



Proiect No.11-048

**Dispozitive nanoelectronice bazate pe materiale
oxidice-NANOXI**

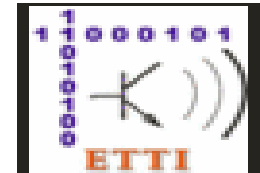
**Coordonator: Institutul National de Cercetare
Dezvoltare pentru Microtehnologii-IMI-Bucuresti
Director proiect: CSI Dr. R. Plugaru**



**Sesiunea CNMP – 23 Noiembrie 2009
Bucuresti**

Parteneri in consortiu

- ▶ Universitatea Politehnica Bucuresti (www.arh.pub.ro)
Conferentiar Dr. Florin Babarada
- ▶ Institutul de Chimie Fizica "ILIE MURGULESCU"
al Academiei Romane (www.icf.ro)
Dr. Mihaiu Maria Suzana
- ▶ Institutul National de Cercetare Dezvoltare pentru Inginerie Electrica
ICPE-CA (www.icpe-ca.ro)
Prof. Dr. Wilhelm Kappel, Ing. Fiz. Iordache Iulian
- ▶ METAV-Cercetare Dezvoltare S.A (www.metav-cd.ro)
Dr. ing. fiz. Vasile Eugeniu



Buget/Cofinantare

2.000.000 lei/59.375

<http://www.imt.ro/nanoxi/>



Obiectivul/rezultatul final al proiectului

► Obiectiv general: obtinerea de dispozitive nanoelectronice demonstratoare de tip MOSFET utilizand filme oxidice ultrasubtiri (< 15 staturi atomice) dopate cu metale de tranzitie sau cu pamanturi rare.

Elementele de noutate/originalitate

A. Experiment

► Obtinerea prin metoda fizica magnetron sputtering si metoda chimica sol-gel a filmelor oxidice semiconductoare transparente de ZnO si ZnO dopate cu Al, Ti sau Mn cu grosimi intre 20 - 100 nm.

► Depunerea prin metoda magnetron sputtering a condus la filme cu grosimea de 100 nm, compacte, uniforme, aderente la substrat de Si/SiO₂, sticla si Sital, cu structura dorita de tip wurtzita. Elemente de noutate: fabricarea dupa un procedeu original a tintelor de ZnO si tehnologia de depunere a filmelor. Au fost depuse doua cereri de brevete pentru: "Obtinerea tintelor pentru depunere de oxid de zinc prin magnetron sputtering (ICPE-CA)" si "Tehnologie de obtinere a filmelor ultrasubtiri dopate de tip ZnO: Mn prin magnetron sputtering (ICPE-CA)".

► Prin metoda sol-gel am obtinut un control la nivel de strat atomic a grosimii filmelor de ZnO si ZnO:Al. Filmele obtinute sunt poroase si au grosimi de 30 - 100nm.



B. Modelare/simulare prin metode computationale

- ▶ Au fost realizate calcule de structuri de benzi de energie pornind de la principiile primare (first principles calculation) in cadrul DFT (Teoria functionalei de densitate) utilizand un cod de potential total bazat pe metoda LCAO. Element de noutate: predictia teoretica a efectelor elementelor dopante asupra proprietatilor de conductie electrica si magnetism in ZnO si in TiO₂.
- ▶ Dezvoltarea unei noi metodologii pentru modelarea la scara atomica si nanometrica a curentilor de strapungere in nanodispozitive, folosind un program de calcul ATLAS.



Beneficiarii rezultatelor, potentialul de aplicare in economie

- ▶ **Pentru industria IT:** Crearea unei baze de date cuprinzand tehnologii experimentale si metode teoretice de modelare/predictie a materialelor pentru aplicatii in nanodispozitive.
- ▶ **Pentru parteneri in proiect:** Punerea in functiune a unor noi echipamente de cercetare si dezvoltare pentru realizarea tehnologiilor de obtinere a materialelor nanostructurate. Crearea unei expertize in utilizarea metodelor experimentale de investigarea a obiectelor la nivel nanostructura (microscopie electronica (SEM, TEM, HRTEM), AFM, spectroelipsometrie, spectroscopie de tunelare (SPM), IR, UV-VIS, PL, difractie de raze x). Crearea unei expertize in utilizarea codurilor care trateaza problema interactiilor cuantice in solid.
- ▶ **Formare tineri cercetatori:** prezentare cursuri, editare capitole de carti, activitate de pregatire master si doctorat.



Stadii de realizare. Etapele conform planului de realizare.

- ▶ **Etapa I/2007:** Elaborarea modelelor pentru obtinerea si caracterizarea filmelor oxidice ultrasubtiri si achizitionarea de echipamente.
- ▶ **Etapa II/2008:** Obtinerea si caracterizarea structurala a filmelor oxidice ultrasubtiri.
- ▶ **Etapa III/2009:** Modelarea/simularea parametrilor de material.
- ▶ **Etapa IV/2009:** Analiza datelor experimentale si a rezultatelor modelarilor/simularilor de material.
- ▶ **Etapa V/2010:** Realizare de dispozitive demonstratoare.



▶ **Etapa I/2007:** Elaborarea modelelor pentru obtinerea si caracterizarea filmelor oxidice ultrasubtiri si achizitionarea de echipamente

▶ **Buget de stat/Cofinantare:** 162.500/0

▶ **Rezultate**

Studii de necesitate publica - de interes national:

Modele pentru obtinerea si caracterizarea filmelor oxidice ultrasubtiri.

"Caracterizarea filmelor subtiri oxidice".

"Modelarea filmelor subtiri oxidice".

