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D2-P-TUE-P1-22 Quantitative analysis of the stepped-strained 6H-SiC/AlN interface in HEMT structures

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D2-P-TUE-P1-26 Three-dimensional structure characterization of nanotubular metal oxide films

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D2-P-TUE-P1-27 X-ray Peak Broadening Analysis and Characterization of Sub-Micron Y2O3 Particles Synthesized by Ultrasonic Spray Pyrolysis Method

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D2-P-TUE-P1-28 In-situ environmental Transmission Electron Microscopy characterization of catalyst materials

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D2-P-TUE-P1-29 Structural characterization and nanoscale bandgap measurements of (ZnO)1-x (GaN)x thin films

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D2-P-TUE-P1-1

Synthesis of Nano iron copper core shell by using K-M reactor

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In this study, Nano iron-copper core shell was synthesized by using Kinetic energy micro reactor (K-M reactor). The reaction between nano pure iron with copper sulphate pentahydrate (CuSO4.5H2O) beside NaCMC as stabilizer at K-M reactor gives many advantages in comparison with traditional chemical method for production of nano iron-Copper core shell in batch reactor. Many factors were investigated for its effect on the process performance such as initial concentrations of nano iron and copper sulphate pentahydrate solution. Different techniques were used for investigation and characterization of the produced nano iron particles such as SEM, XRD, UV-Vis, XPS, TEM and PSD. The produced Nano iron-copper core shell particle using micro mixer showed better characteristics than those produced using batch reactor in different aspects such as homogeneity of the produced particles, particle size distribution and size, as core diameter 10nm particle size were obtained. The results showed that 10 nm core diameter were obtained using Micro mixer as compared to 80 nm core diameter in one fourth the time required by using traditional batch reactor and high thickness of copper shell and good stability.

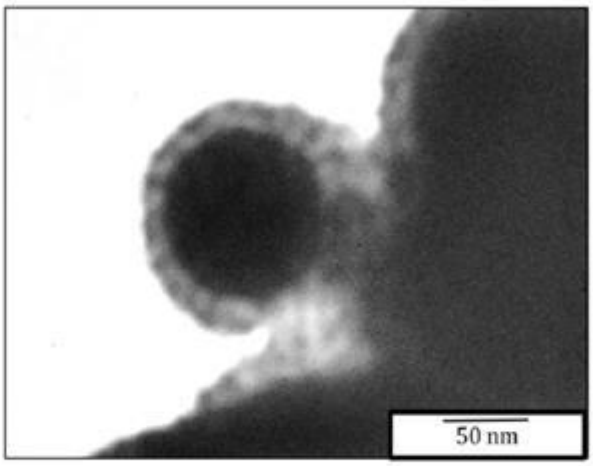

Figure 1: Figure illustrating Fe/Cu composite nanoparticles with iron as core and copper as shell. The initial concentration of CuSO4 is 10 mmol/L(B)

D2-P-TUE-P1-2

Shockley partial dislocations in gallium nitride

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Gallium nitride is a material that has attracted much interest, during the last two decades, as it is used for the fabrication of several electronic and optoelectronic devices [1]. The growth of GaN is usually achieved on structurally and thermally mismatched foreign substrates by means of heteroepitaxy. Consequently, GaN grown layers contain high densities of structural defects, particularly dislocations [2]. Depending on the magnitude of its Burgers vector, with respect to the lattice constant, a dislocation can be perfect or partial bounded by a stacking fault. Dislocations have been proven to impact the performances of the GaN based-devices. This constitutes a strong motivation behind the tremendous effort put by the III-nitrides research community in order to understand the behavior of dislocations.
In this contribution we report on Shockley partial dislocations [3] in wurtzite gallium nitride. We focused on basal Shockley partials, i.e. dislocations with lines running along the <11-20> direction.We have performed atomistic simulations, based on density functional theory (DFT), over different core configurations of the 90° and the 30° partial dislocation. Both glide and shuffle configurations, with gallium or nitrogen cores, were considered. Single period unreconstructed and double period reconstructed configurations were investigated as well [4]. The atomic core structure and the electronic properties of all considered core configurations will be presented and systematically compared. The previous DFT atomistic models were used as input for HRTEM image simulations and compared with experimental images.

Key words: Dislocations, Shockley partials, core configurations, reconstruction, GaN, DFT

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D2-P-TUE-P1-3

Nanoscale characterization of the surface structure of 1T-TaS2

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Transition metal dichalcogenides are among the most prominent candidates for deriving the after-graphene 2D materials with promising new possibilities. In this work, a bulk 1T-type Tantalum Disulfide (1T-TaS_2) sample was examined as a first step of a broader research in 2D materials' properties. Atomic Force Microscopy (AFM), Scanning Tunneling Microscopy (STM), Scanning Tunneling Spectroscopy (STS) and X-ray Photoelectron Spectroscopy (XPS) measurements were obtained in order to investigate the presence of the Charge Density Waves phases (CDW), the Spin-Orbit Coupling (SOC) effect and the Local Electron Density of States (LDOS) in the sample's surface. The surface of the bulk sample presented a step structure, known as TLK (Terrace-Ledge-Kink), consisting of steps of atomic layers, with some layers stacked on top of others. CDW structure was obtained at 105 K by means of STM. The phase present at this temperature was the Commensurate CDW phase, in agreement with the related scientific literature. The results obtained from the STS measurements allow access to the map of the LDOS and consequently to the characteristic I-V and I-dV/dI curves on each point of the sample's surface. The sample presented an overall semiconducting behavior, while metallic behavior was also detected locally. From the XPS spectrum it is concluded that the SOC effect is present in the sample. Additionally, the XPS spectrum indicates that contamination is present on the sample's surface. However, due to its physisorption on the surface it does not affect the other methods employed in this work. The data acquired here are important in the comparison between the physical properties of the bulk 1T-TaS_2 and its 2D counterpart.

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D2-P-TUE-P1-4

Investigation of the Stranski-Krastanow growth of SiGe/Si and Ge/Si by a comparison of analytical transmission electron microscopy with segregation modelling

