-thermoelectric performance of nanostructured bismuth antimony telluride bulk alloys. *science*, *320*(5876), 634-638. https://doi.org/10.1126/science.1156446
[7] Snyder, G. J., & Toberer, E. S. (2008). Complex thermoelectric materials. *Nature materials*, *7*(2), 105-114. https://doi.org/10.1038/nmat2090
[8] Biswas, K., He, J., Blum, I. D., Wu, C. I., Hogan, T. P., Seidman, D. N., & Kanatzidis, M. G. (2012). High-performance bulk thermoelectrics with all-scale hierarchical architectures. *Nature*, *489*(7416), 414-418. https://doi.org/10.1038/nature11439
[9] Goldsmid, H. J. (2010). *Introduction to thermoelectricity* (Vol. 121, p. 46). Berlin: Springer. https://doi.org/10.1007/978-3-642-00716-3
[10] Yapryntsev, M. N., Lyubushkin, R. A., Soklakova, O. N., & Ivanov, O. N. (2017). Synthesis and electrical properties of Bi_2Te_3-based thermoelectric materials doped with Er, Tm, Yb, and Lu. https://doi.org/10.1134/s106378261706029x
[11] Sinduja, M., Amirthapandian, S., Magudapathy, P., Srivastava, S. K., & Asokan, K. (2018). Tuning of the thermoelectric properties of Bi2Te3 nanorods using helium ion irradiation. *Acs Omega*, *3*(12), 18411. https://doi.org/10.1021/acsomega.8b02379
[12] Pan, J., Li, B., Zhai, S., Fang, X., Liu, J., Zhang, H., & Wang, X. (2025). Modulation of the Reverse Saturable Absorption Properties of Bi2Te3 Nanostructures through Crystallinity Engineering. *Journal of Alloys and Compounds*, 181215. https://doi.org/10.1016/j.jallcom.2025.181215
[13] Czajka, R., Horák, J., Lošt'ák, P., Karamazov, S., Vaniš, J., & Walachová, J. (2000). Characterization and nanometer-scale modifications of Bi 2 Te 3 surface via atomic force microscopy. *Journal of Vacuum*

Science & Technology B: Microelectronics and Nanometer Structures Processing, Measurement, and Phenomena, *18*(3), 1194-1197. https://doi.org/10.1116/1.591359

[14] Chuang, P. Y., Su, S. H., Chong, C. W., Chen, Y. F., Chou, Y. H., Huang, J. C. A., & Wu, Y. C. (2018). Anti-site defect effect on the electronic structure of a Bi 2 Te 3 topological insulator. *RSC advances*, *8*(1), 423-428. https://doi.org/10.1039/c7ra08995c

[15] Yang, J., Wu, F., Zhu, Z., Yao, L., Song, H., & Hu, X. (2015). Thermoelectrical properties of lutetium-doped Bi2Te3 bulk samples prepared from flower-like nanopowders. *Journal of Alloys and Compounds*, *619*, 401-405. https://doi.org/10.1016/j.jallcom.2014.09.024

[16] Ji, X. H., Zhao, X. B., Zhang, Y. H., Lu, B. H., & Ni, H. L. (2005). Synthesis and properties of rare earth containing Bi2Te3 based thermoelectric alloys. *Journal of alloys and compounds*, *387*(1-2), 282-286. https://doi.org/10.1016/j.jallcom.2004.06.047