"Experimentarea de noi concepte (principii) de dispozitive nanoelectronice."

• ***Publicatii***

Articole ISI: 1

ISSN/ISBN: 2

Participari la conferinte: 2 (E-MRS Varsovia, Polonia 2007, CAS 2007, Romania)

• ***Achizitii realizate***

Echipamente pentru cercetare-dezvoltare (Diffractometru de raze X tip X'Pert PROMPD - METAV CD-S.A.).

Calculatoare electronice, echipamente periferice, Program FPLO de modelare/simulare dedicat materialelor (IMT, UPB).



▶ **Etapa II/2008:** Obținerea și caracterizarea filmelor oxidice ultrasubțiri.

▶ **Buget de stat/Cofinantare:** 750.883/43.750

▶ **Rezultate**

- *Tehnologii IT performante*

Calcul de structura de benzi de energie în solid prin metode ab initio. (Model conceptual computational).

Modelarea și simularea filmelor subțiri oxidice. (Model conceptual computational).

- *Nano- și micro sisteme:* Tehnologii de obținere a tintelor pentru depuneri de straturi subțiri prin metoda magnetron sputtering. (Model experimental).

Tehnologii de obținere a filmelor oxidice ultrasubțiri prin metoda sol-gel. (Model experimental).

Curs organizat de către IMT București în cadrul proiectului: "Materiale oxidice și aplicații pentru micro-nanoelectronica" 25-26 noiembrie 2008, București

Propunere brevet: "Obținerea tintelor pentru depunere de oxid de zinc prin magnetron sputtering." (ICPE-CA)

- *Publicatii*

Articole ISSN/ISBN: 6

Comunicări științifice: 5

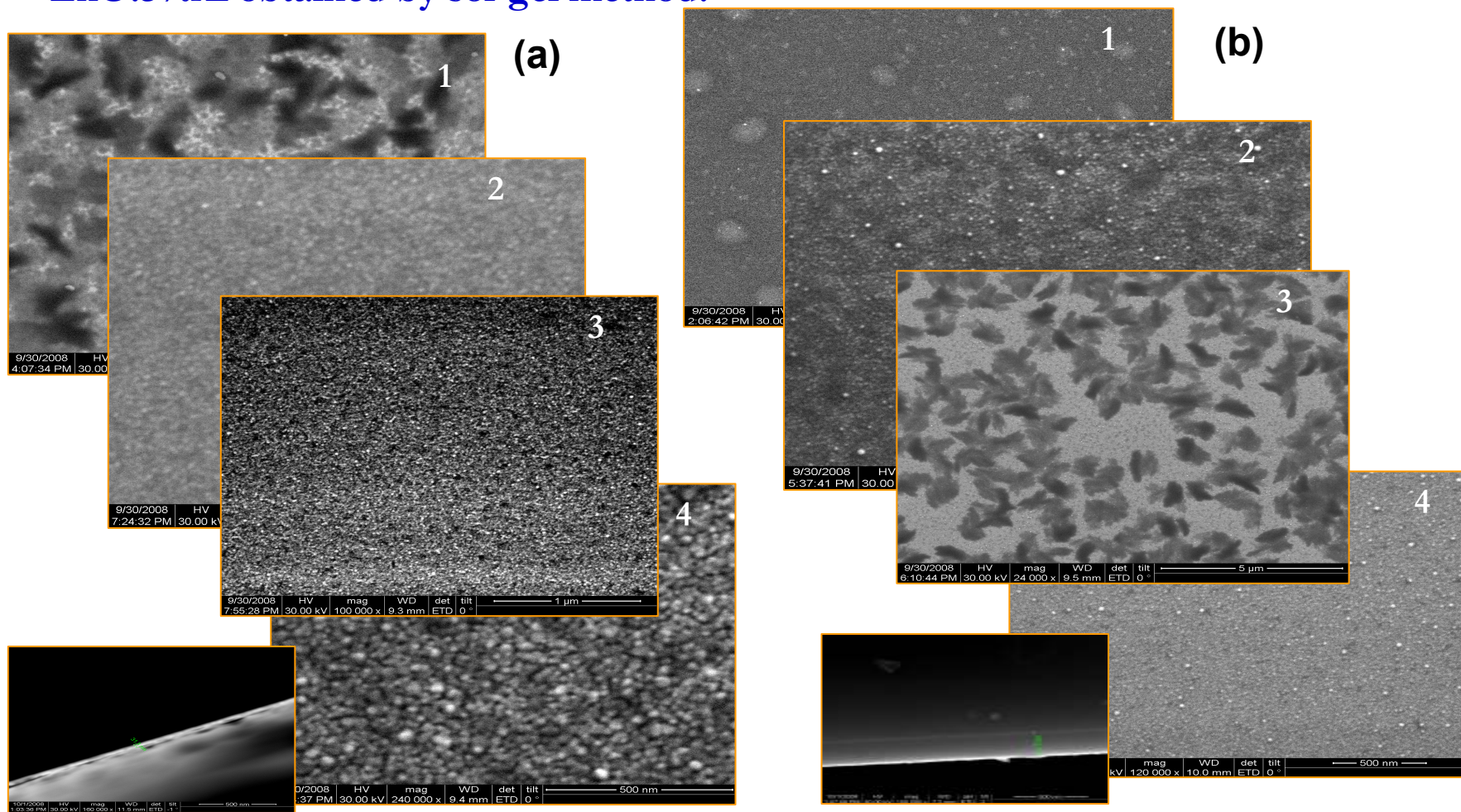
Participări la conferințe: 12

- *Achiziții realizate*

Sistem de caracterizare electrică pentru semiconductoare și sistem de microprobere. Model 4200 SCS/C/Keithley, EP6/ Suss MicroTec (IMT)

Calculatoare electronice și echipamente periferice, software, echipament electronice pentru diseminare (UPB, ICF)). Completări la echipamentul de difracție de raze X (ICPE).