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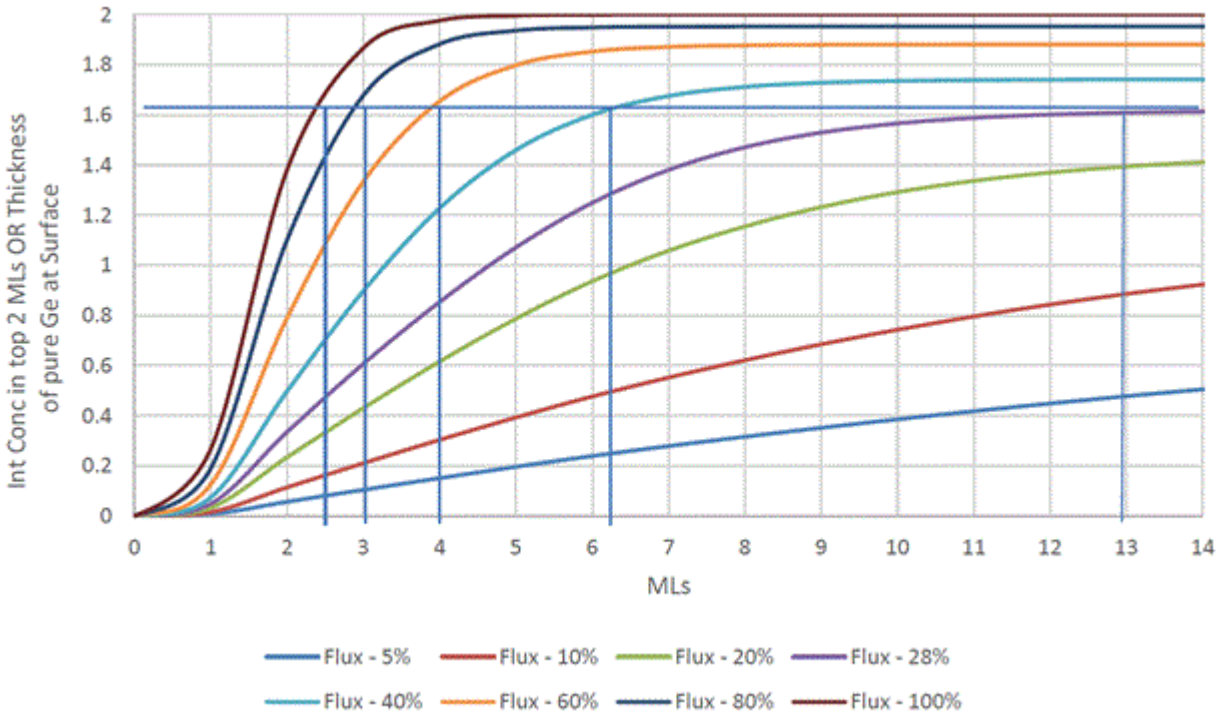
We have performed a transmission electron microscopical analysis of a range of SiGe/Si(001) and Ge/Si(001) samples that undergo the Stranski-Krastanow transition from flat layer to island growth. With the help of a quantification of the X-ray maps of those layers we have determined the total amount of deposited germanium at which islanding commences, and we show by modelling that it is the strain due to the total amount of Ge atoms deposited that drives the islanding process. At 600 °C [400 °C], 1.62 [1.75] monolayers of Ge segregated towards the surface are sufficient to trigger islanding, as shown in the simulation below for different growth fluxes at 600 °C.



D2-P-TUE-P1-5

Nanoscale characteristics of solution-grown In2O3/ZnO heterojunctions

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Nanosized solution-grown metal-oxide heterojunctions exhibit considerably higher electron mobilities than their single layer semiconductor counterparts and, therefore, can be exploited as thin film transistors in large-area optoelectronics. As the presence of the heterointerface appears to be the origin of the mobility enhancement, a rigorous comprehension of its nanostructure is critical. To this end, the structural characteristics of low-dimensional In_2O_3/ZnO heterojunctions were explored by High-Resolution Transmission Electron Microscopy (HRTEM) and quantitatively evaluated by Geometric Phase Analysis (GPA). In_2O_3 and ZnO layers were grown by ultrasonic spray pyrolysis and spin-coating, respectively, atop Si(001)/SiO_2 substrates. HRTEM imaging and fast Fourier Transform analysis identified the 6 nm thick underlayer as cubic In_2O_3, exhibiting the Ia-3 crystal symmetry, and the 8 nm thick overlayer as wurtzite ZnO. The In_2O_3 layer comprised remarkably flat and elongated crystallites with an average length of 35 ± 5 nm along the lateral direction, resembling an epitaxial-like morphology. While no predominant growth texture could be defined for In_2O_3 crystals, there is a trend among them to grow with their [001] direction nearly parallel, or occasionally perpendicular to the normal on the SiO_2 surface. Conversely, the spherical-shaped nanocrystals of ZnO were randomly oriented on In_2O_3. From GPA phase and amplitude images, the formation of distinct In_2O_3 and ZnO layers without intermixing was evidenced, and a minimum nanoscale roughness in both SiO_2/In_2O_3 and In_2O_3/ZnO interfaces was determined. Moreover, GPA and HRTEM images revealed the lack of misfit dislocations at the heterointerface. Hence, there is no periodic structural interface between the two lattices and bonding is achieved by the coalescence of ZnO nanospheres arriving at the In_2O_3 surface at random contact angles. The superior crystal quality of In_2O_3 layers and the absence of interfacial defects lead to exceptional electronic properties, as evidenced by X-ray photoelectron core level and valence band spectra.

D2-P-TUE-P1-6

Microstructural evolution in InGaN epitaxial films on AlN and GaN templates

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The microstructure of InGaN epitaxial films with high alloy contents is crucial in the effort towards highly efficient solar cells and optoelectronic devices with tunable band gaps across the optical spectrum. However, the indium distribution in the film is subject to complex phenomena such as compositional pulling, segregation and clustering, owing to the immiscibility between GaN and InN. In the present contribution, we compare the structural properties and strain content of InGaN films grown to a large thickness using plasma-assisted molecular beam epitaxy (PAMBE). The epilayers were deposited up to an indium content of ~0.4 on (0001) GaN/sapphire and AlN/sapphire templates, and their structural properties were compared regarding the influences of the substrate and growth conditions. Experimental observations were performed using transmission electron microscopy (TEM), high resolution TEM (HRTEM), and scanning TEM (STEM). Strain determination was achieved by geometrical phase analysis (GPA). Non-local film parameters were obtained by high resolution X-ray diffraction (HRXRD). We show that the films are single-phase but their composition is graded for several nanometers, with the grading being modulated by the availability of indium at the growth front. The available indium can be controlled by lowering the growth temperature or by increasing the incident indium flux. The compositional gradient defines the critical thickness for the appearance of plastic relaxation through basal stacking faults that induce the emanation of a-type threading dislocation inverse half loops. The high mismatch between InGaN and AlN, combined with no interdiffusion, promote a well-ordered heteroepitaxial interface while maintaining the two-dimensional growth mode, albeit with formation of some sphalerite-structured interfacial pockets.

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D2-P-TUE-P1-7

TEM STUDY OF THE STRUCTURAL DEFECTS FORMATION IN ELECTRON IRRADIATED CADMIUM TELLURIDE

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The purpose of work is to study the influence of electrons with energy of 400 keV on the formation of structural defects in CdTe crystals. Samples were examined and irradiated in a JEOL 4000EX-II electron microscope operated at energy of 400 keV and beam densities of between 1·1019 e/cm2s and 4·1019 e/cm2s and in JEOL JEM-2100 electron microscope operated at energy of 200 keV.

It is shown that under electron irradiation the small dislocation loops in size of 3-10 nm and a density of ~ 6·1010 cm-2, as well as voids and fine particles of a new phase in size ≤10 nm are formed.

