العنوان:	INVESTIGATION DISLOCATION STRUCTURE EVOLUTION DURING NANOINDENTATION
المؤلف الرئيسي:	Zafar, Hassaan
مؤلفين آخرين:	Khan, Shafique(super.)
التاريخ الميلادي:	2014
موقع:	الظهران
رقم MD:	651514
نوع المحتوى:	رسائل جامعية
اللغة:	English
الدرجة العلمية:	رسالة ماجستير
الجامعة:	جامعة الملك فهد للبترول والمعادن
الكلية:	عمادة الدراسات العليا
الدولة:	السعودية
قواعد المعلومات:	Dissertations
مواضيع:	الهندسة الميكانيكية، التفكك
رابط:	https://search.mandumah.com/Record/651514

ABSTRACT

Full Name : Hassaan Zafar
Thesis Title : Investigating Dislocation Structure Evolution during Nanoindentation
Major Field : Mechanical Engineering
Date of Degree : May 2014

Dislocation structure evolution during nanoindentation is investigated using a three-dimensional multi-scale discrete dislocation plasticity model. This model combines two length scales, discrete dislocation dynamics and continuum finite element analysis. The multiplication, growth and movement of dislocations on different slip planes, in the vicinity of the nanoindentation site, are studied. Moreover, topographical maps of the nanoindented surface are generated to observe the patterns formed by exiting dislocations. Nanoindentation models are developed for spherical, cylindrical, conical and Berkovich indenter tips. Different initial configurations of dislocation sources are employed in the study.

It is observed that the dislocation activity significantly depends upon the initial configuration of the dislocation sources. Secondly, the orientation of the crystal influences the topography of the nanoindented surface. The accuracy of nanoindentation size effect model developed based on two-dimensional simulations is also investigated. It is found that the hardness results for two-dimensional simulations deviate from those of the three-dimensional model. This is because the important phenomena of cross-slip and strain hardening are ignored in two-dimensional models.

ملخص الرسالة

الاسم الكامل: حسان ظفر

عنوان الرسالة: البحث في ظهور و تطور الخلل خلال الغرز بالنانو

التخصص: الهندسة الميكانيكية

تاريخ الدرجة العلمية: مايو 2014

لقد تم دراسة تنامي الخلل الحاصل في المواد خلال عملية الغرز بالنانو بإستخدام نظرية مرونة الخلل ثلاثية الأبعاد. هذه النظرية تعتمد على بعدي طول و ديناميكية الخلل وتحليل العناصر المحدودة. تم دراسة تضاعف و نمو و حركة الخلل في محيط منطقة الغرز. و من ثم تم رسم طوبوغرافيا للسطح المغروس لملاحظة الترتيب الذي أحدثه الخلل. تم إستحداث نظرية غرس لكل من رأس الغرس الكروي و الأسطواني و المخروطي و البيركوفيج . تم توظيف المصادر المتعددة للخلل في الدراسة.

لقد لوحظ أن نشاط الخلل يعتمد بشكل كبير على طبيعة المصدر الأساسي (المنشأ) لهذا الخلل. و لقد لوحظ أيضًا أن إتجاه البلورات في المادة تؤثر على طبوغرافية السطح المغروز بالنانو. إنّ دقة نظرية تأثير حجم الغرز بالنانو طُورت بالإعتماد على المحاكاة ثنائية الأبعاد. لقد وجد أن قيم الصلادة قد إنحرفت عن المفروض لو تم اعتماد النظرية ثلاثية الأبعاد و ذلك لأنه تم تجاهل أهمية مفهوم الإنزلاق المتقاطع و التقوية بالسلاسة في نظرية الأبعاد الثنائية.

العنوان:	INVESTIGATION DISLOCATION STRUCTURE EVOLUTION DURING NANOINDENTATION
المؤلف الرئيسي:	Zafar, Hassaan
مؤلفين آخرين:	Khan, Shafique(super.)
التاريخ الميلادي:	2014
موقع:	الظهران
رقم MD:	651514
نوع المحتوى:	رسائل جامعية
اللغة:	English
الدرجة العلمية:	رسالة ماجستير
الجامعة:	جامعة الملك فهد للبترول والمعادن
الكلية:	عمادة الدراسات العليا
الدولة:	السعودية
قواعد المعلومات:	Dissertations
مواضيع:	الهندسة الميكانيكية، التفكك
رابط:	https://search.mandumah.com/Record/651514