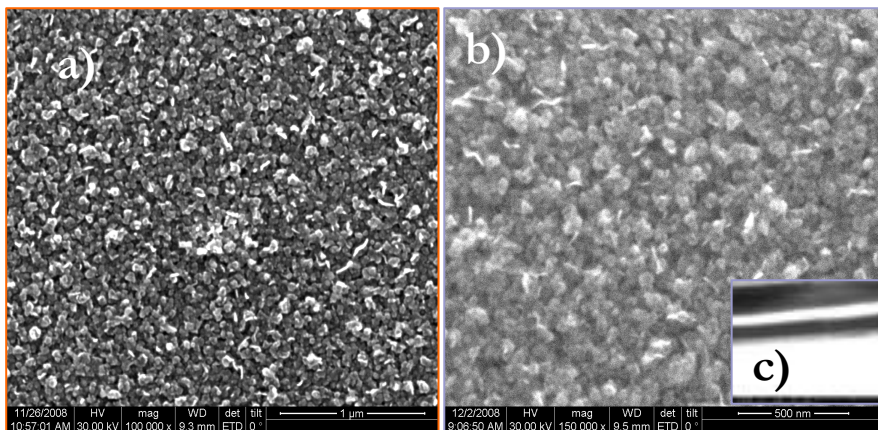
SEM, EDX, AFM, Spectroellipsometry and Spectrofotometry studies of ZnO and ZnO:5%Al obtained by sol-gel method.



Evolution of ZnO (a) and ZnO: 5%Al (b) thin films morphology. The films have been obtained by deposition of 4 successive layers using sol-gel method. Each layer was treated after deposition at 500°C in ambient atmosphere for 1 hour.

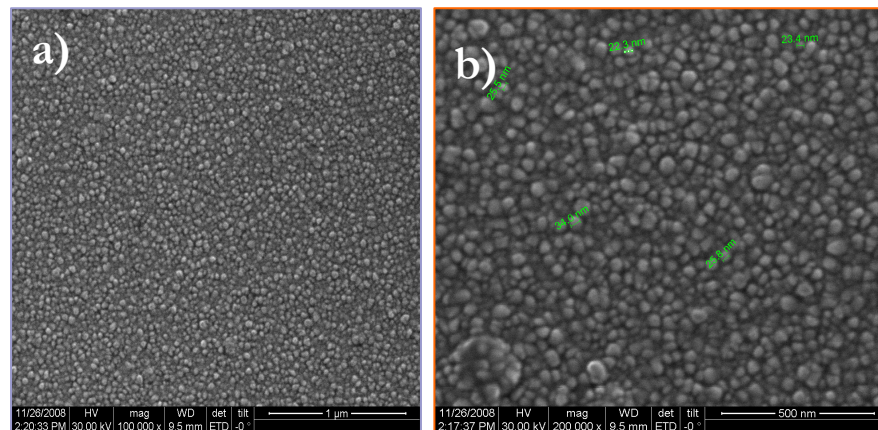
E-MRS 2009 Conference
Strasbourg, France

ZnO films deposited by DC magnetron sputtering from Zn target



SEM images of ZnO film deposited from Zn metallic target and oxidized in air at 450°C, 3h (a, b). The film thickness in the SEM cross section image is 92.5 nm (c).

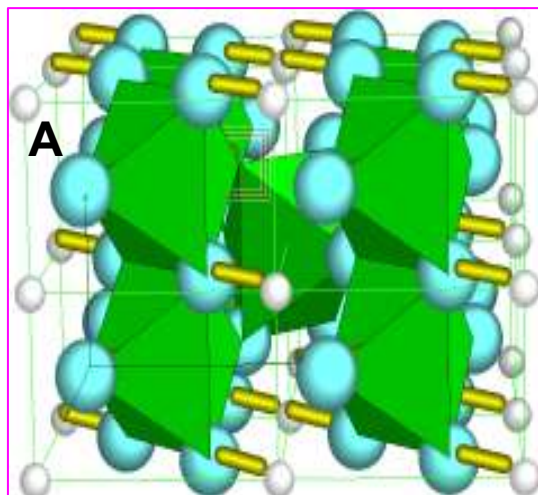
ZnO films deposited by RF magnetron sputtering from ZnO target



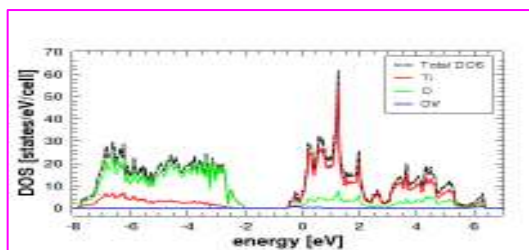
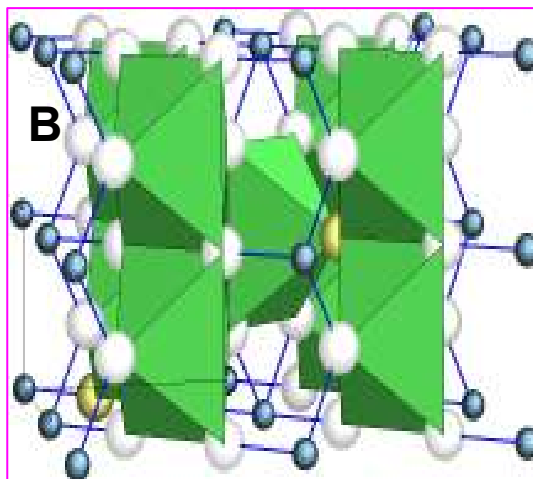
SEM images of the as deposited ZnO film surface (a). Relative uniform grains size about 22-35 nm (b).