From electron microscopic images taken with high resolution it follows that dislocation loops are primarily located on the {112} and {111} planes and have Burgers vectors such as a/2<110> and a/3<111>, respectively. The formation of new phase fine particles during electron irradiation is also possible, such as they may result from the coalescence of point defects (including impurity atoms) generated by the electron beam. These features can be identified from an analysis of moiré fringe contrast as phase of CdTe (hexagonal or trigonal).

It should be noted that the impact of electrons on CdTe less efficiently than ZnS, which is explained by the difference in the stacking fault energy of CdTe and ZnS and is consistent with previous results under irradiation of A2B6 semiconductor crystals by electrons with an energy of 100 keV.

Regularities of structural defects formation in CdTe can be used to solve problems of management type, density and spatial distribution of defects in the crystal structure, which is important for the implementation of the limiting parameters of microelectronic devices.

D2-P-TUE-P1-8

Nanoscale evaluation of interfaces in Fe/Pt bilayers for spin-pumping

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The generation of spin current via the spin-pumping effect in ferromagnetic metal/non-magnetic metal bilayers is a key topic of research in spintronics community. In such bilayer systems, the structural quality of interfaces is crucial, significantly affecting the transmission of spin currents. In this respect, the nanostructure of Fe/Pt bilayers, grown on MgO(100) substrates by e-beam evaporation, was investigated by High-Resolution Transmission Electron Microscopy (HRTEM) techniques, to unveil the impact of growth temperature on the interfacial structural properties.

For Fe(12nm)/Pt(12nm) bilayers grown at 300^{o}C, HRTEM imaging and electron diffraction analysis showed a full epitaxial growth, where the Fe lattice is in-plane rotated by 45^{o} relative to MgO and Pt, to minimize lattice mismatch. Furthermore, the MgO/Fe interface is sharp, while the Fe/Pt interface presents a 0.9 nm RMS roughness. Strain measurements by Geometric Phase Analysis (GPA) and direct HRTEM lattice spacing measurements demonstrated that the bilayer is stress-free, and the in-plane lattice strain is absorbed by misfit dislocations. No intermixing or formation of foreign phases were observed at the Fe/Pt interface.

Conversely, in Fe(12nm)/Pt(12nm) bilayers grown at 450^{o}C, the MgO/Fe interface is not planar but comprises two to five monolayers high steps, forming (100) terraces. The Fe surface is rough and includes pits with 5-15 nm diameters. These pits seem to be filled with disordered material that derives from overlapping of Fe and Pt projected lattices in front and/or behind the pits. Occasionally, the pits contain material with different symmetry that was identified as Fe_3O_4, by fast Fourier Transform analysis and HRTEM image simulations. Iron oxide may either originate from oxidation of the Fe surface, or from outdiffusion of O_2 from the MgO surface, through open-core screw dislocations, which could also explain the formation of MgO surface steps. The consequences of interfacial disorder on the magnetic properties are discussed.

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D2-P-TUE-P1-9

Determination of Bi and Al distribution in (Ga,In)As core nanowires with (Ga,Al)As and Ga(Bi,As) shells by FIB, STEM and EDX

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The incorporation of Bi in GaAs nanowires reduces the band-gap and increases the spin-orbit splitting energy, which leads to enhancement in designing optical devices such as high-efficiency lasers or semiconductor optical amplifiers operating at telecommunication wave spectrum. We have investigated Al and Bi elemental distribution and concentration in core-shell nanowires (NWs) containing Ga(As,Bi) and (Ga, Al)As shells using scanning transmission electron microcopy (STEM). The principal (Ga,In)As NW cores have been grown on GaAs(111)B substrates by Au-catalyzed vapor-liquid-solid (VLS) growth mode. Both core and shells have wurtzite crystal structure although some zinc-blend segments are also present mainly in the upper part of the core. The core-shell heterostructures with Ga(Bi,As) shells deposited on the side-walls of the (Ga,In)As core NWs have been investigated both in planar and cross-sectional geometry. The cross-section of individual nanowires was performed by Focused Ion Beam (FIB). Al and Bi elemental distribution analysis was carried out by Annular Dark Field imaging STEM images, evaluating the intensity distribution in the image. STEM image simulations using Bloch wave and multislice algorithms of structural core-shell nanowire model have been performed to confirm the experimental contrasts observed. STEM Z-contrast intensity was additionally calibrated using experimental data from EDX and EELS. Local Al segregation and Bi incorporation models is proposed in this work. We observed that Bi incorporation is more effective in zinc-blende than in wurtzite (Ga,Bi)As shell. This implies a preferential segregation of Bi excess as droplets (nanocrystals at ambient conditions) in the wurzite parts of NWs. Additionally, Al atoms segregation has been clearly observed in wurzite areas containing stacking faults.

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D2-P-TUE-P1-10

Fe-X (X=Mn, Co, Cu) nanoclusters by density functional theory calculations

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We present results from density functional theory calculations referring to the magnetic properties of 13, 55, 147 and 309 atoms Fe-X (with magnetic Co and Mn or non magnetic Cu substitutions) icosahedral nanoclusters. Aiming in finding the nanocluster with the optimum magnetic moment (mB) we explored the various sizes considering several compositions and atomic conformations for Fe with Co, Mn and Cu substitutions. Starting with the FeCu nanoclusters, it came out that configurations with agglomerated Fe atoms inside the Cu-Fe and the pure Cu surface shell are energetically favoured while the highest magnetic moment, 4.0MB (GGA), was found in the Cu12Fe case with the Fe atom located at the surface cell. The bigger Cu297Fe12 cluster shows 3.18mB for the configuration having Fe atoms surrounded by Cu that occupy the surface shell's edges. The magnetic moment is mainly due to Fe's spin up - down electronic density of states difference close to the Fermi level (EF). In particular, the spin-up Fe d electronic density of states are fully occupied yielding wavefunctions with homogeneous change distribution and Fe 4p occupation while the spin-down is almost unoccupied exhibiting dangling bonding states close to EF. The structural and magnetic properties of the Fe nanoclusters with magnetic Co or Mn substitutions were also evaluated. These results could be used for the design of environmental sustainable smart alloys with superior magnetic properties e.g. by depositing Fe or FeCu on Cu nanoclusters or including new elements that provide the possibility of keeping the Fe Spin up-down electronic occupation difference close to EF

Acknowledgments: This work was supported by the SELECTA (No. 642642) H2020-MSCA-ITN-2014 project

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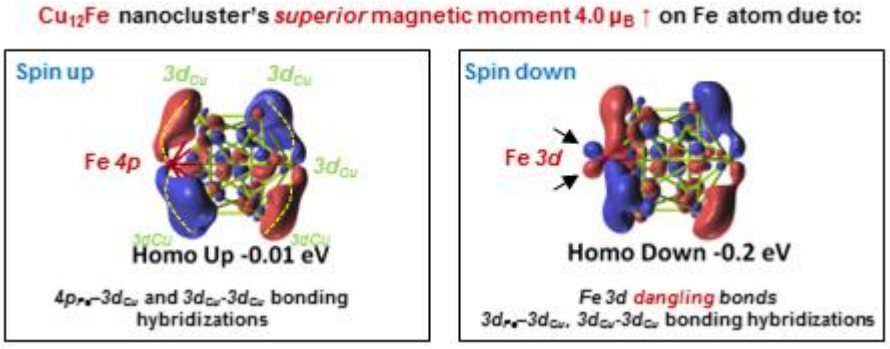

