NEW TECHNOLOGIES
RESEARCH CENTRE
UNIVERSITY
OF WEST BOHEMIA

Oponentní posudek na disertační práci:

Ing. Mgr. Javier Varillas Delgado
A Molecular Dynamics Study of Nanocontact Plasticity and Dislocation Avalanches in FCC and BCC Crystals

In this field nanoindentation which uses an indenter with a known geometry to plunge into a specific site of the specimen by applying an increasing load is widely used to determine the mechanical properties of given material. The macroscopic changes of material during the nanoidentation are however driven by the microscopic modifications of the local crystal structure. Molecular dynamics simulations turned out to be very important tool to understand these microscopic changes of the materials. The main aim of this PhD thesis, detailed study of plasticity and dislocation avalanches in various fcc and bcc metals. In particular, a fundamental insight into the microscopic origin of permanent nanoimprints and differences between fcc and bcc crystals. In addition, detailed statistical analysis of MD simulation shed light into temperature dependent mechanisms characterising dislocation avalanche emission and propagation in these crystals. This topic is surely very timely as it is shown by detailed list of references presented in this thesis.

Thesis is clearly written and starts with short introduction, where author brings his research into broad context of material properties research. Following two chapters are devoted to the basic backgrounds of the dislocation glide theories and molecular dynamics, methods which serves as a formal basis for the investigations presented here. These chapters are supported by detailed appendix. In particular, Chapter concerning MD is very clearly written and it is clear that Mr. J. Varillas Delgado internalised whole theoretical methodology on a very high level. In addition, methods used in this thesis are very suited and unique to solve the main aim of thesis.

Main results of the thesis are summarized in the chapter 4, 5 and 6 and are based on three scientific manuscripts and in two of them J. Varillas Delgado is a first author. In the chapter 4, author concentrates to the interesting study of pile-up and slip-trace pattering around nanoindentations for various surfaces. The strength and uniqueness of this part is a detailed systematic study and comparison between three surface orientations of variety of fcc and bcc metals. It is however not clear why author choose particularly Fe, Ta, Cu and Al. I am bit missing discussion about magnetism of Fe which is known to have crucial influence on the crystal plasticity. Chapter 5 and 6 are than devoted to the understanding of nanohardness and dislocation avalanche. Both chapters are again very clearly written and all data are carefully analyzed. In particular, author used methods of statistical physics to answer above mentioned questions. In both chapters however I am bit missing detailed link to the experimental data. Unfortunately, author does not consider to write concluding chapter which should summarize all results of the whole thesis and that is why I do miss some more general outlook of work presented here, predictions found in the thesis and possible suggestions for new experimental as well as theoretical work. This issue should author summarize during his PhD exam.

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To summarize, submitted work of J. Varillas Delgado is very well written and discuss many important aspects of the nanoindentation from the microscopic point of view. All together, he published 1 manuscript in Acta Materialia which is an important journal in the field and has high impact factor. Two other manuscripts are either in referee process or are being prepared. All together, his publication record is satisfactory. Submitted content-rich thesis undoubtedly reflects his great competence also proofs his achieved scientific independence. Accordingly, I suggest the submitted thesis to be accepted and the dissertation of J. Varillas Delgado to be defended.

Additional questions:

– Results of chapter 5 and 6 are not compared in detail with experimental data. Please comment on it. Please review possible experimental tools which can be used to study effects discussed in the thesis.

– Why did you choose particularly Fe, Ta, Cu and Al? Why not other technologically relevant fcc and bcc metals. What about hcp metals?

– bcc Fe is known to be ferromagnetic material. Feromagnetism has crucial influence on the crystal pastic-ity. Is it possible in general include magnetism into MD simulations, please review it.

– EAM: How did you choose these particular potentials. How are they created and tested? How critical is the choice of the potential on the presented results. Do they have predictive power?

– Authors study in details three different surfaces but potentials for EAM are created and optimized for bulk. Please comment on possible limitations of this approximation.

– Author mentioned density functional theory. Could you please make short introduction into this method. It is important to understand how EAM are created.

– What about shape of the indenter. What do you expect if you consider squared, conical etc. indenters

– Author used open source package LAMMPS. Did you also contributed with your own developments?

Plzeň, 24.4.2019, Doc. Dr. Ján Minár

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FAKULTA STROJNÍ
ZÁPADOČESKÉ
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Oponentní posudek k obhajobě disertační práce

Reviewer's Report on PhD Dissertation Thesis

Západočeská univerzita v Plzni

Jméno/Name: Javier Varillas

Název/Title: Molecular Dynamics Study of Nanoimprint Formation and Dislocation Avalanche Emissions in FCC and BCC Crystals

Fakulta/Faculty: Fakulta Strojní

Studijní program/Study program: P2301 Strojní inženýrství

Studijní obor/Study field: 2303V015 Inženýrství speciálních technologií a materiálů

Školitel/Supervisor: Prof. RNDr. Josef Voldřich, CSc.

Oponent/Reviewer: Dr. Ranganathan Parthasarathy
Adjunct Professor, Department of Civil Engineering
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Nashville, TN 37209
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Obsahová stránka/Thesis Content

The thesis is fundamentally sound, and has extensive details validating the theory using experimental results from the literature. The literature review is also very detailed.

Aktuálnost tématu/Topicality of the subject

The thesis addresses the mechanics of defect initiation, propagation and interaction in crystal plasticity, which is important for designing continuum scale constitutive relationships for crystalline solids, and also for developing new metal alloys on the basis of strength, hardness, and toughness over various temperature ranges.

Postup řešení problému/Methods

The procedure used viz. Molecular Dynamics simulation has been clearly described, and the appendix is sufficiently detailed.

Význam rozvoj vědního oboru a pro praxi/Significance for the research field and applications

Due to the great extent of both breadth and depth in discussing effects of crystal structure, strain rate, temperature, and size effects, the results from this thesis should be highly significant in understanding atomic level mechanisms of crystal plasticity and applying them in developing continuum scale constitutive relationships. The work should be of strong interest to developers of semiconductor devices, and high temperature structural alloys, for example.

Formální a jazyková úroveň/Formal and language level

On the whole, the language is very clear. There are a few grammatical errors which could be corrected.

Publikační činnost/Publications

To my knowledge, two outstanding journal papers have already been published from this work, and the work has sufficiently unique results for several more.

Poznámky, připomínky/Comments, notes

Highly detailed thesis with extensive validation of simulation using experimental results.

To conclude, it is my opinion that the results in this thesis fulfills all requirements for a doctoral degree. I hereby recommend that the dissertation prepared by Javier Varillas, entitled "Molecular Dynamics Study of Nanoimprint Formation and Dislocation Avalanche Emissions in FCC and BCC Crystals," be accepted as fulfilling in part requirements for the degree of doctor of philosophy.

„**philosophiae doctor (Ph.D.)**“

Questions:

1. What was the basis for choosing the temperatures 77 K and 900 K in the simulations?
2. Depending on the indenter diameter, how does the interaction volume below the sample change, and how does it affect the movement and interaction of dislocations?
3. Section 3.2.3: Did the atoms with a vertical component zbox – cimp lose bonding with the simulation box? Why were they eliminated to continue the simulation?
4. Page 30, line 2 and in general: Were local strains at atomic level calculated using the atomic displacement fields to identify the onset of plastic behavior?

19th April 2019 in Nashville, TN (USA)

Reviewer