Metallic Zn (Aldrich, 99.99%) was used as target in DC magnetron sputtering process. ZnO target used in RF magnetron sputtering deposition process was obtained from ZnO powder (Umicore Zinc Chemicals, 99.99%). The ZnO powder was mechanically milled, then pressed as a disc with the diameter of 4.5 cm and thickness of 3.5 - 4 mm. The target was sintered at 1200°C for 1 h.

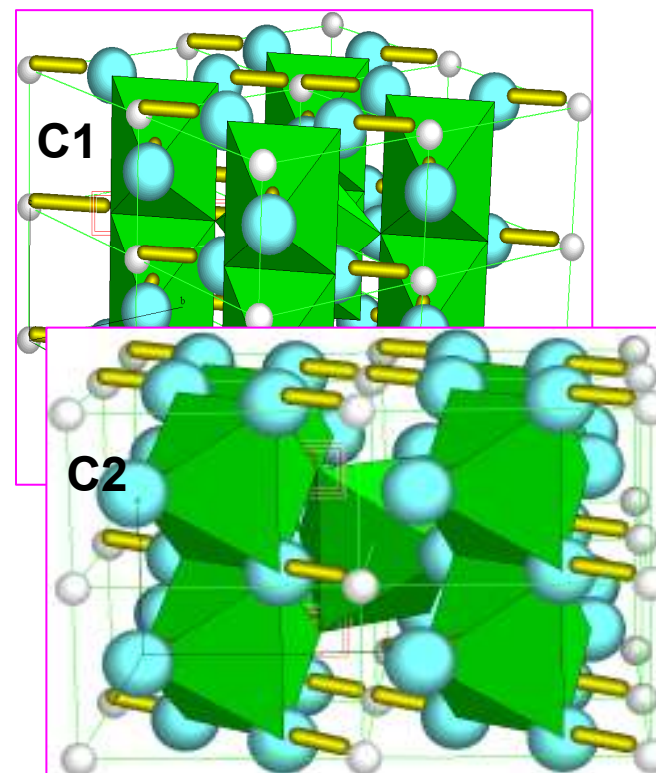
TiO₂ Supercells 2×2×2 of the basic cell at the equilibrium volume with several OV distributions were used as structural models in the calculations



Supercell A, containing a single vacancy, illustrates the layout of 3.125 % isolated OVs.



Supercell B, with 6.25 % OVs, with large separation distance between the OVs to probe the onset of vacancy-vacancy interactions and finite size effects.



Supercells C1 and C2, also with 6.25 % OVs arranged as isolated pairs with perpendicular and parallel orientation, respectively, to the crystallographic c-axis, to investigate symmetry and clustering effects.