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D2-P-TUE-P1-11

Imaging AFM-Methods yielding young's modulus maps of an epoxy/boehmite nanocomposite with high spatial resolution

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Mechanical properties of epoxy can be enhanced by adding inorganic particles as filler, such as boehmite AlO(OH). The properties of the epoxy phase are usually expected to remain unchanged by the presence of inorganic nanoparticles. Only in the short range interaction, i.e. in the interphase of particle and polymer deviating properties are expected. This assumption is widely accepted, but only since measurements of the mechanical properties usually yield values from the macroscale which do not have the spatial resolution to distinguish the nanoparticle from the epoxy phase. Techniques like, e.g., nanoindentation, AFM force-distance curves (FDC) and dynamic AFM methods such as tapping mode or force modulation are able to resolve the different phases of a nanocomposite including the interphase. However, they yield only relative data such as stiffness instead of a modulus. A more recent dynamic method which is implemented in this study is the Intermodulation AFM (Im-AFM) yielding an amplitude-dependent force spectroscopy (ADFS). By exciting the AFM cantilever with two frequencies (± 5Hz of the cantilevers resonance), the resulting oscillation is comprised of a spectrum of amplitudes which equals a force spectrum. The damping of the oscillation in dependence of the amplitude is transferred to the frequency domain. In frequency domain elastic effects can be distinguished from inelastic effects leading to a calculated ADFS-curve. ADFS curves can be treated as FDC curves and therefore yield – when fitted with the appropriate model e.g. Hertz Model - absolute values for the mechanical properties. Young's modulus can be mapped with a spatial resolution of <10nm. Such maps give insight into the mechanical properties of different phases of the composite, as in this case an unexpected low young's modulus for the boehmite nanoparticles and a long range effect of the nanoparticles onto the epoxy matrix, resulting in homogeneous and inhomogeneous stiffening.

D2-P-TUE-P1-12

A comparative approach to determining the mechanical properties of ultra-thin coatings

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Utilization of protective coatings has become one of the usual ways for improvement and modification of the behavior, performance and lifetime of work pieces in various industrial areas. In the past decades, rapid advances in fabrication of hard coatings, including diamond-like carbon films and ultra thin graphene layers, led to commercially available and cost effective coatings with thicknesses down to several nanometers .

Quantitative quality control of these coated components demands thereafter reliable nanomechanical characterization of these thin and ultra-thin coatings. Nanoindentation technique [1] belongs to one of the well standardized material testing methods, which is especially suitable for relatively thin coatings. However, the nanomechanical measurement of ultra-thin coatings (coating thicknesses far less than 100 nm) using nanoindentation technique is still full of challenges. In the case of elastic modulus measurement of thin materials, the laser acoustic measurement method [2] has proven to be effective.

In this manuscript, our efforts to offering qualified nanomechanical testing of ultra-thin coatings using the nanoindentation technique and the laser acoustic method are detailed. Quantitative approaches for performing ultra-shallow nanoindentation (i.e. the maximum indentation depth is less than 10 nm) are presented, methodology for characterization of the project tip area function of a pyramid-like indenters for ultra-shallow indentation are proposed and experimentally investigated, Finite Element Analysis (FEA)-based date interpretation approach for extracting the nano-material properties from ultra-shallow indentation is testified. The relationship between the nanoindentation material testing results and those obtained by the laser acoustic method for ultra-thin DLC coatings has been experimentally investigated and discussed.

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D2-P-TUE-P1-13

The impact of strain on the elastic constants of GaN and InN

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Due to lattice mismatch, the active regions of optoelectronic devices based on III-Nitride semiconductors consist of strained heterostructured nanostructures, i.e. short period superlattices (SPS), quantum wells (QWs) and quantum dots (QDs),. The strain induced in such systems modifies their electronic band structure and alters their electronic properties. Thus, it is important to investigate the elastic properties of these materials under different strain states. The aim of the present work is to investigate the strain effect on the elastic constants and bulk modulus of wurtzite InN and GaN, using density functional theory (DFT) with modified pseudopotentials which accurately represent their band structure. The dependence of the elastic constants on the strain state is not limited up to the previously reported range of strain variable δ=0.02 [1], but is investigated in an extended range of strain up to δ=0.1 elaborating the strain state of pseudomorphic InxGa1-xN/GaN multiple quantum wells. The values of the elastic constants and the bulk modulus of GaN and InN are derived by fitting the calculated Energy Densities Ui (i = 1÷5). The sensitivity of each elastic constant is illustrated in the explored range of strain. Calculation of the elastic constants values, with a δ step equal to 0.005, reveals which elastic constant is more sensitive to strain alterations. The results of the extracted elastic constants and the bulk modulus in GaN and InN are presented, distinguishing tensile (δ positive) from compressive (δ negative) strain states. The proposed method is materials' independent and could be used for elastic properties calculations of any other heterostructure among the various III-Nitride alloys.

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D2-P-TUE-P1-14

Optimization of Specimen Preparation Method and Working Conditions for Transmission Electron Microscopy Study of Organic-Inorganic Perovskite CH3NH3PbI3

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CH3NH3PbI3 perovskites (HPVK) are showing significant results in the photovoltaic field [1]. Their optoelectronic properties depend on factors such as fabrication process or crystal structure. Crystal structure has a determinant effect in properties like the band gap [2]. However, studying the quality of it in this kind of material through (S)TEM techniques is a complex problem because of the instability under the beam.

In this communication, we have analyzed different preparation methods and work conditions for an optimal (S)TEM study. Electron transparent specimens suitable for the study were prepared by conventional milling. Fig. 1 (a) shows a High Angle Annular Dark Field Scanning TEM (HAADF-STEM) image of the sample where the layered structure can be observed. However, we have found during the analysis some amorphous areas within the active layer (see Fig. 1 (b) and (c)). This result was in discordance with what it was expected from previous analysis of the functional properties and thus it is likely that the sample preparation was causing these amorphous zones. Focused Ion Beam (FIB) is the alternative that is being studied in order to prepare the samples. The working conditions at the microscope for an optimal (S)TEM study are being analyzed. Beam voltage is one of the critical parameters that have been taken into account among others. It has been observed that it has a significant effect in the material and thus in the quality of the results obtained.

