10th International Workshop on Nanoscale Pattern Formation at Surfaces

University of Surrey, Guildford, UK
7-10 July 2019

The committees gratefully acknowledge
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RADIATE

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Ion Beam Centre

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Delegates are asked not to leave their baggage unattended and to wear identification badges at all times. The University accepts no liability for loss or damage to property or vehicles and their contents, nor for injury to visitors to the campus except where required by law.

WORKSHOP DESK

The workshop desk is based in the foyer area outside Lecture Theatre M and will be open daily from 0900 on Monday to 1400 hours on Wednesday.

IN AN EMERGENCY OR IF MEDICAL ASSISTANCE IS REQUIRED

If the building alarms sound during the day members of the Surrey team will be available to escort you to a place of safety. If you feel unwell or require medical assistance during the day please make your way either to the workshop desk or approach a member of the Surrey team.

If you need medical assistance when the workshop has closed for the day please make contact with personnel in the Security office who are all first aid trained. In an emergency situation and ONLY in an emergency situation, i.e. the fire service, an ambulance or the police need to be called to the campus, should the Security Office be contacted on the University's dedicated emergency telephone number which is +44 1483 683333 from an external telephone or by dialling 3333 from any internal telephone.

SOCIAL EVENTS

Registration and Welcome Reception
Registration will commence at 1600 hours and a welcome reception will be held from 1800 hours onwards both on Sunday 7 July in Wates House.

Tour of Guildford - Guildford Story
On the tour you will discover the origins of the town and how the town developed to become what it is today. Guildford Castle, the Guildhall and Abbots Hospital all play an important part in this story. The tour will commence at 1815 hours on the Monday. Delegates will be escorted to the venue by members of the Surrey team.

Workshop Dinner
The dinner has been arranged for the evening of 9 July at The Refectory, Guildford Cathedral. Pre-dinner drinks will be served from 1830 hours with the meal to follow at 1930 hours. The Refectory can be accessed via the steps underneath and behind Wates House.

MEALS AND REFRESHMENTS

Breakfasts for delegates staying on-site will be served in Hillside Restaurant. Tea, coffee and lunches will be available in Lecture Theatre H during the day at the times stated in the programme.

PRESENTATIONS

Presentations are to be uploaded prior to the relevant session commencing. Members of the Surrey team will be on hand to assist with this. If any further specialised equipment is required, please make your needs known to the workshop desk at your earliest convenience.

POSTER SESSION

The poster session will be held on Monday afternoon at 1610 hours. Posters are to be mounted on Monday and removed on Wednesday at the close of the workshop. Velcro dots will be provided for poster mounting - you must not use pins on the boards. The posters boards will be numbered as listed in this booklet - please ensure that you place your poster on the appropriately numbered board.

PROGRAMME

Sunday 7 July 2019

16:00 Registration Opens
Wates House

18:00 Continuation of Registration
and Welcome Reception
Wates House

Monday 8 July 2019

09:00 Welcome
J G England, Workshop Chair, University of Surrey

Session 1 Ion Beam Processes
Chair: J G England

09:25 I01 Self-Organized Silicide Nanodot Patterns by Medium-Energy Ion Beam Sputtering
A Redondo-Cubero, K Lorenz, F J Palomares, B Galiana, D Bahena and L Vázquez

10:05 O01 Ion Beam Nanostructuring of Co_xSi_{1-x} Surfaces: Role of Stoichiometry and Sample Swinging
B K Parida and S Sarkar

10:30 O02 Nano Patterning on the Rocked Surface by the Ion Beam Sputtering
S Jo, E Lee, J Jun, S M Yoon, J Seo and J-S Kim

10:55 Coffee

Session 1 (continued) Ion Beam Processes
Chair: M Bradley

11:30 I02 Interaction of Highly Charged Ions with 2D Materials - Towards a Complete Picture of Nanostructure Formation
R A Wilhelm, S Creutzburg, J Schwestka, A Niggas, L Madauß, H Inani, M Tripathi, C Mangler, R Heller, S Facsko, J Kotakoski, P L Grande, M Schleberger and F Aumayr

12:10 O03 Effect of Surface Orientation and Surface Features on the Sputtering Yield of Tungsten Surfaces
F Granberg, J Jussila, A Lopez-Cazalilla and K Nordlund

12:35 O04 Ion Beam Modification of Metal Oxide Based Nanostructured Surface for Frontier Applications
S Chatterjee, P Das and M K Rajbhar

13:00 Lunch and Posters

Session 2 Biological Applications
Chair: C Teichert

14:00 I03 Dynamics of DNA Origami Lattice Formation at Solid-Liquid Interfaces Studied by High-Speed Atomic Force Microscopy
A Keller

14:40 O05 Protein Adsorption on Nanopatterned Surfaces
Y Yang, M Yu, Q Qin, G Grundmeier and A Keller

15:05 O06 Ripple Formation on Ti-Based Surfaces at MeV Energy Heavy-Ion Implantations
M A Garcia, J Rickards, R Cuerno, R Trejo-Luna, J Cañetas-Ortega, L R De la Vega and L Rodríguez-Fernández

15:30 O07 Superhydrophobic PTFE Surface Achieved by Low Energy Ar^+ Ion Beam Irradiation
V Pachchigar, M Ranjan and S Mukherjee

15:55 Poster Introductions

16:10 Poster Session

18:00 Guided Tour of Guildford

Tuesday 9 July 2019

Session 3 **Non-Ion Beam Patterning**
Chair: K Nordlund

09:00 I04 Self-Organised Surface Nanopatterning Upon Implact of Ultra-Short Laser Pulses
J Reif

09:40 O08 Light-Assisted Charge Spreading in Self-Assembled Arrays of Organic Semiconductor Nanoneedles on 2D Materials
C Teichert, A Matković, M Kratzer, J Genser, B Kollmann, D Lüftner, P Puschnig, Z Chen, O Siri and C Becker

10:05 O09 Nanopatterning of $SrTiO_3$(100) Surface with Crystalline Titanium Oxide (TiO) Nanowires in the Process of Thermal Reduction
F Krok, D Wrana, C Rodenbücher, B R Jany, K Cieslik, O Kryshtal, G Cempura, A Kruk and K Szot

10:30 O10 2D Diffraction Patterns of Single-Crystal Si Wafers Isotropically Irradiated with Monochromatic X-Rays
M Tosaki, F Ishizuka and Y Isozumi

10:55 Coffee

Session 4 **Electronic Applications**
Chair: F Buatier de Mongeot

11:30 O11 Ultra-Low Threshold Cold Cathode Electron Emission From Au Nanoparticles Decorated Ion-Beam Patterned Nanofaceted-Si Substrates
M Saini, R Singh, K P Sooraj, M Ranjan, S K Srivastava and T Som

11:55 O12 Morphology Modification of Si Nanopillars Under Ion Irradiation at Elevated Temperatures
X Xu, K-H Heinig, W Möller, H-J Engelmann, N Klingner, A Gharbi, R Tiron, S Facsko, G Hlawacek and J von Borany

12:20 O13 Anisotropic Nanoscale Resistive Switching Behaviour of Au-Ion Implanted Ripple-Like TiO_x ($x < 2$) Films
D Hasina, M Saini, A Dutta and T Som

12:45 Lunch and Posters

Session 5 **Theory**
Chair: R Cuerno

14:00 O14 Triangular Patches of Ripples, Terraces and Elongated Pyramids Produced by Ion Sputtering
R M Bradley

14:25 O15 Non-Linear Theory of Ion-Induced Solid Flow
J Muñoz-García, R Cuerno and M Castro

14:45 O16 Surface Coverage of Ion Irradiated Solid Films
L Repetto, R Lo Savio, G Firpo, E Angeli, P Guida, D Pezzuoli, D Repetto and U Valbusa

15:10 O17 Direct Observation of Ion-Induced Self-Organization and Ripple Propagation Processes in Atomistic Simulations
F Djurabekova, A Lopez-Cazalilla, A Ilinov, C Fridlund and K Nordlund

