To honor Prof. Aifantis, Antalya, 2015



<u> Nano-Stimulus => Atom-Simulus</u>

semiconductors equipped with and atomistic simulations Towards plasticity of nanoindentation

What is it about?

R. Nowak(**说**漫 野貘) Nordic Hysitron Laboraton

Aalto University, Finland



Mechanics meets Electronics Fundamentals of nanoindentation and in nanoscale:

application for Electronic materials



NORDIC HYSITRON LABORATORY

what is possibly in common Mechanical behavior with **Electronics**?

1) Mechanical properties frequently essential to design optoelectronic devices 2) Nanoscale contact deformation provides new means for nanopatterning substrates

3) "Phase-change materials" – future of optoelectronics. Localized high-pressure control.



4) Implementation of nanoindentation for internal stress (difussion/reaction barriers for electronics) ... measurements, interlayer film thickness







EXAMPLE great challange Manipulation of nanostructure -

LETTERS

າ

Mechanical properties of ultrahigh-strength gold nanowires

BIN WU1*, ANDREAS HEIDELBERG1.2* AND JOHN J. BOLAND^{1†} Centre for Research on Adeptive Nanostructures and Nanodevices (CRAM) and the Department of Chemistry, Trinity College Dublin, Dublin 2, Ireland "AGEF e.V.-Institut an der Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf, Germany "These authors contributed equaly to this work"







Nanoindentation with SPM imaging



Contact probing of solid surfaces **MICRO-SCALE**









WHERE IS PHYSICAL BACKGROUND HERE?

H.R. Hertz, Miscellaneous Papers, Macmillan, London (1986), chaps. 5 and 6 H. Hertz, J. reine und angewandte Mathematik 92, 156-71 (1882)



Bulychev, V.P. et al. Int. Lab. **41**, 1409-12 (1975) R.B. King, Int. J. Solids Structures **23**, 1657-64 (1987)

 $E_{eff} \, {\checkmark} A$ エ \mathbf{C} dPdh $\frac{1}{2}$





EPI-based previous research

M. Sakai and R. Nowak, Fracture toughness and brittleness of ceramic materials, Proc. Int. Ceram. Conf. AUSTCERAM 92, ed. by M.J. Bannister, CSIRO Publications, 922-931(1992)

R. Nowak and M. Sakai, Energy principle of indentation contact: The application to sapphire, **J.** Mater. Res. 8, 1068-1078 (1993)

indentation fracture and hardness of α-alumina single crystals, Nucl. Instr. Meth, Phys. Res. B80, 1085-W. Ensinger and R. Nowak, On the influence of the low energy Tantalum ion implantation on 1090 (1993)

W. Ensinger, R. Nowak, Y. Horino and K. Baba, Modification of mechanical properties of single crystal aluminum oxide by ion beam induced structural changes, **Ceram. Forum Int. 70**, 164-167 (1993) R. Nowak and M. Sakai, The anisotropy of surface deformation of sapphire: Continuous indentation of triangular indenter, Acta metall. et materialia 42, 2879-2891 (1994) R. Nowak, C.L. Li and S. Maruno, Low-load indentation behaviour of HfN thin films deposited by reactive r.f. sputtering, J. Mater. Res. 12, 64-69 (1997)

They are commented at this point merely to introduce the main ideas and to explain the scale of We will return again to these theories later on difficulty

OUR MAIN GOAL REMAINS -2 N 5 a sin se





The Japanese Laboratory inside The European University







PRL May 2007

Nano-structured Materials & Thin Films? What are NORDIC HYSITRON Laboratory

Evolution of definition? Evolution of our understanding?



Contact probing of solid surfaces **NANO-SCALE**



Eeff

 $1 - v_1^2$ Б

Targeted Advanced Materials and Structures





- New multiferroic thin films prepared in Japan by sol-gel **BiFeO₃-PbTiO₃**
- Crystalline substrates for electronics (Al₂O₃, Si, SiC)
- Outer layer of human bones
- Nano-balls (SiO₂) and Nanowhiskers (W₁₈O₄₉)
- Surface of semiconductors

Targeted Advanced Materials and Structures



- <u>New multiferroic thin films</u> <u>prepared in Japan by sol-gel</u>
- Crystalline substrates for electronics (Al₂O₃, Si, SiC)
- Outer layer of human bones
- Nano-balls (SiO₂) and Nanowhiskers ($W_{18}O_{49}$)