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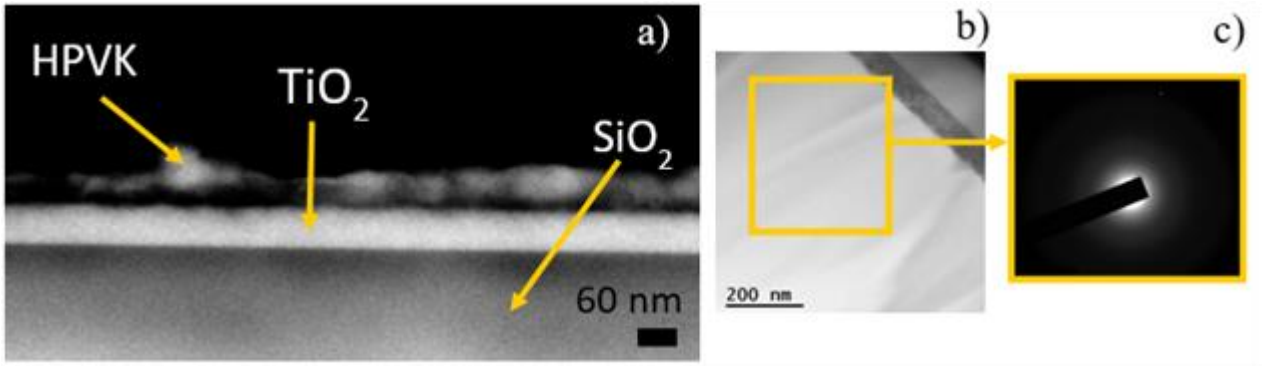
Figure 1. a) HAADF-STEM image of CH3NH3PbI3 perovskite; b) Image of the perovskite zone where diffraction studies have shown that it has an amorphous structure (c) Diffraction pattern of the marked area in Fig. 1 b).



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D2-P-TUE-P1-16

Poly-Si Films consisting of Si whiskers crystallized by Ni Metal Induce Lateral Crystallization at temperatures as low as 413oC

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Polycrystalline silicon (poly-Si) films are used in a wide range of applications, like in large-area electronics, including thin-film transistors (TFTs), solar cells and sensors. Solid phase crystallization (SPC) is the most common method to crystallize amorphous silicon (a-Si) films. However, they are hampered by the need of elevated temperatures above 600°C. The SPC temperature of a-Si can be lowered by the presence of a metal, like aluminium, nickel, gold, silver, etc. Therefore Metal Induced Crystallization (MIC) is a process in which an amorphous semiconductor undergoes a transformation to a crystalline state at low temperature under the presence of a metal. Among the metals employed for lowering the SPC process the preferred one is nickel (Ni) due to its low residual metal contamination in the poly-Si region. The morphology and the mode of growth of the uniform poly-Si films was studied after Ni Metal Induce Lateral Crystallization (Ni-MILC) of amorphous Si films at 413°C. At this temperature the Solid Phase Crystallization, which co-exists with the Ni-MILC process at higher temperature, was completely suppressed. The poly-Si film consists of whiskers which can be distinguished into two categories. Those growing fast along the <111> direction, which were already observed in conventional Ni-MILC above 500°C and a second type of whisker also growing by Ni-MILC along any crystallographic direction and having a slower growth rate. The ratio of the growth rates between then can be as high as 10 with the lower threshold at 2.5. The uniform poly-Si films after Ni-MILC at 413°C consist of a mixture of both types of whiskers. The superiority of these poly-Si films after suppression of SPC is discussed.

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D2-P-TUE-P1-17

Simulations reveal the role of composition into the atomic-level flexibility of bioactive glass cements

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Bioactive glass ionomer cements (GICs), the reaction product of a fluoro–alumino–silicate glass and polyacrylic acid, have been in effective use in dentistry for over 40 years and more recently in orthopaedics and medical implantation. Their desirable properties have affirmed GIC's place in the medical materials community, yet are limited to non-load bearing applications due to the brittle nature of the hardened composite cement, thought to arise from the glass component and the interfaces it forms. Towards helping resolve the fundamental bases of the mechanical shortcomings of GICs, we report the 1st ever computational models of a GIC-relevant component. Ab initio molecular dynamics simulations were employed to generate and characterise three fluoro–alumino silicate glasses of differing compositions with focus on resolving the atomic scale structural and dynamic contributions of aluminium, phosphorous and fluorine. Analyses of the glasses revealed rising F-content leading to the expansion of the glass network, compression of Al–F bonding, angular constraint at Al-pivots, localisation of alumino–phosphates and increased fluorine diffusion. Together, these changes to the structure, speciation and dynamics with raised fluorine content impart an overall rigidifying effect on the glass network, and suggest a predisposition to atomic-level inflexibility, which could manifest in the ionomer cements they form.

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D2-P-TUE-P1-18

Transmission electron microscopy study of Co doped ZnO nanorods

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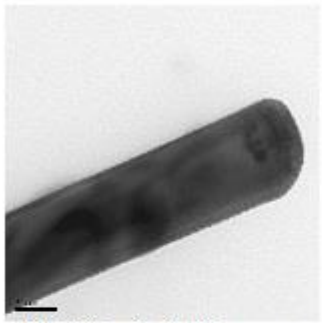
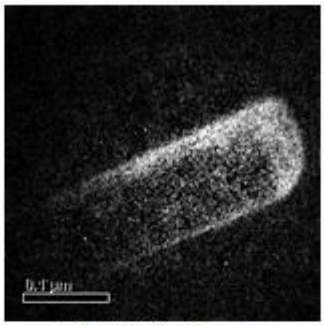
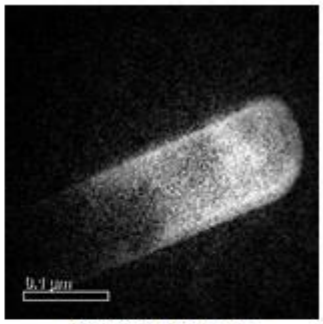
Dilute magnetic semiconductors obtained by incorporating magnetic impurities in host semiconductors have attracted wide spread attention. Among the various candidate systems ZnO doped with transition metal elements, especially Co, have shown potential for room temperature ferromagntism. Herein we report a transmission electron microscopy study of Co doped ZnO nanorods grown by a high pressure pulsed laser deposition method using 2.5 and 5 at% Co-doped ZnO targets. The ZnO nanorods are single crystalline and grow normal to the substrate, along the c-axis. The incorporation of Co results in antiphase boundaries and increases the dislocation density. Energy Filtered TEM (EFTEM) imaging shows that Co forms a Co:ZnO shell surrounding the ZnO core of the nanorods. Electron Energy Loss Specroscopy is utilized in order to investigate the valency of the Co ions in the ZnO matrix. Comparing the Co L3/L2 while line intensity ratio of the Co:ZnO nanorods with those of standard compounds it is found that the valency of Co equals 2. Moreover the analysis of the shape of the L3/L2 edges shows that Co does not form metallic clusters. The above results lead to the conclusion that Co substitutes Zn in the ZnO crystal matrix.