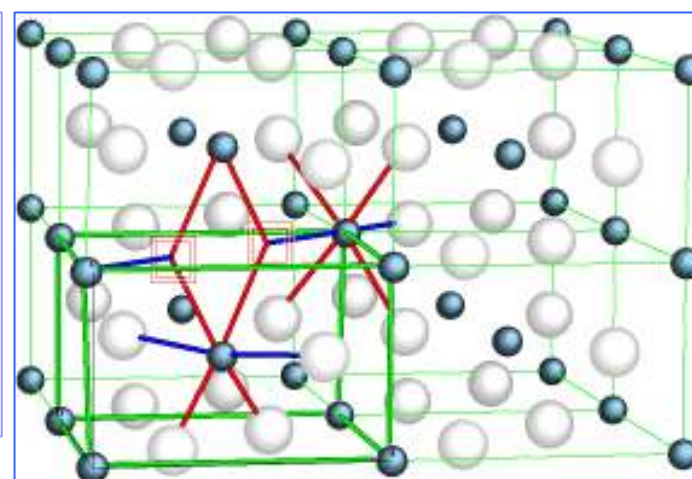
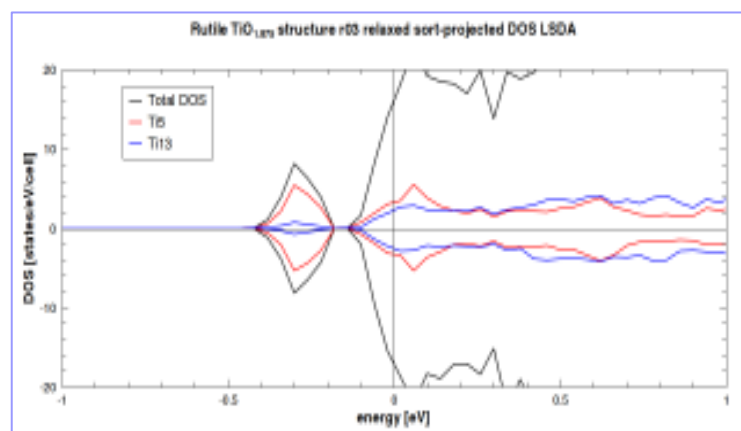
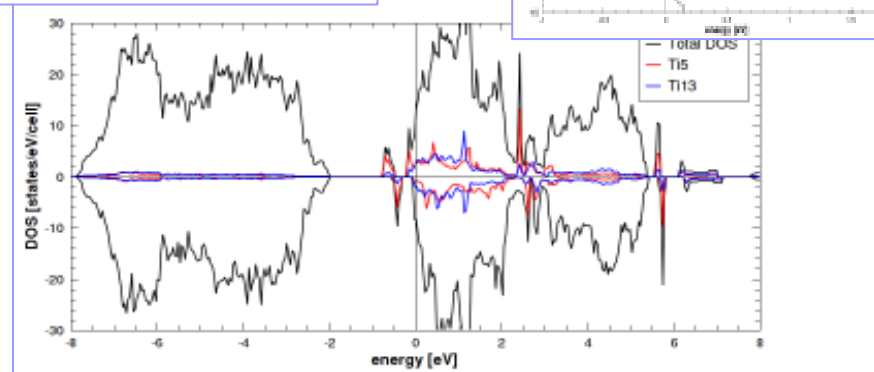
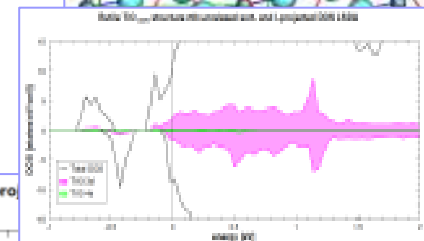
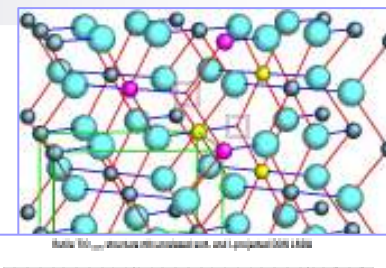
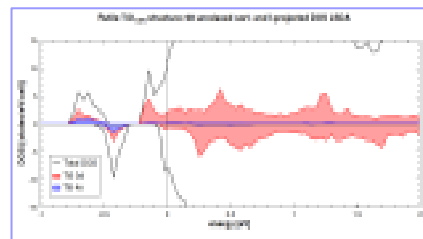
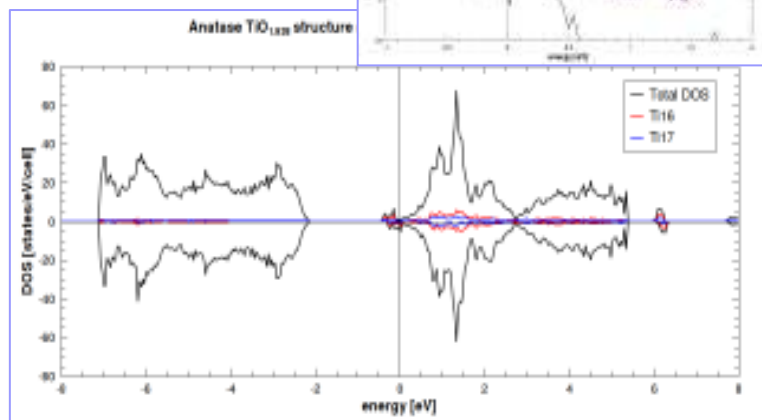
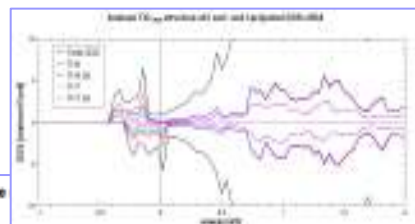
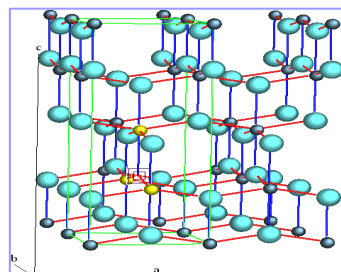
CAS 2008 Conference,
Romania

FPLO Workshop 2008
Dresda, Germania

Stress induced magnetism in $\text{TiO}_{2-\delta}$

A- TiO_2

R- TiO_2

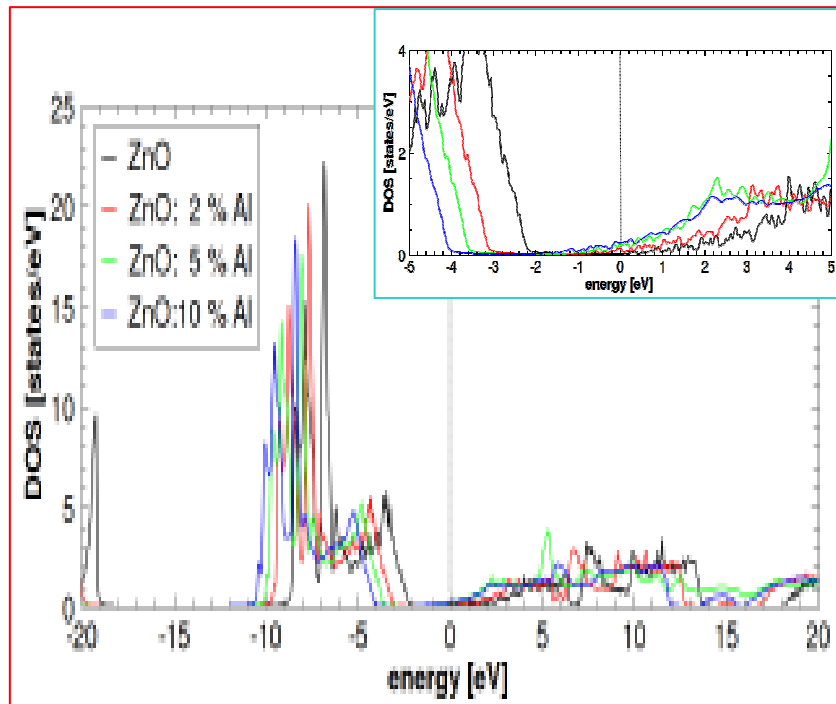


Locally relaxed
r03 structure.