Surface of semiconductors



Advanced Materials and Structures Evaluated by our Group



New multiferroic thin films prepared in Japan by sol-gel

<u>Crystalline substrates for</u> <u>electronics (Al₂O₃, Si, SiC)</u>

- Outer layer of human bones
- Nano-balls (SiO₂) and Nanowhiskers (W₁₈O₄₉)
- Surface of semiconductors

Advanced Materials and Structures Evaluated by our Group





- New multiferroic thin films prepared in Japan by sol-gel
- Crystalline substrates for electronics (Al₂O₃, Si, SiC)
- **Outer layer of human bones**
- Nano-balls (SiO₂) and Nanowhiskers (W₁₈O₄₉)

Surface of semiconductors





prepared in Japan by sol-gel New multiferroic thin films

electronics (Al₂O₃, Si, SiC) Crystalline substrates for

Outer layer of human bones

Nano-balls (SiO₂) and Nanowhiskers (W₁₈0₄₉)

Surface of semiconductors Net

(Nagao-JAPAN, Nordlund-FINLAND, Nowak-?) 2006 - Physical Review B 2005 - founded

EVOLUTION

2007 - Physical Review Letters

(Chrobak-POLAND, Nordlund-FINLAND, Nowak-?)

2009 - Nature Nanotechnology

(Nowak, Chrobak, Nagao-?/Poland/JAPAN Vodnick, Berg - USA HYSITRON INC.

2011 - Nature Nanotechnology





What makes NHL Special?

- initial idea
- Japanese-style devotion
- lucky selection of individuals as members
- our stubborn non-orthodox approach close to Finnish SISU-style 1

Nordic Hysitron Laboratory = Hunters of Curiosities





Nordic Hysitron Laboratory



TRIBOINDENTER HYSITRON

000

to a new discovery !!! The fatal attraction









Per aspera ad astra

Hunting a curiosity



To come to laser via nanomechanical treatment?



The subject stems from experimental research

The goal was to introduce initial defects to GaAs surface in PATTERNING), and subsequently, to employ MBE to grow a regular, controlled way (NANOINDENTATION quantum dots in the defined location

NORDIC HYSITRON LABORATORY





Corcoran et al., Phys. Rev. B 55, R16057 (1997)

Is it hot-topic???

NORDIC HYSITRON LABORATORY

- Shan et al., Mechanical annealing and source-limited deformation in submicrometre-diameter Ni crystals, **Nature Mater. 7**, 115 119 (2007)
- Minor *et al.* A new view of the onset of plasticity during the nanoindentation of aluminum. *Nature Mater.* 5, 697-702 (2006).
- P. Schall, I. Cohen, D.A. Weitz and F. Spaepen, Visualizing dislocation nucleation by indenting colloidal crystals, *Nature* 440, 319-323 (2006)
- M. Cross, A. Schirmeisen, P. Grütter and U.T. Dürig, Plasticity, healing and shakedown in sharp-asperity nanoindentation, *Nature Mater*. 5, 370-376 (2006) G.L.W. Cross, A.
- S. Suresh, Crystal deformation: Colloid model for atoms, Nature Mater. 5, 253-254 (2006)
- I. Szlufarska, A. Nakano and P. Vashista, A crossover in the mechanical response of nanocrystalline ceramics, **Science 309**, 911-914 (2005)
- W. Gerberich and W. Mook, A new picture of plasticity, Nature Mater. 4, 577-578 (2005)
- Schuh, J.K. Mason and A.C. Lund, Quantitative insight into dislocation nucleation from high-temperature nanoindentation experiments, *Nature Mater.* 4, 617-621 (2005) C.A.
- J. Li, K.J. Van Vliet, T. Zhu, S. Yip and S. Suresh, Atomistic mechanisms governing elastic limit and incipient plasticity in crystals, *Nature* 418, 307-310 (2002)
- a crystal, **Natu** Gulds Ŕ





Nature 418, 307-310 (2002).

4

The widely accepted mechanism of pop-in in metals is related to the nucleation of the <u>initial dislocations</u>











Our QD-oriented nanoindentation project entirely unsuccessful! Why? (!)



Û

GaAs structure

GaAs compound is an important semiconductor widely used to make devices such as: infrared light-emitting diodes

Ga – magenta As – yellow

- laser diodes
- high efficiency solar cells

The combination of GaAs with germanium and indium gallium phosphide is the basis of a triple junction solar cell which holds the record efficiency of over 32% and can operate also with light as concentrated as 2.000 suns.

devices of high structural quality GaAS are important to make Mechanical properties of





H. Leipner at al., Phys. Rev. B 172101 (2003)

or g is 2

Molocular Dynamics simulation of the tip - GaAs contact



 diamond cube indenter with edge length 28 A
indenter was shifted by 1A in [001] direction
and then structural relaxation within 20 000 time steps took place MD simulation of zinc-blende GaAs: Indented surface: (001) Ibulk dimensions: 316x316x158 A Itotal number of atoms: 700 425













Slip vector analysis

 $s(i) = \frac{1}{4} \sum_{j=1}^{4} [x(i, j) - x^{0}(i, j)]$

Slip vector gives information about

Burgers vector of dislocations.