15:35 Coffee

Session 6 Quantum Applications
Chair: S Facsko

16:00 O18 A New FIB for Deterministic Single Ion Implantation
N Cassidy, R P Webb, R Curry, P Blenkinsopp, I Brown, B Murdin, M Gallucci Masteghin and D Cox

16:25 O19 Exotic LM(A)IS Sources for Ion Implantation: How FIB Milling Patterning Can Promote New Qubit Proposals
M Gallucci Masteghin, N Cassidy, R P Webb and D Cox

16:50 O20 Investigating the Formation of Isotopically Pure Patterned Areas for Quantum Computers Using Ion Implantation and Layer Exchange
J G England, D Cox, N Cassidy, B Mirkhaydarov and A Perez-Fadon

18:30 Pre-Dinner Drinks and Workshop Dinner at Guildford Cathedral Refectory

Wednesday 10 July 2019

Session 7 **Optical Applications**
Chair: F Krok

09:00 I05 Faceted Nanoscale Wrinkles on Amorphous Templates for Optoelectronics, Biosensing and Nanomechanics
M C Giordano and F Buatier de Mongeot

09:40 O21 Light Trapping in Nanopatterned 2D Materials and Thin Film Optoelectronic Devices
F Buatier de Mongeot, C Mennucci, D Chowdury, M Bhatnagar, G Manzato and M C Giordano

10:05 O22 Low Energy Ions for Fabricating Ordered Plasmonic Structures for Second Harmonic Generation and Sensing Applications
M Ranjan and K P Sooraj

10:30 O23 Preparation of a New Kind of Two-Dimensional Metal/Dielectric Nanocomposite Surface-Relief Grating Couplers and Their Vertical Input Coupling Properties
G Wang, J Wang and C Liu

10:55 Coffee

Session 8 **Semiconductors**
Chair: T Som

11:30 O24 Ion-Induced Surface Nanostructures of Germanium(001)
R de Schultz, D Erb and S Facsko

11:55 O25 Controlled Nanoporosity Induced by Ion Irradiation of Ge Thin Films
S Mondal, M Secchi, D Giubertoni, M Crivellari, A Picciotto and G Pepponi

12:20 O26 Comparison of Si and Ge Surface Patterns Produced by Ion Irradiation in the Reverse Epitaxy Regime
S Facsko, X Ou, R de Schultz and D Erb

12:45 Closing Comments

13:00 Lunch

14:00 Tour of the University of Surrey Ion Beam Centre

POSTERS

P01 Morphology, Density, and Temporal Evolution of Topological Defects in Reverse Epitaxy
D Erb, G Malsch and S Facsko

P02 Production of Homogeneous Plasmonic Gallium Nanoparticles Using Hexagonal Pit Templates
S Catalán-Gómez, C Bran, M Vázquez, J L Pau and A Redondo-Cubero

P03 Realization of Wafer-Scale Gratings with Sub-59 nm Period Through Vacancy Epitaxy
S Facsko, X Ou, Q Jia, J Feng, H Huang, X Yang, J Grenzer, K Huang, S Zhang, J Lin, H Zhou, T You, W Yu, P Jonnard, M Wu, A Giglia, Z Zhang, Z Liu, Z Wang and X Wang

P04 Texturization of Polycrystalline Ti-Based Surfaces by Low-Energy Ion-Beam Irradiation: Implications in Biomedical Implants
M A García, R Gago, M Arroyo-Hernández, E Herrero, M T Iglesia, D Esteban-Mendoza, J Rickards and Rodolfo Cuerno

P05 Adsorption of Fullerene on Surface and Edges of Graphene
F F Umarov, V G Stelmakh and I J Yadgarov

P06 Carbon Atom Hydrogenation Influence on Graphene Deposition
F F Umarov, V G Stelmakh and I D Yadgarov

SESSION 1

ION BEAM PROCESSES

Chairs: J G England
M Bradley

I01 SELF-ORGANIZED SILICIDE NANODOT PATTERNS BY MEDIUM-ENERGY ION BEAM SPUTTERING

A Redondo-Cubero[1], K Lorenz[2], F J Palomares[3], B Galiana[4], D Bahena[5] and L Vázquez[3]

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[2]IPFN and INESC-MN, Instituto Superior Técnico, Universidade de Lisboa, 2695-066 Bobadela LRS, Portugal
[3]Instituto de Ciencia de Materiales de Madrid, CSIC, 28049 Madrid, Spain
[4]Departamento de Física, Universidad Carlos III de Madrid, Avenida de la Universidad 30, 28911 Leganés, Spain
[5]Laboratorio Avanzado de Nanoscopia Electrónica (LANE), CINVESTAV, Av IPN 2508, 07360 DF México, México

Self-organization mechanisms play an important role in the development of current low-dimensional structures. Ion beam erosion is a well-studied process leading to dot patterns at the nanoscale. In the case of silicon substrates, these dot patterns develop at normal incidence with the incorporation of metal impurities, which lead to the formation of silicides [1]. However, the exact control of those patterns in terms of the physical parameters is not fully understood.

Here we report on the production of silicide nanodot patterns by medium-energy ion beam sputtering (IBS) of silicon targets with simultaneous and isotropic metal supply. The advantage of using medium-energy ions lies on the enhancement of the physical magnitudes of the nanodots, regarding both the structure and the surface metal content, when compared to those obtained at low energies [1,2]. This fact enables a better assessment of the structural and compositional properties of the patterns and their dependence with the different irradiation conditions. In order to further understand the metal-assisted IBS surface patterning, we have performed the irradiations under different conditions, by changing the ion species (Xe/Ar), the metal (Mo/Fe) and target temperature.

The obtained patterns have been intensely characterized by transmission and scanning electron microscopies as well as by atomic and magnetic (for the Fe case) force microscopies, and X-ray photoelectron spectroscopy. From these analyses, it can be confirmed that the dots are silicide-rich structures, although the flat areas between them also contain silicides but in a lesser extent. The pattern ordering was analysed using the Voronoi tessellation [3]. It was found that ordering depends on the target temperature, ion species as well as in the local metal content. In particular, its change with the temperature depends also on the metal species. Likewise, the silicide distribution within the dot structure changed with the target temperature. Although some morphological features are similar to those found for low-energy IBS, in the latter case their eventual correlations are difficult to assess because of the reduced dimensions and metal content. Thus, metal-assisted medium-energy IBS dot patterning could be a useful technique to advance the understanding of this interesting nanofabrication method.

[1] Gago R, Redondo-Cubero A, Palomares FJ, Vázquez L, Nanotechnology, 25 (2014) 415301.
[2] Redondo-Cubero A, Galiana B, Lorenz K, Palomares FJ, Bahena D, Ballesteros C, Hernandez-Calderón I, Vázquez L, Nanotechnology, 27 (2016) 444001.
[3] Redondo-Cubero A, Lorenz K, Palomares FJ, Muñoz A, Castro M, Muñoz-García J, Cuerno R, Vázquez L, Journal of Physics: Condensed Matter, 30 (2018) 274001.