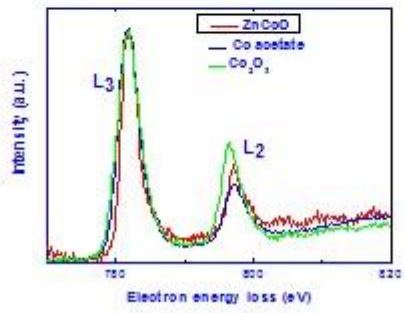
TEM bright field image of Co:ZnO nanorod



EFTEM Co map



EFTEM O map



EELS of L3/L2 Co edges

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D2-P-TUE-P1-19

APT and t-EBSD of self-faceting grain boundaries in a Ni-based alloy

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Polycrystalline metallic materials contain a high density of grain boundaries (GBs) that influence material's mechanical, kinetic properties. Solute segregation via specifically designed heat treatment is used to manipulate GB structures and compositions, enabling useful material response. The introduction of a slow cooling process to the alloy manipulates the motion of GBs in terms of solute decoration; they are partially facetted or serrated, but still planar. We refer here to as 'self-faceting GBs' or 'GB faceting engineering' via solute segregation along GBs. This GB faceting that occurs prior to the particle formation, can improve the cohesive strength of GBs in the polycrystalline materials, thereby suppressing crack propagation along GBs.
In this study, we report how solute decoration leads to a GB motion in Ni-Cr alloy during very slow cooling from high temperature. The facetted GBs in the sample subject to the diffusion heat treatment outlined here lead to a lowering of creep strain rate, as compared to faceting-free GBs in the same alloy composition subject to the conventional heating and cooling process. Using atom probe tomography (APT) and transmission electron backscatter diffraction (t-EBSD), the structural and chemical states of both faceting GBs and faceting-free GBs are characterized. Specially, the crystallographycally characterized GBs via t-EBSD are quantified by APT of the same samples at the same location. It reveals that the segregation coefficient of the solute elements segregated to the GBs changes with time when the employed heat treatment is high enough for atomic transport. To interpret the mechanism responsible for the GB faceting, the changes in strain energy, mobility, and structure will be discussed.

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D2-P-TUE-P1-20

Indentation-induced plastic deformation and fracture in (0001) and (10-10) GaN single crystals at the microscale and nanoscale

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Indentation techniques at the microscale and nanoscale were utilized to induce localized deformation on polar c-plane and nonpolar m-plane surfaces of GaN single crystals, at the load range from 10-4 N to 2 N. Two orientations of the indenter tips were used, in order to study the effect of crystal anisotropy on the elastic, plastic and cracking behavior. Cracking was more sensitively dependent on the orientation of the indenter tip, compared to hardness. The indentation induced plastic deformation and fracture sequences were studied by cathodoluminescence imaging and optical microscopy, respectively. Polar GaN was harder than nonpolar GaN, while pop-in discontinuities occurred at lower loads and were narrower at polar compared to nonpolar GaN. Dislocation arrangements were more isotropic at the polar than the nonpolar orientation, since dislocations propagate along the basal plane, in both cases. Polar GaN was more susceptible to crack initiation compared to nonpolar, when indented with a Vickers indenter, while nanoindentation did not produce cracking in all cases. Indentation at the high load regime fostered radial and lateral crack formation at both indenter orientations at polar GaN. Post-indentation lateral crack propagation was observed in situ at polar GaN. Nonpolar GaN presented anisotropic crack propagation pattern for both indenter orientations.

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D2-P-TUE-P1-21

Numerical and Experimental Elastic Strain Profiling in III-V Semiconductor Nanostructures

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Knowledge of the elastic stress/strain fields and nanoscale composition in III-V semiconductor nanostructures, such as quantum dots (QDs) and nanowires (NWs), are necessary to elucidate their response as active elements in microelectronic and optoelectronic devices. The objective of this research was to numerically simulate the induced by the lattice mismatch elastic fields of III-V nano-heterostructures, using the Finite Elements Method (FEM), and to compare them with experimental results obtained by applying Geometric Phase Analysis (GPA) on High Resolution Transmission Electron Microscopy (HRTEM) images. Particularly, the elastic stress and strain fields of (211)-oriented InAs/GaAs QD superlattices and (111)-oriented GaAs/AlxGa(1-x)As and GaAs/InxGa(1-x)As core-shell NWs grown on Si, were calculated by FEM and the results were correlated to the molar fraction of each active element. Due to the specific geometry of these nanosystems, three-dimensional (3D) finite element meshes with prismatic and hexahedral elements were constructed for core-shell NWs and QDs, respectively. FEM simulations were performed by modifying the elastic characteristics of any (hkl)-oriented system relative to the conventional <001> coordinate system, using the anisotropic elastic model in the frame of thermo-elasticity theory. The stress/strain field distributions in the nanostructures were studied as a function of variable shell chemical composition and the relative shell-to-NW diameter, in the case of core-shell NWs, while in QD superlattices the effect of a GaAs capping layer was explored. The FEM calculated elastic strain fields were in good agreement with the nanoscale strain maps obtained by GPA using the biaxial stress model. This allows the construction of reliable 3D compositional profiles of the involved nanostructures.

Acknowledgements
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D2-P-TUE-P1-22

Quantitative analysis of the stepped-strained 6H-SiC/AlN interface in HEMT structures

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Wide band gap semiconductors, such as SiC and GaN, exhibit many attractive properties, making them ideal candidates for high power and high frequency applications [1-2]. As 6-inch SiC wafers are being introduced into the market, a decrease of the substrate off-cut for SiC heteroepitaxy is desirable to reduce the manufacturing costs [3]. Therefore, multilayer (5 layers) and multicomponent structures (based on GaN and related materials) were grown on 6H-SiC (with a misorientation of 1 deg. off from the (0001) plane) substrates using the MOVPE method, for high power applications. The layers were grown epitaxially, as it was confirmed from the corresponding electron diffraction patterns. HRTEM and STEM images reveal the presence of steps in the 6H-SiC/AlN interface, with the area around them being in some cases strained.

In this study, quantitative analysis of the 6H-SiC/AlN interface is presented based on experimental HRTEM and STEM micrographs, showing and proving the steps sites, the layers' sequence and any strain relaxation situation existing. A structural model based on this analysis is proposed and simulated HRTEM images are also obtained. The corresponding atomic models proposed are found to describe well the 6H-SiC/AlN interface, with the corresponding computer simulation images coinciding with the experimental HRTEM images.

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D2-P-TUE-P1-23

Lateral force calibration in atomic force microscope using MEMS microforce sensor.

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In this paper we present a simple and direct method for the lateral force calibration constant determination in atomic force microscopes. The calibration procedure does not require any knowledge about material or geometrical parameters of an investigated cantilever. A commercially available microforce sensor with precise electronics is applied for direct measurement of the friction force exerted by the cantilever's tip to a flat surface of the microforce sensor measuring beam. Due to the third law of dynamics, the friction force of the equal value tilts the AFM cantilever. Therefore, torsional (lateral force) signal is compared with the signal from the microforce sensor and the lateral force calibration constant is determined with high accuracy (about 2%). The method is easy to perform and could be widely used for the lateral force calibration constant determination in many types of atomic force microscopes.