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

العنوان:	INVESTIGATION DISLOCATION STRUCTURE EVOLUTION DURING NANOINDENTATION
المؤلف الرئيسي:	Zafar, Hassaan
مؤلفين آخرين:	Khan, Shafique(super.)
التاريخ الميلادي:	2014
موقع:	الظهران
رقم MD:	651514
نوع المحتوى:	رسائل جامعية
اللغة:	English
الدرجة العلمية:	رسالة ماجستير
الجامعة:	جامعة الملك فهد للبترول والمعادن
الكلية:	عمادة الدراسات العليا
الدولة:	السعودية
قواعد المعلومات:	Dissertations
مواضيع:	الهندسة الميكانيكية، التفكك
رابط:	https://search.mandumah.com/Record/651514

INVESTIGATING DISLOCATION STRUCTURE EVOLUTION DURING NANOINDENTATION

BY

HASSAAN ZAFAR

A Thesis Presented to the
DEANSHIP OF GRADUATE STUDIES

KING FAHD UNIVERSITY OF PETROLEUM & MINERALS
DHAHRAN, SAUDI ARABIA

In Partial Fulfillment of the
Requirements for the Degree of

MASTER OF SCIENCE
In

MECHANICAL ENGINEERING

MAY 2014

KING FAHD UNIVERSITY OF PETROLEUM & MINERALS
DHAHRAN- 31261, SAUDI ARABIA
DEANSHIP OF GRADUATE STUDIES

This thesis, written by **HASSAAN ZAFAR** under the direction his thesis advisor and approved by his thesis committee, has been presented and accepted by the Dean of Graduate Studies, in partial fulfillment of the requirements for the degree of **MASTER OF SCIENCE IN MECHANICAL ENGINEERING.**

Dr. Shafique Khan
(Advisor)

Dr. Zuhair Gasem
Department Chairman

Dr. Numan Abu-Dheir
(Member)

Dr. Salam A. Zummo
Dean of Graduate Studies

Dr. Sulaman Pashah
(Member)

13/5/14
Date

Dedicated to

My Parents and my wife

ACKNOWLEDGMENTS

First of all I would like to thank Almighty Allah (S.W.T) for giving the strength necessary to achieve my goals. Secondly, I express gratitude to my thesis advisor, Dr. Shafique Khan for his guidance and support throughout the thesis work. He has been very kind, encouraging and a source of inspiration to me. Moreover, I would also like to thank my committee members Dr. Numan Abu-Dheir and Dr. Sulaman Pashah for their valuable suggestions and guidance. I would also like express my gratitude to KFUPM and the Mechanical Engineering Department for their support.

I am also grateful to my university fellows for helpful discussions and advices. Finally, I express thanks to my family for the encouragement and prayers.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

ABSTRACT

Full Name : Hassaan Zafar

Thesis Title : Investigating Dislocation Structure Evolution during Nanoindentation

Major Field : Mechanical Engineering

Date of Degree : May 2014

Dislocation structure evolution during nanoindentation is investigated using a three-dimensional multi-scale discrete dislocation plasticity model. This model combines two length scales, discrete dislocation dynamics and continuum finite element analysis. The multiplication, growth and movement of dislocations on different slip planes, in the vicinity of the nanoindentation site, are studied. Moreover, topographical maps of the nanoindented surface are generated to observe the patterns formed by exiting dislocations. Nanoindentation models are developed for spherical, cylindrical, conical and Berkovich indenter tips. Different initial configurations of dislocation sources are employed in the study.

It is observed that the dislocation activity significantly depends upon the initial configuration of the dislocation sources. Secondly, the orientation of the crystal influences the topography of the nanoindented surface. The accuracy of nanoindentation size effect model developed based on two-dimensional simulations is also investigated. It is found that the hardness results for two-dimensional simulations deviate from those of the three-dimensional model. This is because the important phenomena of cross-slip and strain hardening are ignored in two-dimensional models.

