# STUDY ON THE PRODUCTION AND AGGREGATION OF DEFECTS IN ZIRCONIUM NITRIDE

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論 文 名　：**STUDY ON THE PRODUCTION AND AGGREGATION OF DEFECTS IN ZIRCONIUM NITRIDE**
(窒化ジルコニウム中の欠陥ならびに集合体形成に関する研究)

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## 論　文　内　容　の　要　旨

Zirconium nitride (ZrN) is a promising matrix candidate for advanced nuclear fuels and transmutation of minor actinides. In those applications, ZrN should subsist against radiations of energetic particles at high temperatures. Recent extensive researches have shown the excellent radiation resistance of ZrN under radiation environment. However, at present, information on fundamental properties of point defects, such as the production and their kinetic behavior, is limited. For example, no values are available for the displacement threshold energy ($E_d$) of ZrN, although this is an indispensable physical quantity to understand the radiation damage.

This thesis investigated fundamental properties of point defects in ZrN. First, values of $E_d$ were evaluated by using *ab-initio* molecular dynamics (AIMD) simulation. Then *in-situ* microstructure observations were performed under electron irradiation in a high voltage electron microscope. Based on the evaluated values of $E_d$, the nucleation-and-growth process of defect clusters in ZrN was analyzed as functions of electron energy and irradiation temperature to understand the nature of defect clusters and the migration energy of point defects. Microstructure change irradiated with swift heavy ions was also investigated to evaluate the influence of high density electronic excitation. This dissertation consists of seven chapters.

Chapter 1 describes the research purpose of this study, and step-wise organization of the chapters is also outlined.

Chapter 2 reviews theoretical and experimental investigations on radiation damage in ceramic materials, with an emphasis on nitrides.

Chapter 3 describes experimental details, such as for ZrN specimen preparation, electron and ion irradiation conditions. *In situ* TEM observation conditions and data acquisition procedure are also described.

Chapter 4 describes the evaluation of $E_d$ in ZrN by using AIMD simulation technique. Values of $E_d$ were found to depend on types of atoms (Zr and N atom) and crystallographic directions. The weighted average values of $E_d$ for crystallographic directions were evaluated to be 33 eV and 29 eV for Zr and N atoms, respectively. Detailed monitoring of primary knock-on atoms (PKAs) during the collision process disclosed an important role of the sequential replacement collision in the [110] direction. Further, the stable configurations of interstitials were found to be a <111> split-type and tetrahedral sites for Zr and N atoms, respectively. Such difference in interstitial configuration caused the difference in $E_d$ values on the types of atoms.

In Chapter 5, the nucleation-and-growth of defect clusters was investigated as functions of electron energy and temperatures. Electrons with 1250 keV induced stoichiometric dislocation loops with Burgers vector parallel to <110> directions. Migration energy of interstitial atoms for the rate controlling species was evaluated to be 0.48 ± 0.07 eV. On the other hand, electron irradiation with 400 - 800 keV was found to induce nonstoichiometric dislocation loops, presumably consist of solely N atoms. A role of selective displacement damage of N atoms at electron energy below 800 keV was discussed to understand the energy dependent dislocation loop formation in ZrN.

Chapter 6 deals with microstructure change of ZrN irradiated with swift heavy ions. No ion tracks were formed under irradiation of 200 MeV Xe ions, which indicates the excellent resistance of ZrN to electronic excitation damage. On the other hand, different types of defects were formed dependent on the penetration depth of incident ions: dislocation lines and small dot-contrast were observed at shallow and deep penetration depth, respectively. Those microstructure change was attributed to the change in the electronic stopping power against the penetration depth of incident ions.

In Chapter 7, important findings obtained from simulation and experimental investigations in this study were summarized as conclusions. Possible directions of researches for further understanding of defects behavior in ZrN were also highlighted.