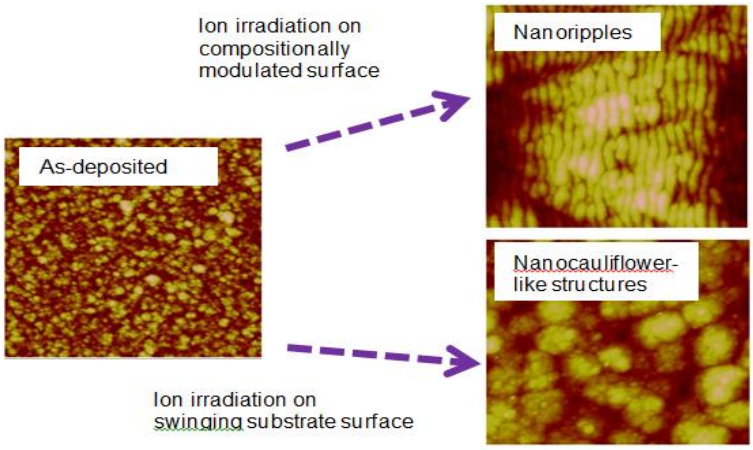
O01 ION BEAM NANOSTRUCTURING OF Co_xSi_{1-x} SURFACES: ROLE OF STOICHIOMETRY AND SAMPLE SWINGING

Basanta Kumar Parida and Subhendu Sarkar

Department of Physics, Indian Institute of Technology Ropar, Rupnagar, Punjab 140001, India

Ion beam sputtering (IBS) has the advantage of creating self-organized nanostructured surfaces in a single step without using any template. Ion irradiation on mono-elemental surfaces result in formation of periodic structures like nanoripples, dots etc. The scenario is however different in case of binary/ternary alloys or compounds due to the difference in sputtering yields and individual diffusivities of the elemental species. Theoretically, the above two instabilities lead to spontaneous modulations in topography and composition which is in- or out-of-phase with the ripple topography [1].

In the present study, we have prepared homogeneous Co_xSi_{1-x} samples having varied stoichiometries by confocal magnetron sputtering [2,3]. These surfaces were irradiated with Ar^+ ions (700 eV) for a fixed ion fluence of 7.5×10^{18} ions/cm^2 and an angle of incidence 67°. We find that there exists a morphological instability on these binary surfaces which triggers the transition of surface structure from nanoripples to ellipsoidal ones. Nanoripples are found to form within a specific stoichiometric range and not for the entire compositional domain.



Further, we have also studied the effect of substrate swinging in the azimuthal direction with respect to the ion beam. $Co_{69}Si_{31}$ binary surfaces are irradiated with 500 eV Ar^+ ions at an oblique incidence of 67°. Stochastic nanoscale dots and nanoscale cauliflower-like structures are observed for different angles of swinging. The surface roughness shows a linear increment with the total swinging angle within the angular range studied. Decrease in aspect ratio of these nanostructures have been observed from as-grown surface to ion beam eroded surfaces. Formation of the cauliflower like structures may be due to the lateral mass transport and bi-periodic momentum transfer from ions to the elemental species. Anisotropicity reduces the pattern symmetries over these substrates.

[1] Shenoy V, Chan W, Chason E, Physical Review Letters, 98 (2007) 256101.
[2] Parida BK, Ranjan M, Sarkar S, Current Applied Physics, 18 (2018) 993.
[3] Parida BK, Ranjan M, Sarkar S, Physica B, 545 (2018) 34.

O02 NANO PATTERNING ON THE ROCKED SURFACE BY THE ION BEAM SPUTTERING

Sujin Jo[1], E Lee[1], Jihee Jun[1], S M Yoon[2], J Seo[3] and J-S Kim[1,3]

[1]Department of Physics, Sook-Myung Women's University, Seoul 04310, Korea
[2]Materials and Life Science Research Division, Korea Institute of Science and Technology, Seoul 02792, Korea
[3]Institute of Advanced Materials and Systems, Sook-Myung Women's University, Seoul 04310, Korea

Nanopatterns formed by broad ion beam sputtering (IBS) include high density of structural defects, a common trait of the self-assembled patterns, and their application is seriously limited. Recent theoretical work [1] proposes a remedy that rocking a substrate during IBS in a prescribed way can produce defect-free pattern. We examine that proposal with Si and amorphous carbon (a-C) substrates. Indeed, rocking of the substrates can markedly improve the order of the ripple patterns, irrespective of the substrate and the incident ion energy. The improvement of the order is observed in one case under the prescribed condition, but in other cases outside the suggested rocking angles. Our numerical study under the more general condition or the extended KS equation indicates that the optimal rocking condition is more widely observed in the parameter space for the rocking, possibly answering the experimental observation. If time allows, we will also discuss how the characteristics of the pattern is determined under given rocking condition.

[1] Harrison et al, Physical Review E, 93 (2016) 040802(R).

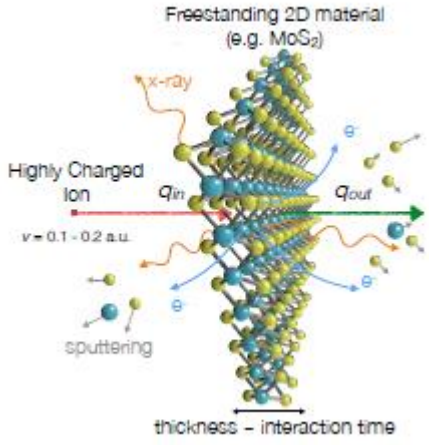
I02 INTERACTION OF HIGHLY CHARGED IONS WITH 2D MATERIALS - TOWARDS A COMPLETE PICTURE OF NANOSTRUCTURE FORMATION

R A Wilhelm[1,2], S Creutzburg[2], J Schwestka[1], A Niggas[1], L Madauβ[3], H Inani[4], M Tripathi[4], C Mangler[4], R Heller[2], S Facsko[2], J Kotakoski[4], P L Grande[5], M Schleberger[3] and F Aumayr[1]

[1]TU Wien, Institute of Applied Physics, Vienna, EU
[2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, EU
[3]University Duisburg-Essen, Faculty of Physics and CENIDE, Duisburg, EU
[4]University Vienna, Faculty of Physics, Vienna, EU
[5]Federal University of Rio Grande do Sul, Institute of Physics, Ion Implantation Laboratory, Porto Alegre, Brazil

Slow highly charged ions (HCI) provide an efficient toolkit for surface modifications at the nanoscale [1]. Due to the potential energy of HCIs, nanoscale surface melting or atom sputtering can be observed in susceptible materials with an efficiency of about 100% (one surface feature per ion). The neutralization of the HCIs driving the potential energy deposition is typically considered to be finished in 'a shallow region' in the surface, i.e. 'on the first nanometers'. To further quantify the HCI neutralization dynamics we recently took a new approach and used freestanding 2D materials as the target.

Due to the atomic thickness of the materials, ions are not stopped in the materials and are available for spectroscopic analysis. At the same time the 2D materials are available for post-irradiation microscopic analysis, which finally allows us to determine (1) the kinetic and potential energy lost by the ion, (2) the energy dissipated by emission of secondary particles (electrons and photons), and (3) the energy spend in the nanostructure formation process.



Sketch of HCI transmission through a single layer of MoS_2. Measurement of the emitted secondary particles and the transmitted primary ion allows reconstruction of the interaction process.

By applying our ion beam spectroscopy, we performed charge state and kinetic energy analysis of ions transmitted through freestanding single layer graphene (SLG) [2], amorphous 1 nm thick Carbon Nanomembranes (CNM) [3], freestanding single layer MoS_2, SLG/MoS_2 heterostructures and others. As a first result we found an ultrafast (sub-10 fs ~ 1 monolayer) neutralization taking place, much

faster than established models would have anticipated [4]. Furthermore, kinetic energy loss is significantly enhanced compared to the value of singly charged ions under the same conditions.

To facilitate a comprehensive understanding of the plethora of observed phenomena and their interplay, we use an energy, angle, and charge state resolved spectroscopy in coincidence with yield and energy resolved measurement of emitted secondary particles [5]. We further developed an atomistic model for ion stopping, charge exchange and electronic decay taking the time-dependent ion charge state explicitly into account [6].

In this contribution I will give an overview about our recent progress in the field of ion scattering from 2D materials and put the results in perspective to nanostructure formation.

[1] Kozubek R et al, Journal of Physics Chemistry Letters, 10 (2019) 904.
[2] Gruber E, Wilhelm RA et al, Nature Communications, 12 (2016) 126101.
[3] Wilhelm RA et al, Physical Review Letters, 112 (2014) 153201.
[4] Wilhelm RA et al, Physical Review Letters, 119 (2017) 103401.
[5] Schwestka J et al, Review of Scientific Instruments, 89 (2018) 085101.
[6] Wilhelm RA, Grande PL, Communications Physics (2019) under review.