ملخص الرسالة

الاسم الكامل: حسان ظفر

عنوان الرسالة: البحث في ظهور و تطور الخلل خلال الغرز بالنانو

التخصص: الهندسة الميكانيكية

تاريخ الدرجة العلمية: مايو 2014

لقد تم دراسة تنامي الخلل الحاصل في المواد خلال عملية الغرز بالنانو بإستخدام نظرية مرونة الخلل ثلاثية الأبعاد. هذه النظرية تعتمد على بعدي طول و ديناميكية الخلل وتحليل العناصر المحدودة. تم دراسة تضاعف و نمو و حركة الخلل في محيط منطقة الغرز. و من ثم تم رسم طوبوغرافيا للسطح المغروس لملاحظة الترتيب الذي أحدثه الخلل. تم إستحداث نظرية غرس لكل من رأس الغرس الكروي و الأسطواني و المخروطي و البيركوفيج . تم توظيف المصادر المتعددة للخلل في الدراسة.

لقد لوحظ أن نشاط الخلل يعتمد بشكل كبير على طبيعة المصدر الأساسي (المنشأ) لهذا الخلل. و لقد لوحظ أيضاً أن إتجاه البلورات في المادة تؤثر على طبوغرافية السطح المغروز بالنانو. إنّ دقة نظرية تأثير حجم الغرز بالنانو طُورت بالإعتماد على المحاكاة ثنائية الأبعاد. لقد وجد أن قيم الصلادة قد إنحرفت عن المفروض لو تم اعتماد النظرية ثلاثية الأبعاد و ذلك لأنه تم تجاهل أهمية مفهوم الإنزلاق المتقاطع و التقوية بالسلاسة في نظرية الأبعاد الثنائية.

CHAPTER 1

INTRODUCTION

Nanoindentation has become a very popular technique to determine the mechanical properties of materials (e.g. hardness and elastic modulus). However, nanoindentation tests cannot directly explain the mechanisms that occur within the material and their effect on the test results. Investigation of the region around the indentation can help us understand how the plasticity initiates and progresses. According to dislocation theory, plastic deformation is directly related to the nucleation, multiplication and movement of dislocations. However, spatial resolution available through advanced electron microscopy is not enough to experimentally study this nucleation and multiplication of dislocations within the nanoindentation zone, during the nanoindentation test. Therefore, the dislocation activity related to a particular slip system cannot be studied experimentally. This has led to the use of modeling and simulation techniques by researchers to explain the dislocation behavior during nanoindentation Modeling and simulation techniques have been used by researchers to explain the dislocation behavior during nanoindentation. These techniques include: (i) Atomistic/Molecular Dynamics (MD) modeling (ii) Discrete Dislocation Dynamics (*DD*) modeling (iii) Finite Element Methods. Atomistic/MD modeling requires extreme computational power and therefore can only simulate the initial stages of the plastic deformation, i.e. the onset of plasticity, at which neither the dislocation structures have fully developed, nor has the dislocation density increased considerably. Moreover, only the nanometer scale is considered since the specimen is defined by only a few thousand atoms. Due to these factors, this method cannot simulate the interaction of a large number of dislocations, associated with the plastic deformations during nanoindentation. On the other hand, *DD* modeling can simulate a large number of dislocations.

Two-dimensional discrete dislocation dynamics models have been used by several researchers but these models have limitations as they are simplified with assumptions and cannot simulate detailed analysis of dislocation activity on all slip systems especially the intersecting slip planes. Moreover, the 2D models consider only edge dislocations disregarding screw or mixed character dislocations.

1.1 Nanoindentation Testing

Nanoindentation test apparatus is widely available now. The typical parts include a loading frame, indenter shaft, loading actuator and sensors to measure positions and displacements. An optical microscope is also installed to accurately position the indenter. Nanoindentation testing can be performed on very small volumes of materials and single crystals. The specimen surface must be well prepared to minimize surface roughness for better results. The commonly used indenter tips have spherical, conical, cylindrical or pyramidal shapes. The most common indenter material is diamond that has been ground into the desired tip geometry. Moreover, the onset of plasticity and subsequent plastic deformations are also topics of interests among researchers. Nanoindentation advances the macro and micro indentation tests by indenting on the nanometer length scale. The resolutions for measuring the displacements and positions are very high. Real time load-displacement data is recorded and plotted while the indentation test is in progress (Fig. 1.1). These curves can be used to extract mechanical properties of the material, such as the hardness and modulus of elasticity. It is very crucial to measure the contact area accurately for best results. This is achieved by imaging the residual impression with a surface probe such as Atomic Force Microsocopy (AFM). The contact area can also be estimated by calculations, if the tip geometry and the final indentation depth is known. In this case, the depth of penetration is recorded, and the area of the indent is determined using the known geometry of the indentation tip.

