Crystallographic Investigation of Orientation-Dependent Defect Evolution in Irradiated MgO

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1. Introduction

Magnesium oxide (MgO) is a promising ceramic material for nuclear applications, including inert-matrix fuels [1] and mineral-insulated cable insulation [2]. In addition, its simple rock-salt crystal structure makes MgO a useful model material for investigating crystallographic effects on irradiation-induced defect formation.

When energetic ions enter a crystalline material along an open crystallographic direction, ion channeling may occur [3]. Under channeling conditions, incident ions undergo glancing interactions with atomic rows, which can influence ion penetration and defect production. Because the atomic-row configurations differ among the [100], [110], and [111] directions in MgO, the irradiation response may depend on crystallographic orientation.

In this study, MgO single crystals with (100), (110), and (111) orientations were irradiated with He^+ ions to investigate the effect of crystallographic orientation on irradiation-induced structural changes. The irradiation damage depth was estimated using SRIM simulations, and structural changes were evaluated by XRD.

2. Experimental

MgO single crystals with (100), (110), and (111) surface orientations were used in this study. Prior to ion irradiation, the specimens were characterized by scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDS), electron backscatter diffraction (EBSD), and X-ray diffraction (XRD).

SEM and EDS analyses confirmed the homogeneous composition of the MgO specimens. EBSD orientation mapping and inverse pole figure analysis were used to verify the single-crystalline nature of the specimens. Representative SEM/EDS and EBSD results for the (100)-oriented specimen are shown in Fig. 1.

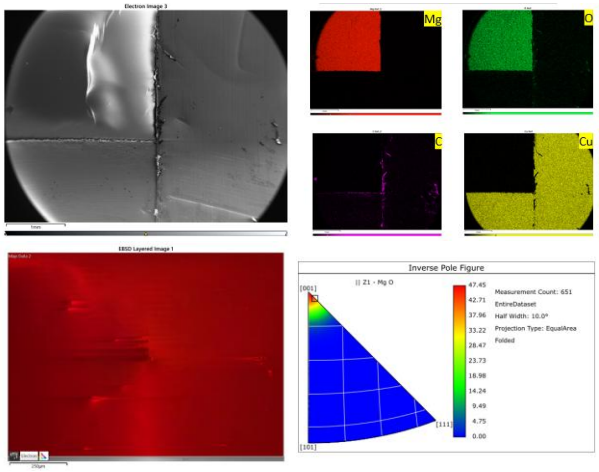


Fig. 1. Initial characterization of MgO single crystals, showing an SEM image and EDS elemental maps at the top, and an EBSD orientation map and inverse pole figure of the (100)-oriented specimen at the bottom.

The crystallographic orientations of the specimens were further confirmed by XRD. As shown in Fig. 2, the unirradiated specimens exhibited diffraction peaks corresponding to the intended (100), (110), and (111) orientations.

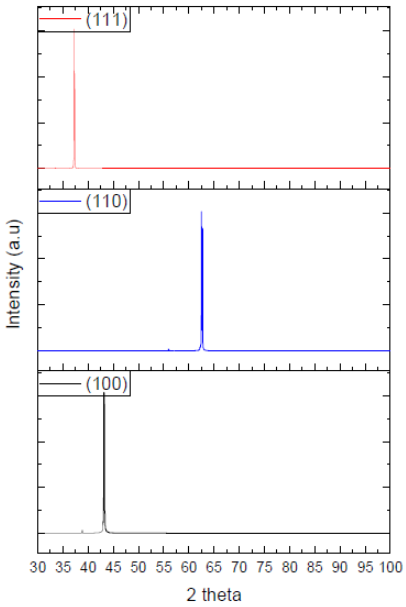


Fig. 2. XRD patterns of unirradiated MgO single crystals with (100), (110), and (111) orientations

The MgO single crystals were irradiated with He^+ ions at energies of 463 and 465 keV for fluences of 5×10^{16} and 2×10^{17} ions/cm², respectively, at the Korea Institute of Geoscience and Mineral Resources. For each irradiation condition, identical conditions were applied to all three crystallographic orientations.