O03 EFFECT OF SURFACE ORIENTATION AND SURFACE FEATURES ON THE SPUTTERING YIELD OF TUNGSTEN SURFACES

Fredric Granberg, Joonas Jussila, Alvaro Lopez-Cazalilla and Kai Nordlund

Department of Physics, University of Helsinki, Helsinki, 00014, Finland

Tungsten is the chosen material for several plasma facing components in fusion reactors, due to its good properties. The harsh environment will affect the surface material, for instance as surface sputtering. The charged particles will hit the surface at place dependent incoming angles and neutrals can hit the surface at random incoming angles. To understand how the surface will react to irradiation, a thorough investigation is needed. Previous studies have been conducted to understand the sputtering, however, they focused mainly on the sputtering of low index surfaces and at mainly perpendicular incoming ion angles.

In this study, we focus on two different sputtering effects. Firstly, the effect of random surface orientation on the sputtering yield was studied. Secondly, the sputtering yield of surface features, to represent tungsten fuzz, was investigated.

The results on sputtering yield of random surfaces are compared to common low index surfaces. To study the effect of ion mass, we study helium for its relevancy to fusion and argon for its higher weight. To get a clearer insight, we study four different energies and eleven different incoming angles. We found that the average sputtering yield for random surfaces are not the same as for any of the low index surfaces nor their average [1]. In addition, the incoming angle will drastically affect the sputtering yields. It was found that channelling will reduce sputtering at certain surface orientation dependent angles. The random surfaces revealed that some surface features can greatly increase the sputtering yield. In addition to the sputtering yield, the corresponding reflective yield was calculated for all different variations. To compare the obtained results to experiments, also the angular distribution of the sputtered W atoms was obtained for all different parameters.

As the random surface investigation revealed, some surface features can drastically change the sputtering yield. To more thoroughly investigate this, we performed simulation of tungsten pillars on top of a tungsten surface. Different heights of the pillars were investigated to study a model system of tungsten fuzz. A detailed study of preferential sputtering was done, to understand the mechanisms involved. We found that the height of the pillar is affecting the total sputtering yield of the system.

[1] Jussila J, Granberg F, Nordlund K, Nuclear Materials and Energy, 17 (2018) 113-122.

O04 ION BEAM MODIFICATION OF METAL OXIDE BASED NANOSTRUCTURED SURFACE FOR FRONTIER APPLICATIONS

Shyamal Chatterjee, Pritam Das and Manoj K Rajbhar

School of Basic Sciences, IIT Bhubaneswar, Jatni, Khordha 752050, India

One-dimensional (1D) materials are highly demanding in the field of nanoscience and nanotechnology for large aspect ratios, high surface-to-volume ratios and possess larger number of reactive surface atoms. Fabrication of nanostructured based devices require nanoscale modification, joining and sometimes control its wetting behaviour for various applications [1-4]. We present here significant surface modifications of copper oxide and strontium manganate nanowires by low energy ion beam [1,5]. With increasing ion fluence we find formation of periodic pattern of nanostructures on copper oxide nanowires. High resolution microscopy X-ray diffraction and Raman scattering measurements reveal formation of crystalline nanoprotrusions of Cu_8O phase [1,5]. With increasing ion energy the nanowires are welded to form wide scale network. The modified nanowire network shows higher electrical conductivity and strong water repelling characteristics. The observed modifications are explained by state-of-the-art TRI3DYN simulations. On contrary, strontium manganate surface remains smooth even at higher ion fluence. However, it shows progressive welding starting at low ion fluence. With increasing ion fluence the surface also become hydrophobic from an initial hydrophilic surface. The underlying physics of aforementioned modification is explained by density functional theory based calculations [1,5].

[1] Rajbhar MK, Das P, Satpati B, Möller W, Facsko S, Böttger R, Ramgir N, Chatterjee S, Applied Surface Science, 478 (2019) 651.
[2] Dhal S, Das P, Rajbhar MK, Möller W, Chatterjee S, Ramgir N, Chatterjee S, Journal of Materials Chemistry C, 6 (2018) 1951.
[3] Dhal S, Chatterjee S, Facsko S, Möller W, Böttger R, Satpati B, Ratha S, Hübner R, Crystal Growth and Design, 17(5) (2017) 2660.
[4] Das P, Dhal S, Ghosh S, Chatterjee S, Rout CS, Ramgir N, Chatterjee S, Nuclear Instruments and Methods in Physics Research B, 413 (2017) 31.

SESSION 2

BIOLOGICAL APPLICATIONS

Chair: C Teichert

I03 DYNAMICS OF DNA ORIGAMI LATTICE FORMATION AT SOLID-LIQUID INTERFACES STUDIED BY HIGH-SPEED ATOMIC FORCE MICROSCOPY

Adrian Keller

Technical and Macromolecular Chemistry, Paderborn University, Germany

Since its introduction in 2006 [1], the DNA origami technique has found its way into many different areas of fundamental and applied research. It enables the rapid, high-yield assembly of arbitrary yet well-defined nanostructures by exploiting the extraordinary specificity of Watson-Crick base pairing. While such DNA-based molecular nanostructures have very promising applications as fully biocompatible and biodegradable drug delivery vehicles and biosensors, they are nowadays also increasingly explored for materials science-related applications. As a particularly attractive approach, molecular lithography techniques enable the transfer of the DNA origami shapes into other organic and inorganic materials, including polymers, metals, and oxides, thus facilitating the synthesis of a broad range of nanomaterials [2]. The fabrication of functional nanodevices such as nanoelectronic circuits or plasmonic metasurfaces by these molecular lithography-based approaches, however, further requires the controlled arrangement of the DNA origami nanostructures on a solid substrate, which still represents a serious experimental challenge.

A promising approach for the controlled arrangement of DNA origami nanostructures into regular lattices on mica surfaces was developed by Aghebat Rafat et al [3]. It is exploiting the competitive binding of mono- and divalent cations to the mica surface in order to tune the electrostatic interactions between the adsorbed DNA origami and the substrate, thereby enabling the formation of densely packed DNA origami monolayers. Using this technique, regular DNA origami masks can be assembled and employed in molecular lithography [4]. This talk will summarize our recent and ongoing attempts to investigate the dynamics of DNA origami lattice formation on mica surfaces by high-speed atomic force microscopy. In particular, we study the influence of cation species and concentrations on lattice assembly and the dynamics of lattice defects [5] with the aim to further enhance the order of the resulting DNA origami masks. Possible strategies for transferring these highly ordered masks to other substrate materials will be discussed as well.

[1] Rothemund PWK, Nature, 440 (2006) 297-302.
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O05 PROTEIN ADSORPTION ON NANOPATTERNED SURFACES

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The biocompatibility of artificial materials in contact with human tissue is strongly influenced by not only its biological surrounding but also its chemical and physical surface properties. Various approaches for improving the biomaterial-tissue interaction have been explored so far that mostly focused on enhancing the surface's bioactivity by chemical and mechanical treatments. However, also the nanoscale surface morphology has been recognized as a significant parameter affecting protein adsorption and cell response, such as cell migration, proliferation etc [1,2].

To investigate the diverse influences of surface chemistry and surface topography on protein adsorption, we employ flat as well as nanorippled SiO_2 and TiO_2 model surfaces. Nanorippled Si substrates were synthesized by 500 eV Ar^+ ion irradiation at 67° incidence and a fluence of 1×10^{17} cm^{-2} [3]. Using magnetron sputter deposition, Ti films with a thickness of 20 nm were then grown on such nanopatterned Si substrates, which under optimized conditions may perfectly reproduce the ripple patterns [4]. The so-fabricated nanopatterned Ti and Si surfaces with native surface oxide were characterized by atomic force microscopy (AFM) and X-ray photoelectron spectroscopy (XPS). The nanopatterned oxide surfaces and their corresponding flat counterparts were then employed to study the influence of surface chemistry and nanotopography on protein adsorption. To this end, a variety of globular proteins with different molecular weights and isoelectric points were selected. Adsorption dynamics was monitored in-situ using ellipsometry while the morphology of the adsorbed protein films was assessed by ex-situ AFM. Additionally, conformational changes of the adsorbed proteins were investigated in-situ by attenuated total reflection infrared (ATR-IR) spectroscopy employing flat and nanorippled ATR crystals.