[1] J.A. Zimmerman et al., Phys. Rev Lett, 87, 165507 (2001)

There is no slip planes in our system









there is no dislocation affected volume .⊆ Pop-in events in GaAs –unexplored mechanism of incipient plasticity What is origin of the pop-in? rocksalt-like 4 Å



Pop-in events in GaAs – unexplored mechanism of incipient plasticity



There is transformation from GaAs-I to GaAs-II phase [1-3]

SEMICONDUCTING

CONDUCTING



zinc-blende structure with bond angles of \sim 110 degrees

rocksalt structure with bond angles of 90 degrees

The average hydrostatic pressure in thin volume (28x28x17 A, *U* - domain) under indenter was equal to 18 GPa

S.T. Weir *et al.*, Phys. Rev. B 39, 1280 (1989)
J.M. Benson *et al.*, Phys. Rev. B 44, 4214 (1991)
S.B. Zhang *et al.*, Phys. Rev. B 39, 1450 (1989)

Pop-in events in GaAs – unexplored mechanism of incipient plasticity





The existence of \sim 70 degrees bond angles was confirmed by BADF analysis for U - domain.

\$

Valentini, Gerberich & Dumitrica, Phase-transformation plasticity response in uniaxially compressed silicon nanospheres. Phys. Rev. Lett. 99, 175701 (2007).



NORDIC HYSITRON LABORATORY





Chrobak, Nordlund and Nowak Phys. Rev. Lett. (2007)







where indentation was performed, as schematically presented in Figs. 4 and 5. Qbs are grown by MBE, and further the remaining SiO_2 part would be removed by etching (Figs. 6 and 7). The method offers possibility of control of the hole since it no longer sharply deposited SiO₂ coating, instead in the GaAs wafer (see Figs. 2 and 3). Subsequently, the depends on tip shape and size and can be moderate by etching process (relatively large SiO₂ film would be selectively etched in order to expose the GaAs surface at the spot The essence of the idea proposed in NAKAMA-EXT is to perform indentation in the tip will act merely as a marker for etching process).



SiO₂ GaAs-substrate Fig. 1 SiO₂ mesa structures prepared by ORC on GaAs substrate

Fabrication of mesa-structured SiO2-on-GaAs templates for nano-indentation This task concerns the fabrication of SiO2on-GaAs templates with SiO2 mesa-structure. SiO2 is first grown on epi-ready n-GaAs(100) substrate by plasma-enhanced chemical vapour deposition (PECVD). Subsequently, the surface of GaAs wafer is patterned either by standard photolithographic methods and etching or by nanoimprint lithography (NIL) to form variable sized SiO2 mesa structure.





















θ









The schematic explanation of the phenomena responsible for a singularity in mechanical (pop-in) and electrical (current spike) response in nanoindented GaAs. The initial GaAs-conducting contact is of Schottky type (A). Under the imposed pressure the junction leaks in B-stage of the indentation due to introduced metallization of a certain part of zinc-blende structure, while the appearance of metallic rocksalt structure (C) halts the CS-spike current and restores the Schottky contact.

pop-in instant

before pop-in

initial contact





HIMITSU







provides a way to new, hitherto unrecognized applications

when deformed in the nano-scale

The discovery of GaAs as phaseswitching material

"phase-change material"? a locally stress-controlled





polymers and other free volume materials by nanoimprint manufacturing

Graham L.W. Cross, Nature Nanotechn. 2011



This has practical implications for the fabrication and ultimate strength of nanostructures formed in glassy

RN

To honor Prof. Aifantis, Antalya, 2015

The discovery of GaAs as phase-switching material

when deformed in the nano-scale provides a way to

new, hitherto unrecognized applications

The discovery of GaAs as phase-switching material when deformed in the nano-scale provides a way to new, hitherto unrecognized applications

RN

This has practical implications for the fabrication and ultimate strength of nanostructures formed in glassy polymers and other free volume materials by nanoimprint manufacturing

Graham L.W. Cross, Nature Nanotechn. 2011



INSTEAD OF CONCLUSIONS

Thank you very much for your kind attention