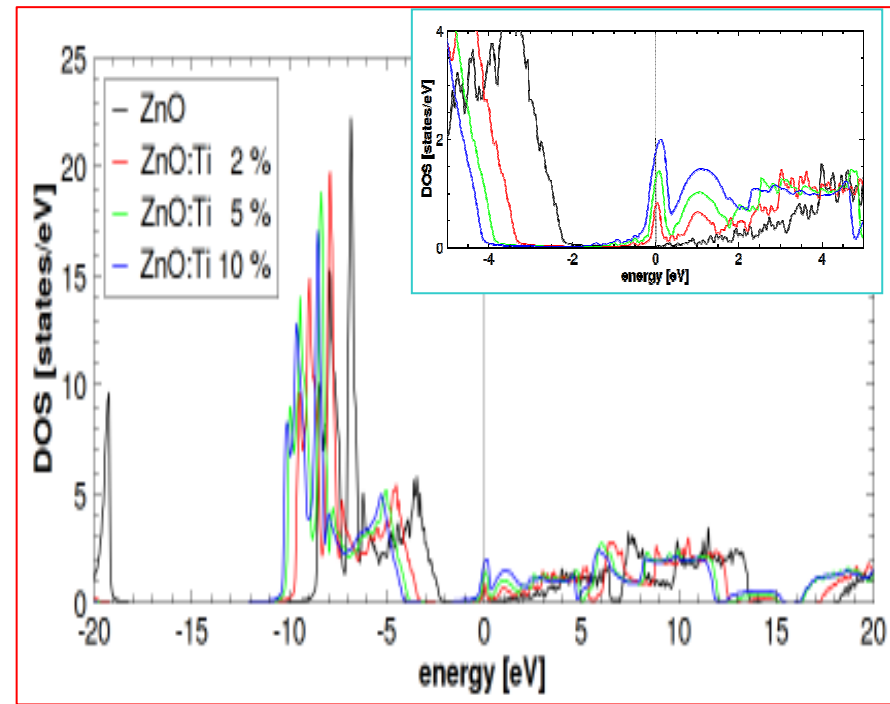
E-MRS Conference 2009,
Strasbourg, France

Electronic structure of ZnO doped with Al, Ti, Mn

- LDA calculations on wurtzite-type ZnO doped with Al, Ti and Mn in the concentration range 2-10 at.%, assuming substitutional disorder at Zn site, in order to separate the dopant effects on electrical conductivity and magnetism in ZnO.



Total DOS of Al-ZnO $x=2, 5$ and 10% . DOS of pure ZnO is also shown.

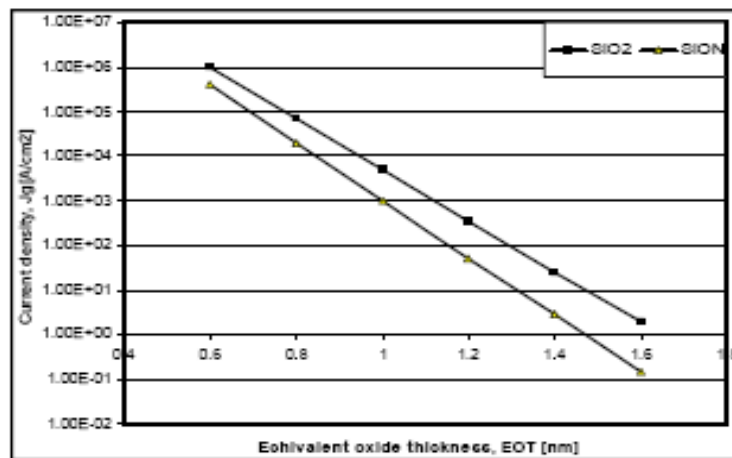


Total DOS of Ti-ZnO, $x=2, 5$ and 10% Ti. DOS of pure ZnO is also shown.

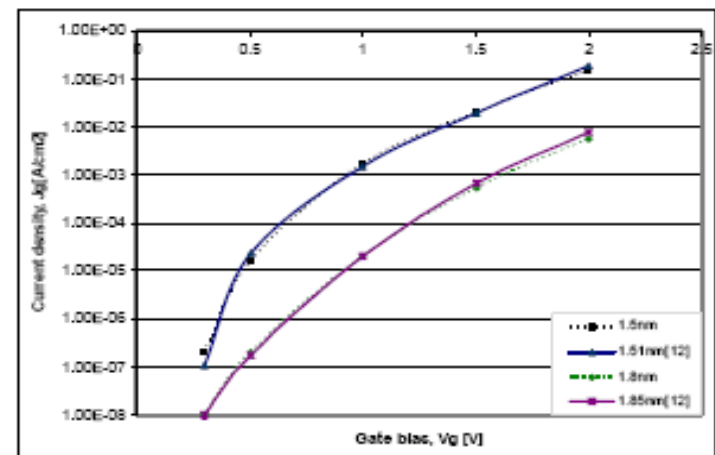
- Al and Ti behave as donors. A density of states arises at the Fermi level, $N(E_F)$, increasing with dopant concentration. The valence band shifts to lower energy.

Tunnelling leakage current characterization of silicon oxide and high-k dielectrics for advanced semiconductor devices.

Numerical simulations were performed using ATLAS devices simulator software package from Silvaco. An iterative approximate method was used to calculate the 1D MOS structures main electric parameters without using the Schrödinger-Poisson equations.



Tunnelling current gate leakage in inversion channel for oxide and oxynitride at $V_g=1V$.



Calculated data and experimental gate leakage currents for high-k stacks with Al_2O_3 .