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O06 RIPPLE FORMATION ON Ti-BASED SURFACES AT MeV ENERGY HEAVY-ION IMPLANTATIONS

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Surface modification of biomedical materials is of interest for orthopedic implants where characteristic structures of nano, up to micrometer, sizes can promote cell adhesion, spreading and proliferation. Physical methods for surface modification including ion beam sputtering (IBS) continues to be a relevant process for biomedical applications. In this work [1], we investigate the formation of surface ripples on biocompatible polycrystalline titanium and its alloy (Ti-6Al-4V) targets after high-energy noble-ion implantation conditions for which nuclear stopping is still prevalent. Surface ripples with micrometer sizes emerge after Au ion implantation at low fluence, evolving into sawtooth structures at intermediate and high fluences. Experimental conditions studied include the dependence on the angle of incidence in addition to the comparison on the use of Vickers' indentation procedures. The formation of surface ripples is similar to low and medium energy irradiation conditions on semiconducting materials. With this analogy in mind, the relative importance of sputtering, surface mass-rearrangement, and ion implantation has been quantitatively estimated in a continuum model.

This work acknowledges financial support from project PAPITT-UNAM projects IN-111717 and CONACyT (México) Postdoctoral Fellowship.

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O07 SUPERHYDROPHOBIC PTFE SURFACE ACHIEVED BY LOW ENERGY Ar^+ ION BEAM IRRADIATION

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Superhydrophobic polytetrafluoroethylene (PTFE) surfaces were developed using low energy Ar^+ ion beam irradiation. The ion beam energy was varied from 300 eV to 800 eV both at normal and oblique angle of incidence of ion beam. The irradiation time and ion fluence were varied between 30 s to 780 s and 1×10^{16} ions/cm^2 to 3×10^{18} ions/cm^2, respectively. A remarkable change in surface wettability was observed and surface became hydrophobic to superhydrophobic in just 30 s time with 800 eV ion irradiation. The surface morphology revealed the formation of hierarchical micro and nanostructures on its surface. Detailed wetting behaviour of irradiated PTFE was studied using contact angle, surface free energy and rolling speed measurement. A systematic increase in the contact angle was observed with increase in beam energy, irradiation time and surface roughness. With initial contact angle of 105°, 800 eV ion beam irradiation has increased the contact angle value to 150° just after 30 s irradiation time. In case of oblique angle irradiation, for 300 eV, as the angle of incidence is increased from 0° to 40°, there was a systematic increase in the contact angle from 137° to 146°, which was followed by a drastic reduction at 70° of angle of incidence with contact angle of 131°. But, a continuous reduction in contact angle was observed with increase in angle incidence in case of 800 eV. After a threshold irradiation time, the water droplet started rolling from the horizontal surface in each ion beam energy range and was supported by measurement of polar and non-polar components of surface free energy. After 180 s of irradiation at 800 eV, the surface energy of PTFE was reduced to 0.35 mN/m with rolling speed of 31 mm/s. This wetting behaviour of PTFE surface was explained by the Wenzel and Cassie-Baxter theories.

SESSION 3

NON-ION BEAM PATTERNING

Chair: K Nordlund

I04 SELF-ORGANISED SURFACE NANOPATTERNING UPON IMPACT OF ULTRA-SHORT LASER PULSES

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By irradiation with powerful ultra-short laser pulses around the ablation threshold, ordered nanostructures are formed at the surface of solid materials (LIPSS; laser induced periodic surface structures), which are very similar to those created by ion sputtering. Triggered by this similarity we developed an explaining model of self-organised structure formation following the same route as in ion sputtering, based on a transient surface instability induced by the high energetic excitation from the laser input.

Recent results show that it is possible to extend single laser spot (Ø several µm) structures coherently covering large areas of several cm^2. These areas, then, exhibit peculiar functional properties, like modified wettability, colour, tribology etc.

The talk will present some experimental features of the surface patterns and their dependence on irradiation parameters, briefly sketch the model explanations, and then show some applications of surface functionalization.

O08 LIGHT-ASSISTED CHARGE SPREADING IN SELF-ASSEMBLED ARRAYS OF ORGANIC SEMICONDUCTOR NANONEEDLES ON 2D MATERIALS

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Crystalline films of small conjugated molecules offer attractive potential for fabricating organic solar cells, organic light emitting diodes (LEDs), and organic field effect transistors (OFETs) on flexible substrates. Here, the novel two-dimensional (2D) van der Waals materials like conducting graphene (Gr), insulating ultrathin hexagonal boron nitride (hBN), or semiconducting transition metal dichalcogenides come into play. Gr for instance offers potential application as a transparent conductive electrode in organic solar cells and LEDs replacing indium tin oxide, whereas hBN can be used as an ultrathin flexible dielectric in OFETs. Recently, we reported on the self-assembly of crystalline nanowires (NWs) composed of rod-like oligophenylene molecules on exfoliated, wrinkle-free Gr [1,2] and hBN [3], both transferred onto SiO_2. The NWs are several 10 nm wide and a few nm high, they can extend to several 10 µm in length. The discrete NW directions with respect to armchair and zigzag directions of the substrates were determined by atomic-force microscopy (AFM) in conjunction with density functional theory calculations.

Here, we study the growth of an oligoazaacene derivate dihydrotetraazaheptacene (DHTA7), which - due to nitrogen containing groups - forms crystals through H-bonding and dipolar interactions between neighboring molecules. Crystalline NWs of DHTA7 were grown by hot wall epitaxy on insulating ultra-thin hBN flakes. Using conductive AFM (C-AFM) and photo-assisted electrostatic force microscopy (EFM), we demonstrate charge trapping and light-assisted charge spreading within the networks of DHTA7 NWs. For this, we either charged the needles or needle networks by applying a bias via a C-AFM tip in contact mode without scanning or contacting the needles via a graphite plate on top of the hBN. We found that the NWs are not conductive in the dark, while visible light - linearly polarized parallel to the long axis of the molecules, i.e. perpendicular to the nanowires' long axes - allows spreading of the charges across the network for tens of micrometers. The results indicate that - due to light excitation - charges that were trapped in the localized defects can spread through the bands of the organic semiconductor. The charge transport can be described by a simple diffusion model, considering the individual NWs as RC-transmission lines [4].

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O09 NANOPATTERNING OF $SrTiO_3$(100) SURFACE WITH CRYSTALLINE TITANIUM OXIDE (TiO) NANOWIRES IN THE PROCESS OF THERMAL REDUCTION

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Transition metal oxides with a tailored non-stoichiometry in the oxygen sublattice are recently of a high interest in all fields of material sciences. New phases formed on reduced oxide crystals or thin films possess interesting optoelectronic properties such as conductivity, absorption and fluorescence and are promising materials for the development of novel memristive and catalytic devices. Particularly interesting are heterostructures of two or more oxides of different structural or electronic properties, however growth of such is challenging, especially when it comes to form nanopatterned structures.