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Electron microscopy of bilayer Cu-Sb film

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Sb-based thin films are used for phase-change memory devices and thermoelectric materials. Cu-Sb films (10-20 nm) were prepared by subsequent evaporation in vacuum with specially made thickness gradients and studied by transmission electron microscopes JEM-2100 (200, 80 Kv) and LVEM5 (5 Kv) including the extinction bend contour method [1] with SAED and SEM.
Sb grains with main orientations around [001], (Fig. 1 a, b), and less transparent isolated microcrystalls Cu2Sb, (Fig. 1 c, d), up to 0.5 µm in size (fig.1 d) are observed in fine grained film. Both types of crystalls have a lattice with internal bending (stronger for Sb areas). Such kind of essential regular internal bending of crystal lattice planes is observed often for crystal growth in amorphous films [2] (~120 degrees per 1 µm and more).
The lattice bending was analyzed primarily using zones axis patterns (ZAPs). At the Fig.1a zone azis are indicated, which were used. The lattice bending around the axis between zones [001] and is 540 per 1 µm and between zones and is 1010 per 1 µm. A local lattice bending of the crystal Cu2Sb 800 per 1 µm. Crystal thicknesses were estimated using measurments of fine structure of extinction bend contours ~10 nm.
In the thinnest part the Sb film has an island structure with a dominant zone axis [001].

Fig.1 EM of Cu-Sb films:TEM of Sb area (a); SAED (b) with spots marked for [001] by circles, for - by squares; EM of Cu2Sb crystal with zone axis [100] (c); SEM of Cu2Sb inclusions (d).

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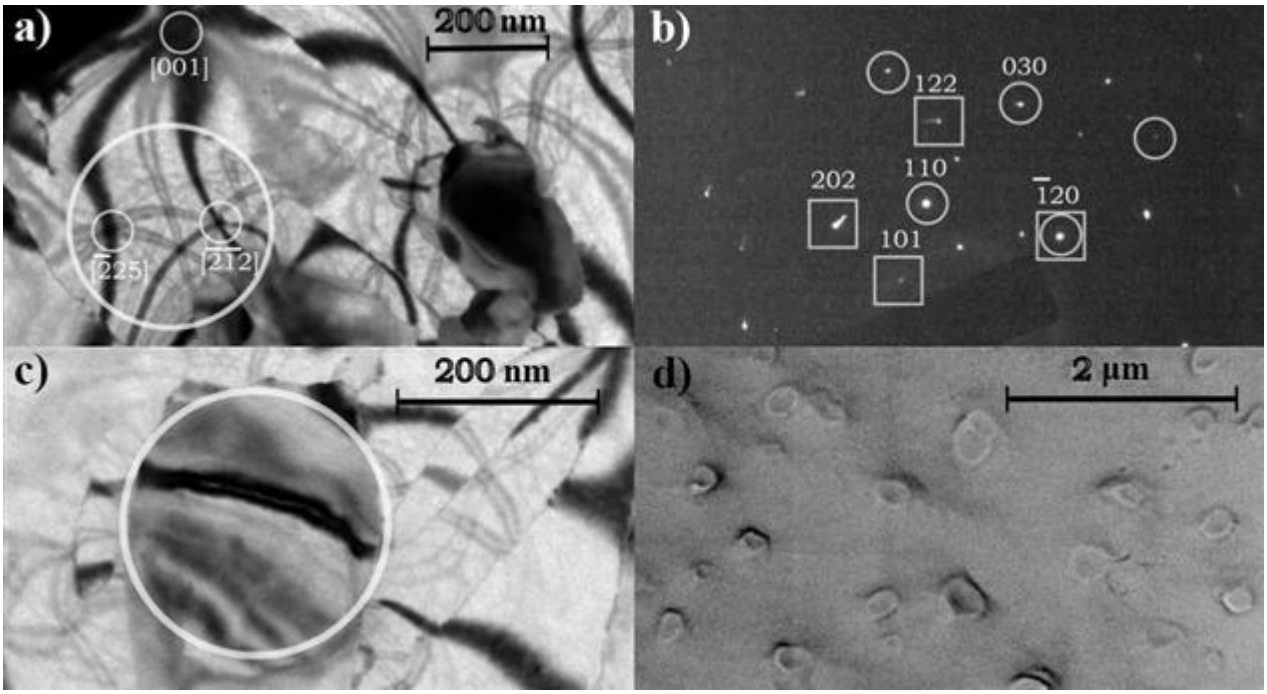

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D2-P-TUE-P1-25

Observation of a novel Al3Zr-η' core-shell particle in Al-Zn-Mg-Cu alloy

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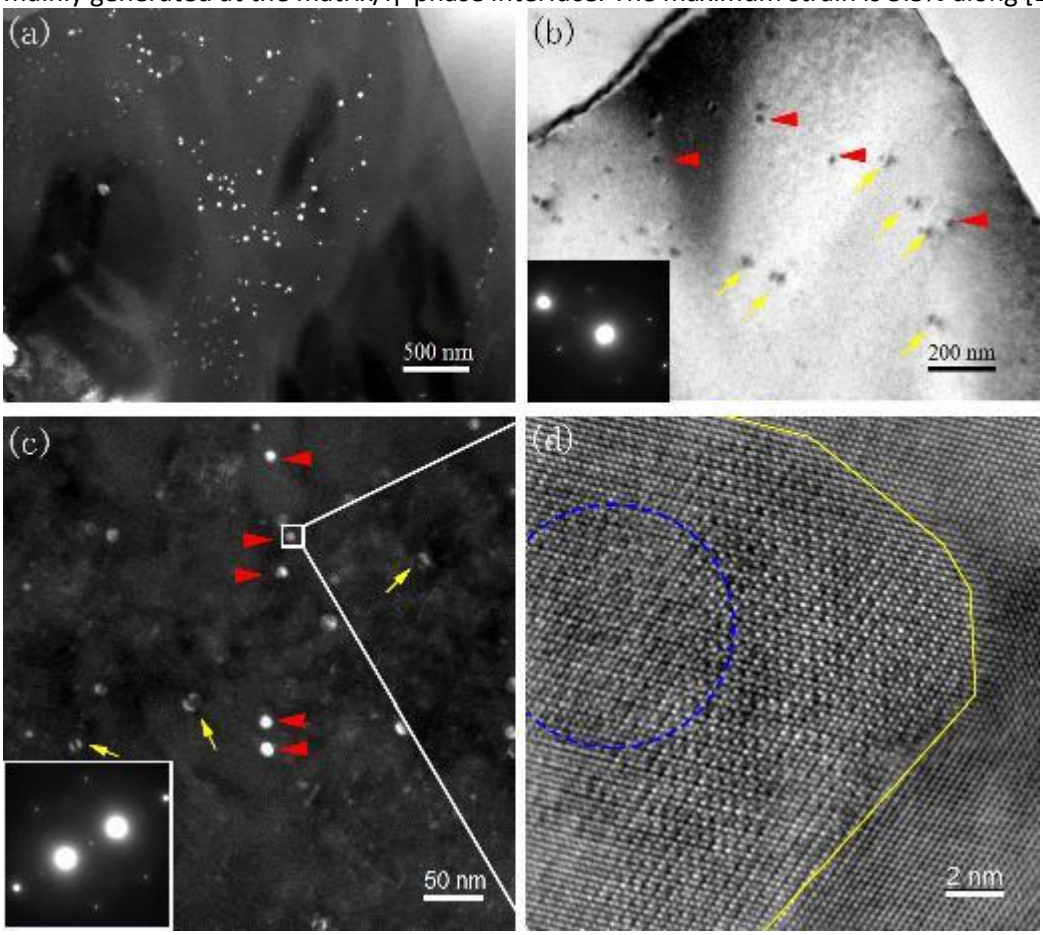
In this study, we observed an Al_3Zr-η' core-shell particle in an Al-Zn-Mg-Cu alloy by using high-resolution transmission electron microscopy (HRTEM). Combining electron diffraction simulation with geometric phase analysis (GPA), the structure of the particles and interfacial lattice distortions between the Al_3Zr-η' core-shell particle and the Al matrix were investigated. The results showed that two types of Al_3Zr particles appeared in the Al matrix: one a standalone Al_3Zr particle coherent with the matrix and the other an as-core Al_3Zr particle acting as nucleation for η' precipitates resulting in a core-shell particle which is semi-coherent with the matrix. The mean strain of the as-core Al_3Zr is -0.16%, which is lower than that of the standalone mean strain of 0.34%. The shell is composed of η' precipitates with four variants. Strains caused by the misfit dislocation are mainly generated at the matrix/η' phase interface. The maximum strain is 5.5% along [111]Al.