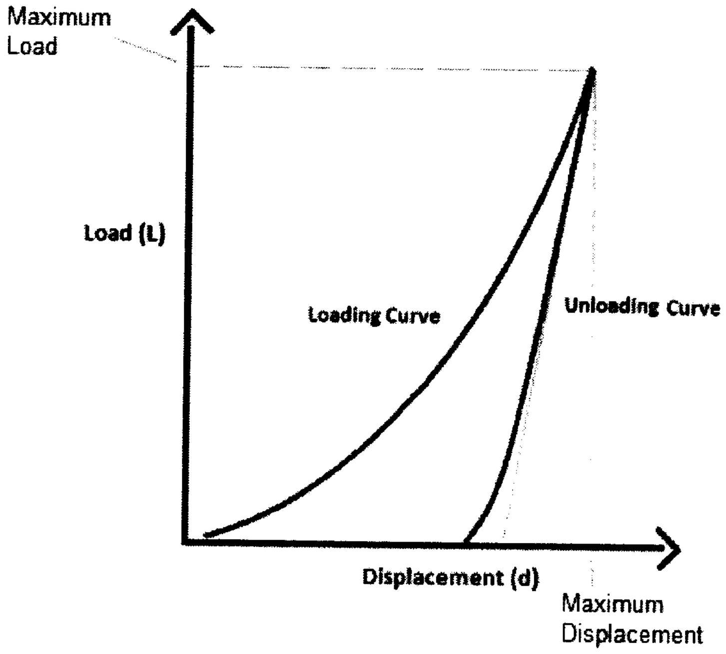

Figure 1.1: Typical load-displacement curve for an instrumented nanoindentation test.

1.2 Dislocation Theory

A dislocation is a crystallographic line defect, or irregularity, within a crystal structure. Dislocations can be envisioned as being caused by the termination of a plane of atoms in the middle of a crystal. In such a case, the neighboring planes are not straight, but instead bent around the edge of the terminating plane. Therefore, the crystal structure is perfectly ordered on both sides of the plane. The dislocation has two properties, a line sense, that defines the direction of the dislocation line, and the Burgers vector that describes the magnitude and direction of distortion to the lattice. Two main types of dislocations exist: (i) edge dislocation (the Burgers vector is perpendicular to the line sense; Fig. 1.2a) (ii) screw dislocation (the Burgers vector is parallel to the line sense; Fig. 1.2b). Dislocations found in real materials are typically mixed, meaning that they have characteristics of both. The Burgers vector in this case lies at an angle to the line sense and thus has both the screw and edge components. When external stress is applied, the dislocations move on their slip planes (by gliding motion) in specific directions, causing plastic deformation. Both Face-Centered Cubic (FCC) and Body-Centered Cubic (BCC) materials have their own specific slip planes and slip directions, combinations of which are called the slip systems. The dislocations interact among themselves to form jogs, junctions, dipoles etc. Moreover, two dislocations with equal Burgers vectors and opposite line senses on the same slip plane can come closer and cancel each other, leaving behind a perfect crystal lattice. This process is called dislocation annihilation. The screw dislocations can slip on to another intersecting slip plane by a process known as cross-slip. Dislocations that account for the plastic deformation during nanoindentation are known as Geometrically Necessary Dislocations (GND).

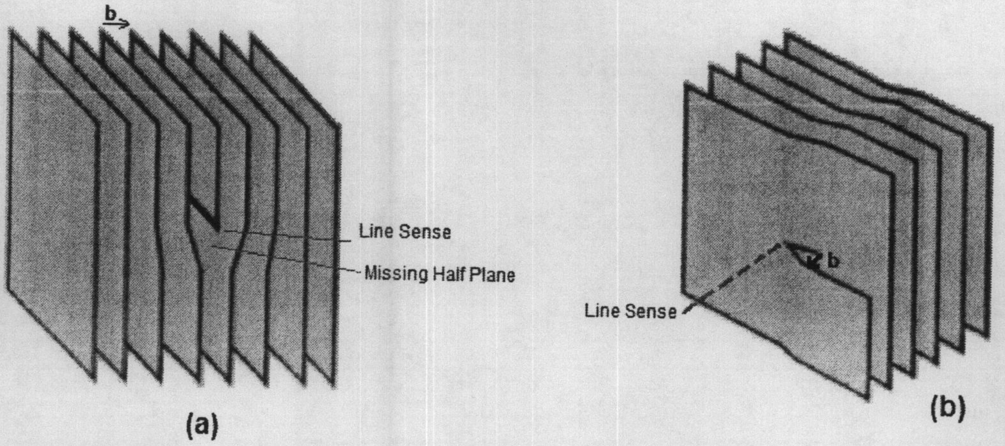

Figure 1.2: (a) Schemetic of an edge dislocation; (b) Schemetic of a screw Dislocation.

