博　士　学　位　論　文

Doctoral Thesis

内容の要旨

及び

審査結果の要旨

Thesis Abstracts

and

Summaries of the Thesis Review Results

第13号

The Thirteenth Issue

平成21年6月

June, 2009

The University of Aizu

はしがき

博士の学位を授与したので、学位規則（昭和28年4月1日文部省令第9号）第8条の規定に基づき、その論文の内容の要旨及び論文審査の結果の要旨をここに公表する。

学位記番号に付した「甲」は学位規則第4条第1項（いわゆる課程博士）によるものであることを示す。

Preface

On granting the Doctoral Degree to the individuals mentioned below, abstracts of their theses and the theses review results are herewith publicly announced, in according to the provisions provided for in Article 8 of the Ruling of Degrees (Ministry Of Education Ordinance No.9, enacted on April 1, 1953)

The Chinese character, “甲”, at the beginning of the diploma number represents that an individual has been granted the degree in accordance with the provisions provided for in Paragraph 4-1 of the Ruling Of Degrees (what in called “Katei Hakase,” or the Doctoral Degree granted by the University at which the grantee was enrolled.)

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Name 氏名	Youhei Nishidate 西舘　陽平
The relevant degree 学位の種類	Doctoral degree (in Computer Science and Engineering) 博士(コンピュータ理工学)
Number of the diploma of the Doctoral Degree 学位記番号	甲 CI 博第 5 号
The Date of Conferment 学位授与日	March 23, 2009 平成 21 年 3 月 23 日
Requirements for Degree Conferment 学位授与の要件	Please refer to the article five of "University Regulation on University Degrees" 会津大学学位規程　第5条該当
Thesis Title 論文題目	Modeling of Self-Positioning Nanostructures 自己形成するナノ構造物のモデリング
Thesis Review Committee Members 論文審査委員	University of Aizu, Prof. G. Nikishkov(Chief Referee) University of Aizu, Prof. M. Osano University of Aizu, Prof. V. Ryzhii University of Aizu, Prof. H. Terasaka 会津大学教授　G. Nikishkov 会津大学教授　小佐野　峰忠 会津大学教授　V. Ryzhii 会津大学教授　寺坂　晴夫

Modeling of Self-Positioning Nanostructures

Thesis Abstract

The *self-positioning* is a phenomenon that occurs in structures which are subjected to a strain/stress imbalance. Multilayer thin films consisting of different materials are rolled-up and form nanohinges and nanotubes. Complicated three-dimensional nanostructures can be fabricated by utilizing the self-positioning phenomenon. We perform modeling of self-positioning structures by the continuum mechanics theory, the finite element method, and the atomic-scale finite element method.

Continuum mechanics solution has been derived for multi-layer thin film structures subjected to initial strains under generalized plane strain conditions. Such solution can be useful for estimating the curvature radius and strains or stresses of self-positioning structures. The generalized plane strain conditions are more realistic than assumptions in previously published solutions. Also, we show that the generalized plane strain solution is identical to previous solutions in some specific cases.

Finite element modeling has been applied for estimation of the curvature radius of self-positioning hinges. Materials used for the self-positioning structures usually involve anisotropy depending on their crystal orientations. We developed a finite element procedure which takes into account the material anisotropy. The finite element procedure has been employed for modeling bi-layer self-positioning nanostructures consisting of GaAs and $In_{0.2}Ga_{0.8}As$ layers. Comparison of curvature radii obtained by the finite element modeling and experimental data shows qualitative agreement.

An atomic-scale finite element procedure has been developed for atomic-scale modeling of self-positioning nanostructures. We adopted the Tersoff inter-atomic potential function and its parameters developed by Nordlund. Since self-positioning deformations involve large displacements, an iteration procedure has been proposed for controlling nonlinear solution. Bi-layer structures composed of GaAs and InAs layers have been modeled for varying total thicknesses and crystal orientations. The atomic-scale modeling shows significant decrease of the curvature radius comparing to the continuum mechanics solution with decrease of the structure thickness. On the other hand, the curvature radius asymptotically approaches the continuum mechanics solution with the structure thickness increase. Also, we found that varying crystallographic axes direction leads to change of the curvature radius by 35% for the GaAs-InAs bi-layer self-positioning structures. Strains estimation techniques are incorporated in the atomic-scale finite element procedure based on mesh free finite element interpolation methods. Contour plots of the strain distributions show large compressive strains at free surfaces due to absence of atoms. Free surface effects become more significant for structures with smaller sizes. Decreasing of the curvature

radius can be attributed to the surface effects.

Summaries of the Thesis Review Results

Dissertation of Y. Nishidate is devoted to modeling of self-positioning structures by a continuum mechanics theory, a finite element procedure, and an atomic-scale finite element procedure. New continuum mechanics solution under the generalized plane strain conditions has been derived for multi-layer nanostructures with initial strains. A finite element procedure for modeling self-positioning structures with material anisotropy has been developed. Modeling of GaAs and $In_{0.2}Ga_{0.8}As$ bi-layer self-positioning structures for varying crystal orientations has been performed. Atomic-scale finite element procedure for modeling of self-positioning nanostructures has been created. The developed AFEM procedure has been used for estimation of curvature radius and strain components of bi-layer self-positioning nanostructures composed of GaAs top and InAs bottom layers. New results indicating influence of structure size have been obtained.

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発行　会津大学

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