▶ Etapa III-IV/2009

III. Modelarea/simularea parametrilor de material.

IV. Analiza datelor experimentale si a rezultatelor modelarilor/simularilor de material

▶ Buget de stat/Cofinantare 261.435/0

▶ Rezultate

- *Produse : Materiale avansate*

Filme oxidice ultrasubtiri dopate ZnO:Al.

Filme oxidice ultrasubtiri dopate ZnO:Mn.

- *Tehnologii IT performante*

Model compact al tranzistorului MOS cu grad ridicat de scalare. (Model conceptual).

Algoritm de aproximare iterativa a curentilor reziduali de tunelare in straturi izolatoare high-k. (Model conceptual).

Modele de sisteme dezordonate pentru simularea si studiul efectului doparii asupra proprietatilor electronice ale materialelor semiconductoare oxidice. (Model conceptual).

Sisteme dezordonate pentru modelarea/simularea proceselor de dopare a semiconductorilor oxidici. (Model conceptual).

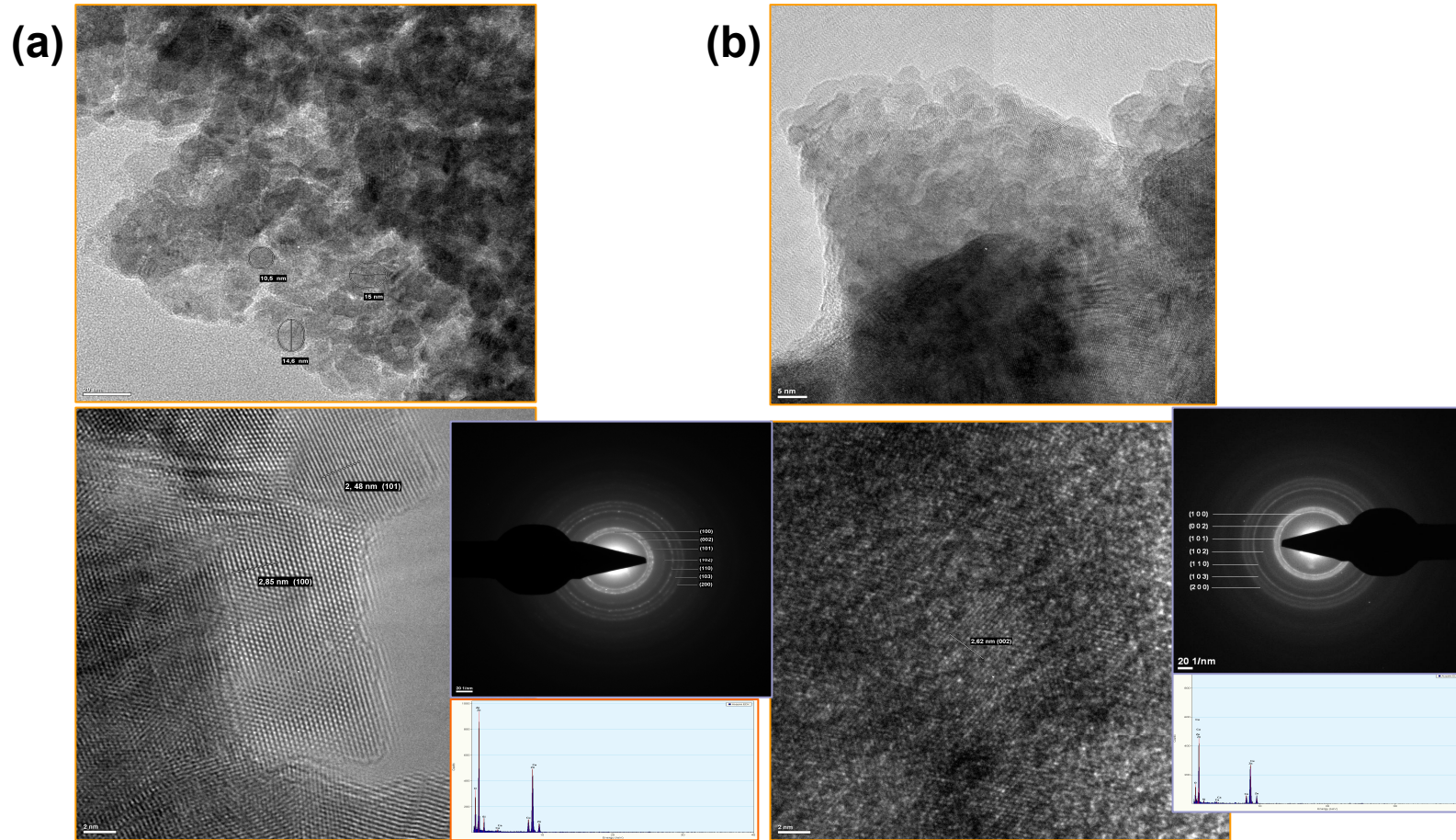
- *Tehnologii avansate de conducere a proceselor industriale*

Proiectarea experimentului pentru noi tehnologii de fabricare a dispozitivelor MOS bazate pe materiale oxidice. (Flux tehnologic).

Modelarea suprafetei de raspuns pentru dispozitive MOS bazate pe materiale oxidice. (Model conceptual).

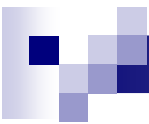
Modelarea procesului de crestere heterogena a filmelor ultrasubtiri prin depuneri multistrat. (Model experimental).

HRTEM, SAED and EDAX analyses of ZnO thin films obtained by DC and RF magnetron sputtering from Zn and ZnO targets.