In the presentation we will report on a new bottom-up method of crystalline TiO nanowires formation on the $SrTiO_3$ surface due to thermally-induced crystal reduction [1]. With the help of the UHV SPM and diffraction methods we have found that thermally-induced mild reduction of a pristine $SrTiO_3$(100) single crystal leads to progressive changes in the surface structure, associated with the insulator-metal transition of the electrical conductivity in the surface region [2]. Furthermore, we have found that the higher temperature reduction (>1000°C) with oxygen partial pressure additionally lowered with the use of an oxygen getter, results in the incongruent sublimation of strontium and decomposition of the perovskite surface [3]. This process leads to the formation of titanium monoxide (TiO) crystalline nanowires on reduced strontium titanate, as shown by the results of HAADF-STEM measurements. It has been found that the TiO/$SrTiO_3$ interface is atomically sharp and the transition from Ti^{4+} to Ti^{2+} happens within two unit cells. The nanowires are oriented along the main crystallographic directions of the $SrTiO_3$(100) surface, forming macroscopic network, whereas nanowires' length and height can be controlled by varying the annealing temperature and oxygen partial pressure. We will discuss the mechanism of the nanowires formation based the incongruent effusion of Sr associated with the crystallographic shearing of TiO_6 octahedra in the subsurface region of $SrTiO_3$ crystal.

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O10 2D DIFFRACTION PATTERNS OF SINGLE-CRYSTAL Si WAFER ISOTROPICALLY IRRADIATED WITH MONOCHROMATIC X-RAYS

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We have developed a simple device that can perform analysis of X-ray diffraction patterns with high resolution and high detection efficiency by using an imaging plate (IP) for a recording detector. In addition to the normal diffraction patterns with the form of circles, ellipses and parabolas appeared on the IP, as shown in the figure. These beautiful geometric 2D patterns were obtained by isotropically irradiating the perfect crystal Si wafer with monochromatic X-rays, which emit from a near point source of ^{55}Fe. The 2D diffraction curve shows the constructive interference of X-rays scattered from lattice planes satisfying the Bragg's condition in many planes of crystalline Si.

We found that each 2D pattern can be expressed by the cross-section of a cone cut with a plane in the direction corresponding to the pattern. The plane is a lattice plane satisfying Bragg's law in the crystal Si wafer. The surface of the cone is formed with part of X-rays from the point source, which are emitted strictly in the direction of Bragg angle for the lattice diffraction. It is interesting that these diffraction patterns can be described by the conic section that goes back to the definition by Apollonius of Perga (262 - 190 BC), who was a Greek mathematician known as 'The Great Geometer'.

We have succeeded in the simulation of the diffraction pattern by the crystal structure analysis approach and the geometrical analysis, especially Bragg diffraction with monochromatic X-rays isotropically irradiated. In this presentation, we will explain the mechanism of making various 2D diffraction patterns on the sheet of IP using the conic section.

X-ray source: Fe-55 (5.9 keV)
Size: about 1 mm in diameter
Imaging plate, IP (40 × 20 cm)
with 100 µm resolution
Distance: the source to IP:5 cm
Si wafer: 10 cm in diameter
Lattice constant: 5.43 Å

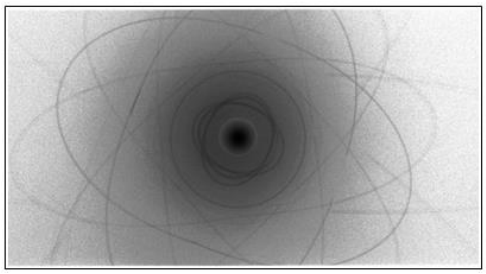

Image of 2D diffraction patterns on the IP.

SESSION 4

ELECTRONIC APPLICATIONS

Chair: F Buatier de Mongeot

O11 ULTRA-LOW THRESHOLD COLD CATHODE ELECTRON EMISSION FROM Au NANOPARTICLES DECORATED ION-BEAM PATTERNED NANOFACETED-Si SUBSTRATES

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Decoration of metal nanoparticles on nanostructured semiconductors unfolds a new horizon for highly efficient cold cathode electron emission devices. In this study, we report a fascinating low turn-on (~0.27 V μm^{-1}) and highly stable field emission from self-organized gold nanoparticles (Au-NPs) on low energy ion-beam fabricated self-organized silicon nanofacets (NFs). Fabrication of Si-NFs is carried out using 500 eV Ar ions at an oblique angle incidence of 71° on silicon substrates at room temperature. A variation in the growth angle (65° - 85°) of Au-NPs provides the functionality of self-organization and tunability in the size of Au-NPs leading to tunable threshold fields (0.27 - 0.51 V μm^{-1}) for cold cathode electron emission. The local probe based dual pass tunneling current microscopy (DPTCM) measurements reveal that tunneling current originates predominantly from the Au-NPs at the apexes and side walls of the Si-NFs. The emergence of tunneling electrons under low turn-on fields can be attributed to the tiny and isolated Au-NPs working as effective electron emitting sites. In addition, these experimental observations are reinforced by electrostatic field-based simulation studies, which suggest that there is a stronger local field enhancement at the apexes of Si-NFs following their decoration with Au-NPs. Thus, the present study reveals that Au-NPs decorated ion-beam fabricated Si-NFs lead to extraordinary cold cathode electron emission performance which should be useful for low-dimensional field emitting devices.

O12 MORPHOLOGY MODIFICATION OF Si NANOPILLARS UNDER ION IRRADIATION AT ELEVATED TEMPERATURES

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Ion beam irradiation of vertical nanopillar structures may be utilized to fabricate a vertical gate-all-around (GAA) single electron transistor (SET) device in a CMOS-compatible way. After irradiation of Si nanopillars (with a diameter of 35 nm and a height of 70 nm) by either 50 keV broad beam Si^+ or 25 keV focused Ne^+ beam from a helium ion microscope (HIM) at room temperature and a fluence of 2×10^{16} ions/cm^2, strong deformation of the nanopillars has been observed which hinders further device integration. This is attributed to ion beam induced amorphization of Si allowing plastic flow due to the ion hammering effect, which, in connection with surface capillary forces, dictates the final shape. However, plastic deformation can be suppressed under irradiation at elevated temperatures (investigated up to 672 K). Then, as confirmed by bright-field transmission electron microscopy, the substrate and the nanopillars remain crystalline, and are continuously thinned radially with increasing fluence down to a diameter of 10 nm. This is attributed to enhanced forward sputtering through the sidewalls of the pillar, and found in reasonable quantitative agreement with the predictions from 3D ballistic computer simulation using the TRI3DYN program.

This work is supported by the European Union's H-2020 research project 'IONS4SET' under Grant Agreement No 688072.

O13 ANISOTROPIC NANOSCALE RESISTIVE SWITCHING BEHAVIOUR OF Au-ION IMPLANTED RIPPLE-LIKE TiO_x ($x < 2$) FILMS

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Due to an increasing demand of high-density data storage, non-volatile memory devices based on resistive switching phenomenon has gained a lot of interest in recent years. These devices combine the advantages of flash and dynamic random access memory (DRAM) devices. Here, we demonstrate tunable resistive switching (RS) behaviour in Au-ion implanted TiO_x films. A two-step fabrication method has been adapted here where Au-ions at various fluences (in the range of 5×10^{14} - 1×10^{17} ions cm^{-2}) are implanted at 45° in radio-frequency (RF) sputter-deposited TiO_x thin films on highly-doped (ρ = 0.05 Ω-cm) p-Si (100) substrates. It is observed that ion implantation leads to the formation of self-organized ripple-like patterns on TiO_x surface above a threshold fluence of 1×10^{16} ions cm^{-2}. This is followed by tunable resistivity (in the range of 7.2×10^{3} - 3×10^{-1} Ω-cm) and work function (in the range of 4.37 - 4.96 eV) of TiO_x films with increasing Au ion-fluence which corroborate well with X-ray photoelectron spectroscopy results, indicating the evolution of Ti-rich films at higher fluences. The devices exhibit stable loop openings under both forward and reverse bias conditions in the respective current voltage (I-V) characteristics - measured at ridges and grooves of the respective ripple patterns using conductive atomic force microscopy (cAFM). It is interesting to note that the threshold voltages for high-to-low resistance state (V_{set}) and that for low-to-high resistance state (V_{reset}) transitions occur at relatively higher voltages with increasing ion fluence. In addition, for each fluence, V_{set} and V_{reset} values turn out to be different at pattern ridges and grooves. Thus, we demonstrate that Au-ion implanted TiO_x films show anisotropic surface morphologies, leading to the evolution of tunable but highly stable nanoscale anisotropic RS behaviour of the devices.