1.3 Dislocation Modeling

1.3.1 Discrete Dislocation Dynamics

Discrete Dislocation Dynamics (*DD*) models approximate the dislocation structures by a finite number of discrete dislocations, each with a defined character. *DD* models simulate movement, interaction and multiplication of dislocations when a load is applied. The behavior of an individual dislocation is closely related to the interaction with other dislocations and stresses due to external loadings. In two-dimensional *DD* models, the dislocation structure is approximated by dislocation points with either edge or screw character and usually only one type of slip planes is considered. Therefore for 2D models, the important phenomenon of cross-slip is ignored.

Three dimensional DD models approximate individual dislocation curves by straight line segments. All the slip planes and slip directions can be considered and cross-slip is taken into account. The motion and interactions of the dislocations is considered in detail on each slip plane.

1.4 Multi-scale Discrete Dislocation Dynamics Plasticity

The three-dimensional Multi-scale Discrete Dislocation Plasticity (*MDDP*) model combines three dimensional *DD* with continuum Finite Element Analyses (*FEA*). The material is considered linear elastic for *FEA*. However, the stresses due to dislocations and plastic strains are superimposed as external loading. The *DD* part simulates the dislocation movement and evolution whereas the *FEA* applies boundary conditions and tracks shape changes of the crystal.

1.5 Research Objectives

The aim of this research is to:

i. Develop models for simulating nanoindentation in the M*DD*P computational code for spherical, flat punch, conical and Berkovich indenters.

ii. Investigate the dislocation structure evolution during nanoindentation using random initial dislocation configuration.

iii. Investigate the dislocation structure evolution during nanoindentation using initial dislocation configuration from atomistic/MD simulation as available in open literature.

iv. Investigate the accuracy of nanoindentation size effect model developed based on 2D simulations.

v. Generate topographical map of nanoindented surface based on exiting dislocations.

1.6 Methodology Followed

Several models were developed for simulating nanoindentation in the *MDDP* computational code for spherical, flat punch, conical and Berkovich indenters using suitable contact mechanics relationships.

Dislocation sources were placed in the computational cell, at different locations, based on different configurations. Indentation loading was applied and a plotting software (Tecplot) was used to visualize the positions of dislocations after each loading step. A computer program was generated and utilized to produce topographical maps based on the density of exiting dislocations at different locations on the nanoindented surface.

CHAPTER 2

LITERATURE REVIEW

2.1 Determination of Mechanical Properties by Nanoindentation

Material response of nanoindentation and related mechanisms is very complicated, especially if heterogeneous and polycrystalline materials are considered. Oliver & Pharr [1, 2] introduced a method for measuring hardness and elastic modulus by instrumented nanoindentation techniques. This technique has been widely adopted and used to determine mechanical behavior on nanoscale because the significance of this technique lies in the fact that the mechanical properties could be determined directly from load-displacement measurements, without the need to image the final impression. For this reason, the method found applications in thin films and small structural elements. Figure 2.1 shows a cross-section through a typical impression made during the nanoindentation test. The material pile up around the indentation site can also be seen.

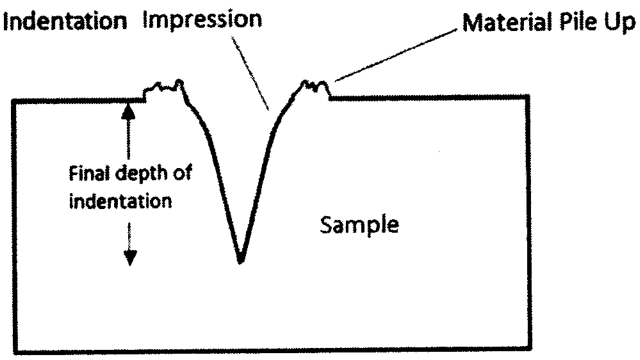

Figure 2.1: Schematic showing section through a typical nanoindentation impression at the end of nanoindentation test.