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Three-dimensional structure characterization of nanotubular metal oxide films

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Metal oxide nanotubes have become very attractive material with potential applications in bioengineering, nanoelectronics, catalysis, energy etc. Extensive research has been carried out especially for titanium oxide nanotubes, however other materials like zirconium oxide and aluminum oxide nanotubes seem to be also very interesting. The properties of nanostructured metal oxide films depend on morphology which results from fabrication conditions [1,2]. Electrochemical oxidation of metal substrate is excellent method for preparation structurally well-defined metal oxide nanotubes with controlled diameter and length. Nanostructured oxide films require advanced electron microscopy techniques for characterization like electron tomography.
In this work nanotubes with diameter below 100 nm were fabricated by electrochemical oxidation of metal at voltage of 15-20V in optimized electrolytes. Three different metals – titanium, aluminum and zirconium were used as the substrate. Morphology of the metal oxide films was characterized by Hitachi HD-2700 dedicated STEM (Scanning Transmission Electron Microscopy). For 3D structure analysis high angle annular dark field scanning transmission electron microscopy (HAADF-STEM) tilt series were collected. SIRT algorithm was used for reconstruction of the real structure. Specimen fabrication was performed on FIB Hitachi NB-5000 (Hitachi High Technology, Japan).
The results of STEM electron tomography clarified some morphological aspects related to nanotubes growth process, i.e. size, shape and connections of nanotubes. The differences in the structure of various metal oxide films were revealed during analysis of 3D images. STEM electron tomography is a suitable technique to visualize and characterize real structure of nanosized objects.

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X-ray Peak Broadening Analysis and Characterization of Sub-Micron Y2O3 Particles Synthesized by Ultrasonic Spray Pyrolysis Method

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The present study focuses on the production and structural characterization of sub-micron Y2O3 particles There is a growing interest on Y2O3 particles due to their excellent chemical stability, good thermal conductivity and high light output. Y2O3 particles were successfully synthesized by ultrasonic spray pyrolysis processes from yttrium nitrate solution. The effect of calcination temperature and solution molarity on morphology and structure of Y2O3 particles were characterized by Scanning electron microscope (SEM), energy dispersive spectroscopy (EDS), Fourier transform infrared spectrometer (FTIR) and X-Ray diffraction (XRD). Also using X-ray broadening, the crystalline sizes and lattice strain evaluate by the Williamson-Hall (W-H), Size-Strain plot method (SSP) and modified debby scherer method (MDS). The particle characterization studies show that Y2O3 particles have a great morphology in terms of spherical shape, narrow size distribution, sub-micron size and non-aggregation characteristics.

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In-situ environmental Transmission Electron Microscopy characterization of catalyst materials

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Dynamic, atomic-scale visualization of structural evolutions in-situ under reactive (gas) environments directly addresses the environment-dependent structure and dynamics of the material properties. This is a crucial R&D step; because in general there is no evidence that the dynamic state of materials can be truly derived from post-mortem (high-vacuum) examinations, where the intermediate steps usually are unknown. The discovery of new cost-effective and highly active catalysts for electrochemical energy conversion and storage is of prime importance to address climate change challenges and develop storage options for renewable energy production. We have therefore used Environmental Transmission Electron Microscopy (ETEM) to study the changes in the material properties on the nano-scale during oxidation and reduction for two catalytic material systems.

Oxygen storage materials (OSMs) are capable of changing oxygen stoichiometry with a variation of temperature or oxygen partial pressure, and have great potential in applications such as heterogeneous catalysts and three-way catalysts [1]. Ca2MnAlO5 (CAM) is a recently developed oxide with oxygen storage capability over 1.3 times that of the best-known OSM, and fast oxygen transport properties. The second material system investigated with ETEM is the hydrotalcite like material system Cu/ZnO/Al2O3. These materials are used in methanol production industry. Methanol has the potential for being used as a chemical carrier of hydrogen for application in fuel cells [2]. The Cu/ZnO/Al2O3 catalyst can achieve higher activity by increasing the Cu dispersion by a coprecipitation method. Although this catalyst have been produced commercially for years, there are a number of unknown factors associated with the oxidation and reduction process at the nano-scale.

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Structural characterization and nanoscale bandgap measurements of (ZnO)1-x (GaN)x thin films

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Bandgap engineering plays an important role in designing novel functional semiconductor materials, offering tunable optical and electronic properties. In recent years, ZnO and GaN, two wide-bandgap semiconductors with similar bandgaps and wurtzite structure, have been at the focus of scientific research due to their versatile applications. Interestingly, recent studies revealed that alloying the two with each other leads to a reduced bandgap due to a strong band bowing effect. In our present work, we studied RF magnetron sputtered (ZnO)1-X(GaN)X thin films deposited on sapphire substrates. Tailoring material properties by controlling nanometer scale structure and composition is of increasing importance. In this respect, film properties were compared to reveal the influence of (a) GaN content (x = 0.15 and 0.2), (b) film thickness, and (c) post-deposition thermal annealing. Structural characterization was performed, applying TEM/STEM methods starting from the mesoscale and down to the atomic scale. The overall morphology of the films revealed a columnar growth that was affected by changes in GaN content, resulting from an almost polycrystalline structure in highly (0001)-oriented columnar grains by increasing GaN content. Due to the immiscibility of alloy constituents, chemically induced phenomena, such as phase separation leading to complex defect microstructures sensitive to the growth conditions are investigated. To this end, (scanning) transmission electron microscopy [(S)TEM] methods were used along with Quantitative HRTEM using geometrical phase analysis (GPA), and energy dispersive x-ray spectroscopy (EDX). Bandgap measurements were acquired by performing electron energy loss spectroscopy (EELS) providing an excellent tool for investigations of local band gap gradients on the scale of a few nanometers. Results were compared to X-ray diffraction and transmission measurements.