SESSION 5

THEORY

Chair: R Cuerno

O14 TRIANGULAR PATCHES OF RIPPLES, TERRACES AND ELONGATED PYRAMIDS PRODUCED BY ION SPUTTERING

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The anisotropic Kuramoto-Sivashinsky (AKS) equation is often used to model the nanoscale patterns produced by bombarding a solid surface with an obliquely-incident, broad ion beam. Intriguing phenomena are observed that are not reproduced by this model, however. Dispersive effects are not included in the AKS equation, but our simulations show that they can lead to the formation of raised and depressed triangular patches traversed by ripples [1]. These patches bear a strong resemblance to nanostructures that are commonly observed in experiments. We have also introduced an equation of motion that differs from the AKS equation by the inclusion of a cubic non-linearity [2]. This additional non-linear term results from an improved approximation to the sputter yield and can have a crucial influence on the dynamics - it can lead to the formation of a terraced topography that coarsens in time, in accord with experimental observations for high ion incidence angles. For different ranges of the parameters, our equation of motion produces unterraced topographies that are remarkably similar to those seen in various experiments, including elongated pyramids and isolated lens-shaped depressions [3].

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O15 NON-LINEAR THEORY OF ION-INDUCED SOLID FLOW

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Nanopattern formation by ion beam sputtering (IBS) is a powerful technique employed to induce surface structures over relatively large areas for a wide range of materials [1]. This technique has many applications in modern technology like magnetic storage, quantum device design or, for example, producing the selective attachment of specific molecules to substrates, with implications in biology and catalysis. For materials like semiconductors that become amorphous under low-to medium-energy irradiation, a description of IBS based on solid flow [2,3] has been proved to successfully explain many experimental observations [4-6]. This view of the process is based on the fact that, as a consequence of the impact of the ions and the subsequent release of energy within the target, residual stress is confined to a thin superficial amorphous layer and is eventually relaxed in macroscopic time scales via viscous flow. Previous viscous flow models have remained limited to the study of the initial (linear) stages of the morphology evolution. In this contribution we derive closed non-linear evolution equations for the depth of the irradiated layer [7]. This mathematical description includes novel terms associated with the spatial distribution of damage that builds up through sustained bombardment and extends classic models of macroscopic fluid-flow systems. Numerical simulations reproduce the main dynamical features of experiments and uncover a relationship between the asymmetric shape of the ripples and their direction of motion along the surface.

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O16 SURFACE COVERAGE OF ION IRRADIATED SOLID FILMS

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Continuous solid films under ion irradiation show a non-uniform thinning that produces characteristic patterns where regions still covered by the film alternate with regions of exposed substrate [1]. The morphology of these patterns can be understood and predicted by exploiting analogies with liquid films dewetting from their substrate. In this latter case, the contrasting actions of surface tension and disjoining pressure can make the film unstable to fluctuations of its thickness [2]. Fluctuations of proper spatial wavelength are amplified up to the film rupture and the following substrate exposure originates the characteristic dewetting patterns. Even if we can suppose active both surface tension and disjoining pressure, and evaporation has a proper analogous in sputtering, still a major difference distinguishes the irradiated solid film from the liquid one: the mobility that allows the material redistribution is acquired only in the region of the ion impact, and it is significant only for a short time after it.

Here we consider the difference between the two ways to proceed towards equilibrium by analyzing how the decrease of surface coverage of irradiated thin films depends on ion fluence. Experimental data are compared with the predictions offered both by the model for real liquids, based on the solution of the thin film equation [3], and by its adaptation that takes into consideration the locality of the process, as needed for ion irradiated solid films [4]. Tracing a proper parallel between the two pictures will allow to exploit the physical insight offered by the thin film equation with respect to the nature of the mobility term in a context that is appropriate for ion irradiated solid films.

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O17 DIRECT OBSERVATION OF ION-INDUCED SELF-ORGANIZATION AND RIPPLE PROPAGATION PROCESSES IN ATOMISTIC SIMULATIONS

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Energetic ion beams can induce self-organization of atoms into ripple- or quantum-dot like nanostructures under prolonged irradiation. The nature of ripple formation on the surface of amorphous materials under tilted ion irradiation is under strong debate over a few decades. Several analytical theories are proposed to explain the phenomenon and develop predictive models of ripple formation. Unfortunately none of the theories is able to capture intrinsically all the processes developed in the system under inclined incidence of irradiating ions. In the present work, we report the first direct observation of ripple formation in the computer simulations using classical molecular dynamics (MD) method. It became possible thanks to the newly developed accelerated algorithm, which allows to speed-up the simulation of involved processes in a controlled manner to enable the full self-organization process under demanding condition of high fluence ion irradiation within the MD timespan. Since this approach does not require the presence of a precursor to trigger self-organization, it can provide valuable first-principles insights on the ripple formation and ripple propagation mechanisms. Analysis of the simulation shows that the ripple formation is dominated by enhanced surface atom displacements, and a pile-up effect. The effects of erosive and redistributive components, as well as the stress buildup will be discussed in detail. We also observe and explain the non-linear change in the build-up rate with fluence.

SESSION 6

QUANTUM APPLICATIONS

Chair: S Facsko

O18 A NEW FIB FOR DETERMINISTIC SINGLE ION IMPLANTATION

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Single isolated dopant atoms implanted into solid state devices have been shown to be a viable architecture for quantum technologies. Ion implantation provides many advantages as a manufacturing method for such devices, such as speed and scalability, but there is currently no way to completely control the number of implanted ions.

The SIMPLE (Single Ion Multispecies Positioning at Low Energy) tool, is a new focused ion beam tool in operation designed for the manufacture of quantum technologies. The tool has a 25 kV LMIG set up for femtoAmp sample currents, with ultra-fast beam blanking, neutral blocking and a highly efficient secondary electron detection system. Deterministic ion implantation is achieved through extraction of single ions through fast beam blanking with low currents, ion implant detection through collection of secondary electron (SE) signal from the target, and high spatial precision in ion placement. Currently the tool has achieved an 80% probability of implanting a single Bi^+ ion into bulk silicon without error, with a 20 nm beam spotsize determining dopant placement precision. A lot of work has gone into maximizing the detection efficiency for secondary electrons and investigating the factors which affect the SE yield.

Currently the system is running with Bi source, and there are In sources available. Alongside the development of the instrument there is also research into developing a series of liquid-metal ion sources for elements with optical and quantum applications including P, Te, Se and Cd.

A second SIMPLE tool has also been installed at the Ion Beam Centre, which operates with a 20 kV duoplasmatron arc source, capable of 50 nm spotsizes. SIMPLE #2 will initially operate with nitrogen source for the fabrication of NV centers in diamond.

O19 EXOTIC LM(A)IS SOURCES FOR ION IMPLANTATION: HOW FIB MILLING PATTERNING CAN PROMOTE NEW QUBIT PROPOSALS

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In 1998, Kane [1] proposed a quantum computer design based on phosphorus donors in silicon. This device requires phosphorus implants spaced 20 nm apart from each other, and 20 nm below the silicon surface. However, even using focused ion beam (FIB) systems for precise implantation, due to the intrinsic straggle of phosphorus ions, this device is impractical. Based on these limitations, new proposals have been made, e.g. Morse et al showing the advantage of using a photonic platform for donor spin qubits in silicon, in which Selenium (Se^+) ions implanted on a standing photonic crystal become robust to manufacturing imperfections. Additionally, these Se^+ implants present other advantages such as “deep” donor optical transitions, emission of highly uniform light, the ability of being optically initialized, and can be operated in slightly higher temperatures.

However, Selenium (or Tellurium) are not commercially available as LMIS for FIB systems. Those materials present too high vapour pressure, which can jeopardize the microscope and result in a short life time of the source. Bearing this in mind, we have established our own source fabrication laboratory to produce alloys that may solve these problems. The aim of this LM(A)IS fabrication lab is to make our own sources to satisfy demand on our single ion implantation instrument (SIMPLE) to produce implanted devices for quantum and other applications.