HRTEM images of ZnO films obtained by DC (a) and RF magnetron sputtering (b). The films structure is wurtzite, with nanocrystals orientation (100) (a), and (002) (b).

**E-MRS 2009 Conference
Strasbourg, France**



► *Publicatii*

Articole ISSN/ISBN: 4

Comunicari stiintifice: 6

Participari la conferinte: 9

Capitole de carti: "Semiconductor Processes and Devices Modelling " din cartea Semiconductor Technologies, Ed. Intechweb, ISBN978-953-7619-X-X, 26 pg. (2009).

Lucrari extinse (2) acceptate vor fi publicate in seria "Nanoscience and Nanotechnology", Editura Academiei Romane (2009).

"Experimental and Density Functional Theory Studies of the Structure, Optical and Electronic Properties of Wide Band Gap Oxides for Nanodevices"
"First principles study of the electronic structure of Al/Ti:ZnO"

Propunere de Brevet: "Tehnologie de obtinere a filmelor ultrasubtiri dopate de tip ZnO: Mn prin magnetron sputtering." (ICPE-CA)

Achizitii realizate

Materiale consumabile pentru experimente (IMT, ICF, UPB)

Cheltuieli de diseminare (IMT, ICF)

Calculatoare si periferice (UPB)

Etapa V/2010: Obtinerea dispozitivelor demonstratoare.

Buget de stat/Cofinantare
825.000/15.625

Participarea tinerilor cercetatori



- **CURS: Materiale oxidice si aplicatii pentru micro-nanoelectronica**

25-26 noiembrie 2008 Bucuresti (IMT-UPB)

Topica:

- Proprietati ale materialelor oxidice.
- Obtinerea si caracterizarea materialelor oxidice.
- Aplicatii. Dispozitive electronice bazate pe materiale oxidice.

Participanti: tineri cercetatori, doctoranzi, studenti masteranzi (UPB, ICF, IMT, ICPE, METAV) (28 de participanti)

- **CURS post-doc: FPLO Hands-on (IFW Dresda, Germania, 2008, 2009).**

- **Teze de doctorat, doctoranzi (6):** Oxizi semiconductor-obtinere, tehnologii, caracterizare, dispozitive.

IMT-drd A. Dinescu, **ICF**-drd. A. Toader, **ICPE-CE** - drd M.N. Iordoc, drd C. Banciu, drd A.A. Teisanu, drd R.B. Vasilescu-Mirea.

Implicarea tinerilor cercetatori in etapele de realizarea ale proiectului

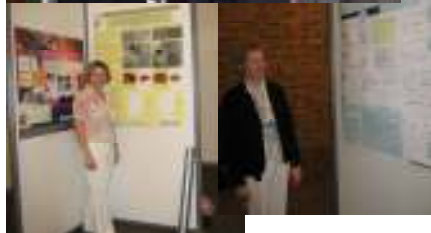
Etapa I/2007 Nr. pers. cu studii superioare 17/ Din care participanti sub virsta de 35 de ani 3.

Etapa II/2008 Nr. pers. cu studii superioare 29/ Din care participanti sub virsta de 35 de ani 8.

Etapa III-IV/2009 Nr. pers. cu studii superioare 22/ Din care participanti sub virsta de 35 de ani 5.

Diseminari: numar de articole publicate/acceptate spre publicare (ISI, reviste), numar de carti publicate/acceptate spre publicare, comunicari stiintifice

Interne



► Conferinta International Semiconductor Conference CAS 2007, 2008, 2009, Sinaia Romania (5 lucrari)

► ROMPHYSCHEM, University of Bucharest, Faculty of Chemistry, 15th July 2008, Bucharest, Romania, 2008. (1 lucrare).

► A 8-a editie a Seminarului National de Nanostiinta si Nanotehnologie 27 aprilie 2009, Amfiteatrul I.H. Radulescu, Biblioteca Academiei Romane (1 lucrare)

Carti:

► F. Babarada, capitolul *Semiconductor Processes and Devices Modelling* din cartea *Semiconductor Technologies*, Ed. Intechweb, Viena Austria, ISBN978-953-7619-X-X, 26pg. 2009.

► R. Plugaru, S. Mihaiu, I. Iordache, E. Vasile, F. Babarada, N. Plugaru, *Experimental and Density Functional Theory Studies of the Structure, Optical and Electronic Properties of Wide Band Gap Oxides for Nanodevices*, accepted in *Nanoscience and Nanotechnology (Romanian Academy) 2009*.

► R. Plugaru, N. Plugaru, *First principles study of the electronic structure of Al/Ti:ZnO crystal*, accepted in *Nanoscience and Nanotechnology (Romanian Academy) 2009*.

Internationale

► E-MRS Fall 2007, Varsovia, Polonia (1 lucrare)

► EMMSS2008, Campora S. Giovanni, Italia. (2 lucrari)

► ICL2008, Villach, Austria, 2008. (1 lucrare)

► 4M2008, Cardiff, Anglia. (1 lucrare)

► Electroceramics XI 2008, Manchester, UK. (1 lucrare)

► 2nd International Congress on Ceramics 2008, Verona, Italy. (2 lucrari)

► MICROSCIENCE Conference 2008, London, UK. (1 lucrare)

► E-MRS Spring 2009, Strasbourg, Franta. (2 lucrari)

► FPLO Workshop 2008, 2009, Dresda, Germania. (3 lucrari)

► 15th International Sol-Gel Conference 2009, Porto de Galinhas-Pernambuco-Brazilia. (1 lucrare)

► EMMSS2009, Tenerife, Spania. (1 lucrare)

► International Conference Interactive Computer Aided Learning-ICL2009, Villach, Austria. (1 lucrare)