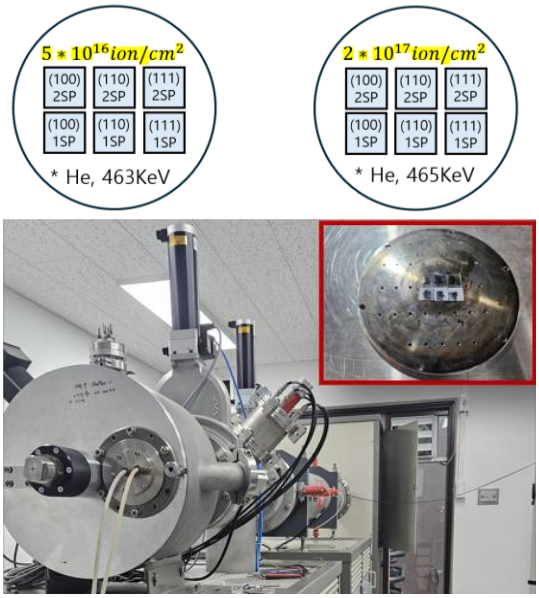


Fig. 3. He^+ ion irradiation conditions for MgO single crystals, showing the specimen arrangement and irradiation parameters for the two fluences (top), and the experimental irradiation setup with the specimen holder inside the irradiation chamber (bottom).

The depth distribution of displacement damage was estimated using SRIM simulations. As shown in Fig. 4, the calculated damage was concentrated in the near-surface region, with the damage peak located at approximately 1.2–1.3 μm below the specimen surface.

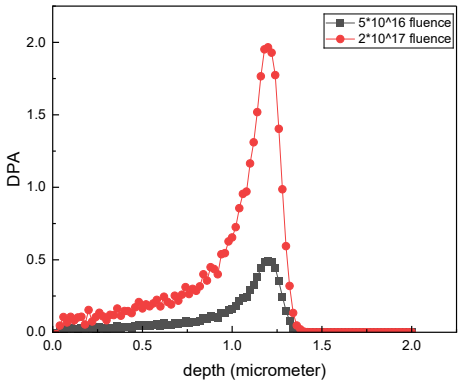


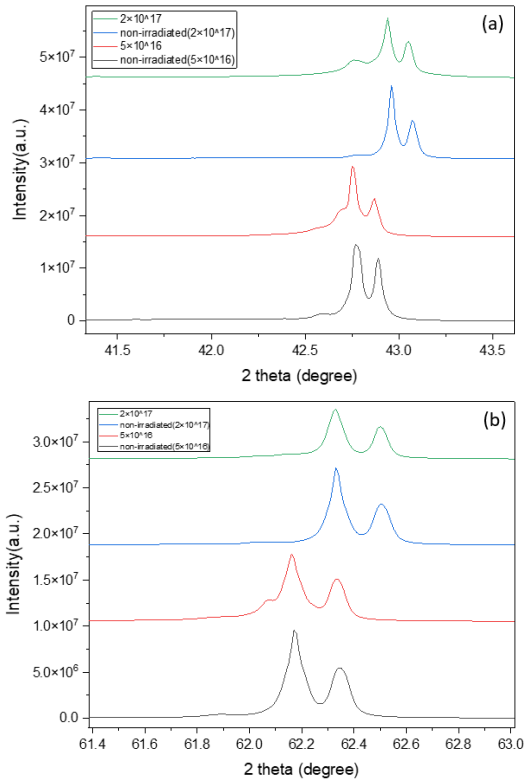
Fig. 4. SRIM-predicted displacement damage profiles in MgO irradiated with 463 keV He^+ ions

Since the SRIM calculation assumes an amorphous target structure, the simulation was used primarily to estimate the characteristic depth of the irradiated region rather than to predict crystallographic orientation-dependent channeling behavior. The relatively shallow irradiation depth should therefore be considered when selecting characterization methods for subsequent analysis of irradiation-induced defects.