2.2 Indentation Size Effect

A decrease in hardness with an increase in indentation depth (for sharp tipped indenters) and decrease in hardness with increase in indenter radius (spherical indenters) is known as indentation size effect. Ouyang et al. [3] found that there are at least two effects that account for the size dependence of indentation hardness for circular indentation: strain hardening and the indentation size effect. Kreuzer & Pippan [4] verified through 2D simulation that indentation size effect at small indentation depths is an important effect of the discrete nature of plasticity.

2.3 Pop-In Events/ Excursions

Another interesting phenomenon is the pop-in events, also known as excursions in the load–displacement graphs i.e. there is sudden increase in displacement at constant load during the loading cycle (as shown in Fig. 2.2). Many researchers have investigated this through experiments and simulations. Gane and Bowden [5] were the first to observe the excursion phenomenon on electropolished surfaces of gold, copper and aluminum. Corcoran et al. [6] showed that yielding behavior during nanoindentation on single-crystal gold is composed of a series of discrete yielding events separated by elastic deformation. The pop-ins observed in the load–displacement curves is associated with dislocation emission, particularly homogeneous dislocation nucleation. Barnoush [7] showed that increasing the dislocation density and tip radius, i.e. the region with maximum shear stress below the tip, results in a reduction in the pop-in probability.

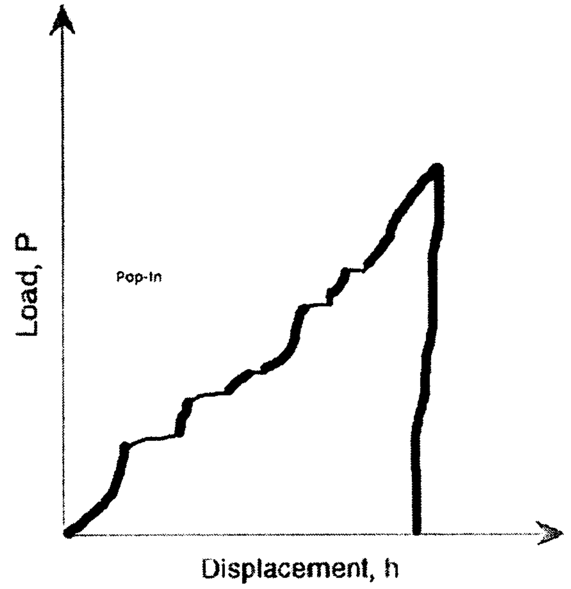

Figure 2.2: Representation of a yielding behavior during nanoindentation with discrete, pop-in events.

2.4 Atomistic/Molecular Dynamics (MD) Simulations

Nanoindentation process has been simulated using atomistic/molecular dynamics modeling. The main focus has been the homogeneous nucleation of dislocations in perfect crystals (without initial defects). Figure 2.3 shows an example of arrangement of atoms in atomistic modeling of nanoindentation. Fuente et al. [8] performed atomistic simulations of the emission of separate dislocation loops by nanoindentation on a (001) FCC surface. They showed that the initial stages of plastic deformation around nanoindentation results in the emission from near the contact point of dislocation half-loops intersecting the surface. Liang et al. [9] investigated elastic–plastic response of a Cu substrate during nanoindentation using molecular dynamics simulation. Wagner et al

العنوان:	INVESTIGATION DISLOCATION STRUCTURE EVOLUTION DURING NANOINDENTATION
المؤلف الرئيسي:	Zafar, Hassaan
مؤلفين آخرين:	Khan, Shafique(super.)
التاريخ الميلادي:	2014
موقع:	الظهران
رقم MD:	651514
نوع المحتوى:	رسائل جامعية
اللغة:	English
الدرجة العلمية:	رسالة ماجستير
الجامعة:	جامعة الملك فهد للبترول والمعادن
الكلية:	عمادة الدراسات العليا
الدولة:	السعودية
قواعد المعلومات:	Dissertations
مواضيع:	الهندسة الميكانيكية، التفكك
رابط:	https://search.mandumah.com/Record/651514

INVESTIGATING DISLOCATION STRUCTURE EVOLUTION DURING NANOINDENTATION

BY

HASSAAN ZAFAR

A Thesis Presented to the
DEANSHIP OF GRADUATE STUDIES

KING FAHD UNIVERSITY OF PETROLEUM & MINERALS
DHAHRAN, SAUDI ARABIA

In Partial Fulfillment of the
Requirements for the Degree of

MASTER OF SCIENCE
In

MECHANICAL ENGINEERING

MAY 2014