3. Results and Discussion

Fig. 5 shows the XRD profiles of the (100)-, (110)-, and (111)-oriented MgO single crystals before and after He^+ irradiation. For each orientation, the diffraction profiles exhibited changes with increasing irradiation fluence.

Slight peak broadening and weak shoulder-like features were observed in the irradiated specimens compared with the unirradiated condition. These changes may indicate irradiation-induced lattice distortion and/or microstrain. However, no clear and systematic dependence on crystallographic orientation was resolved under the present measurement conditions.



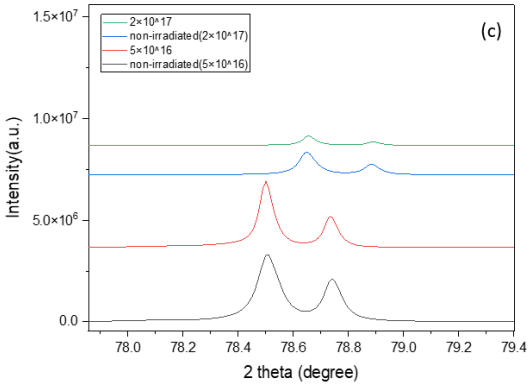


Fig. 5. XRD profiles of (a) (100)-, (b) (110)-, and (c) (111)-oriented MgO single crystals before and after He^+ irradiation at fluences of 5×10^{16} and 2×10^{17} ions/cm²

The limited sensitivity of conventional XRD to the irradiated layer should also be considered. The SRIM results indicate that the irradiation-induced damage is concentrated within approximately 1.2–1.3 μm below the surface, whereas conventional XRD probes a substantially greater depth. Therefore, the diffraction response from the irradiated layer may be diluted by the contribution from the underlying relatively undamaged material.

These preliminary results indicate that He^+ irradiation induces measurable structural changes in MgO single crystals, while further surface-sensitive characterization is required to clarify crystallographic orientation-dependent differences.

4. Conclusion and Future Work

MgO single crystals with (100), (110), and (111) orientations were characterized and irradiated with 463 keV He^+ ions at fluences of 5×10^{16} and 2×10^{17} ions/cm². SEM/EDS, EBSD, and XRD confirmed the initial specimen characteristics and intended crystallographic orientations. SRIM simulations indicated that the irradiation damage was concentrated at approximately 1.2–1.3 μm below the surface.

XRD measurements after irradiation showed slight peak broadening and shoulder-like features, suggesting irradiation-induced lattice distortion. However, a clear systematic dependence on crystallographic orientation was not resolved from the present conventional XRD measurements. Further GIXRD (Grazing Incidence X-ray Diffraction), TEM, and nanoindentation analyses will be conducted to clarify orientation-dependent differences in near-surface lattice response, defect structure, and mechanical properties.

ACKNOWLEDGEMENTS

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REFERENCES

[1] C. Ronchi, J. P. Ottaviani, C. Degueldre, and R. Calabrese, Thermophysical Properties of Inert Matrix Fuels for Actinide Transmutation, *Journal of Nuclear Materials*, Vol. 320, pp. 54-65, 2003.
[2] A. Shaimerdenov, Sh. Gizatulin, D. Sairanbayev, Zh. Bugybay, P. Silnyagin, A. Akhanov, T. Fuyushima, N. Hirota, and K. Tsuchiya, "Characterization of Mineral Insulated Cables at the WWR-K Reactor: First Results," *Nuclear Instruments and Methods in Physics Research Section B*, Vol. 548, 165235, 2024.
[3] D. S. Gemmell, Channeling and Related Effects in the Motion of Charged Particles through Crystals, *Reviews of Modern Physics*, Vol. 46, No. 1, pp. 129–227, 1974.
[4] J. F. Ziegler, M. D. Ziegler, and J. P. Biersack, "SRIM – The stopping and range of ions in matter (2010)," Nuclear Instruments and Methods in Physics Research Section B, Vol. 268, pp. 1818–1823 (2010).