The first step of the LM(A)IS manufacturing is sharpening a tip using a FIB. By using a FIB instead of the electrochemical etching, we are able to use any material as tip, including tungsten, gold, or niobium. Those tips have a high production yield, can help the wettability, and can be shaped using different patterns, such as 4-sided pyramid or conical.

Finally, using FIB we are also direct writing nanopatterned photonic crystals, and single electron transistors. This way, we have a fast prototyping method to test the different LM(A)IS produced as quantum devices.

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[2] Morse KJ et al, Science Advances, 3(7) (2017) e1700930.

O20 INVESTIGATING THE FORMATION OF ISOTOPICALLY PURE PATTERNED AREAS FOR QUANTUM COMPUTERS USING ION IMPLANTATION AND LAYER EXCHANGE

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In 1998 Bruce Kane proposed that quantum computation could be achieved using Qubits that exploit entangled quantum states formed by locating in close proximity two spinning atoms of, for example, P or Bi. The atoms are isolated from environmental perturbations by incorporating them in a low temperature, "solid state vacuum" which can be formed by cryogenically cooling an isotopically pure, defect free crystalline layer consisting of atoms that have no intrinsic electronic or nuclear spin. Such layers composed of pure ^{28}Si, or ^{74}Ge, would be particularly useful as they could be integrated straightforwardly into conventional CMOS for the industrial manufacture of quantum computers systems. Naturally occurring Si is predominantly (92.2%) ^{28}Si, but significantly contains 4.7% ^{29}Si which, possessing nuclear spin, can interfere with the entangled spins. It might be thought that an ion implanter could be used as an isotope separator to selectively deposit low energy ^{28}Si onto a natural Si substrate. However, our group has previously shown that self-sputtering limits the enrichment possible to ~99.5%, and isobaric ions such as $^{14}N_2$ (and even $^{56}Fe^{2+}$) can contaminate the layer. Surface oxidation, if the implanter end-station is not at ultra-high vacuum, could also be problematic. Similar considerations exist for Ge. This talk describes the results of preliminary investigations to exploit a layer exchange technique to overcome these issues. The University of Surrey hosts two advanced implanters that are being developed with the aim of reproducibly and deterministically placing single ions to form such Qubits. The SIMPLE (Single Ion Multispecies Positioning at Low Energy) implanters are modified focussed ion beam tools that can deliver pulsed beams in which there is an average of less than one ion per pulse. A SIMPLE tool fitted with a AuGe liquid metal ion source was used in a non-pulsed mode to implant isotopically pure Ge ion beams to fluences of ~10^{17} ions/cm^2 into an Al metal layer that had been deposited onto a native-oxide free Si wafer. Implants into 5 µm × 5 µm square regions could be completed within a few minutes, enabling experiments over a range of fluences to be undertaken. The implanted regions were annealed under various conditions so that the Ge exchanged places with the Al and grew onto the underlying Si substrate. After Al removal, the exposed Ge layers were analysed for crystal quality and Al content by various means, including TEM. Whilst this approach potentially solved some problems, it introduced others, most notably Al incorporation in the Ge layer. This talk will discuss approaches to minimise Al retention and leverage chemical means for its subsequent removal.

SEM image of eight regions implanted With Ge/25 keV over a range of Fluences between 1 × 10^{17}/cm^2 to 4 × 10^{16}/cm^2 post-anneal and Al removal.

SESSION 7

OPTICAL APPLICATIONS

Chair: F Krok

I05 FACETED NANOSCALE WRINKLES ON AMORPHOUS TEMPLATES FOR OPTOELECTRONICS, BIOSENSING AND NANOMECHANICS

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Wrinkling is very common in nature inducing patterning at the surface of compressively strained elastic layers, such as fruit skin or polymers. Different methods, based on ions- or photons- surface irradiation, have been so far exploited for inducing surface strain in polymers, achieving both random and oriented structures. However, limited control of the pattern formation has been obtained, generally achieving micrometric structures with low height/width aspect ratio.

Here, I will discuss the controlled growth of high-aspect ratio nanostructures at the surface of solid state amorphous glass substrates via ion-assisted wrinkling instability [1]. Highly ordered 1-dimensional (1D) nanoripples are achieved by ion-irradiation near the glass transition temperature, boosting the vertical dynamic of the pattern by more than one order of magnitude with respect to low temperature experiments. Despite the amorphous nature of the surface, asymmetric faceted ridges as long as several micrometers bound the 1D nanowrinkles. The asymmetric faceted profile can be easily tuned by acting on the ion irradiation conditions.

The self-organized nature of the ion-induced wrinkling and the possibility to easily control the facet tilt at the nanoscale represent crucial advantages in view of many large-area applications ranging from optoelectronics and plasmonics to nanotribology and biotechnology. In the talk the possibility to exploit these faceted 1D nanopatterns for driving the growth of tilted plasmonic nanoantennas [2] and conductive nanowire arrays will be discussed. The versatility and the potential of the method will be shown by tuning polarization-sensitive plasmonic resonances from the visible to the Near- and Mid-Infrared spectrum for biosensing (Surface Enhanced Infrared Absorption - SEIRA) [3], directional light scattering and color routing applications. Finally, the crucial role of faceted nanowrinkles for driving the motion of nanoparticles in nanotribology and/or the oriented growth of biological cells in biotechnology will be discussed [4,5].

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O21 LIGHT TRAPPING IN NANOPATTERNED 2D MATERIALS AND THIN FILM OPTOELECTRONIC DEVICES

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Large area nanopatterning approaches, based on defocused Ion Beam Sputtering and on Laser Interference Lithography, are employed in order tailor the growth of uniaxially rippled thin film solar cells and of atomically thin 2D semiconductors. Both classes of materials are actively searched for next generation optoelectronic and photovoltaic applications where non-conventional light trapping schemes are mandatory.

In the first case, we demonstrate that the substrate rippled morphology allows to induce broadband absorption enhancement by exploiting both high haze which determines a strong diffuse scattering at smaller wavelengths, and bio-mimetic moth-eye index grading effects which reduce reflection losses for the photons at larger wavelengths [1].

In the case of atomically thin 2D semiconductors based on MoS_2 new paradigms must be employed in order to achieve efficient light trapping. In this case the 2D semiconductor is patterned to form an atomically flat grating which steers light parallel to the MoS_2 surface upon excitation of Rayleigh modes. Alternatively, the conformal growth of MoS_2 nanosheets on a template pre-patterned with a uniaxial ripple morphology, induces a uniaxial modulation of the electrical, optical and vibrational properties of the 2D semiconductor thanks to strain induced modulation of the electronic bandstructure [2].

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O22 LOW ENERGY IONS FOR FABRICATING ORDERED PLASMONIC STRUCTURES FOR SECOND HARMONIC GENERATION AND SENSING APPLICATIONS

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Nobel metal nanoparticles exhibit distinct optical properties due to localized surface plasmon resonance (LSPR). Potential applications of these structures can be found in thin film solar cells, non-linear optical devices, or sensors [1,2]. The non-linear second-harmonic (SH) response from the ripple patterned surface and metal nanoparticles arrays was measured, using unamplified femtosecond excitation at 800 nm, by rotating the linear polarized input and detecting either the s or p-polarized SH output. A decrease in response with increased ripple structure periodicity was observed for the p-in/p-out configuration, when the plane of incidence was orthogonal to the average ripple orientation [3]. Possible origins of the SHG response will be discussed. Plasmonic field coupling in aligned equidistant chains of metal nanoparticles is higher compared to randomly distributed particles [1,2]. Due to large field enhancement, such metal nanoparticles arrays have also shown their potential applications in plasmonic sensor for detecting the glucose concentration lower than blood glucose level [4].

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O23 PREPARATION OF A NEW KIND OF TWO-DIMENSIONAL METAL/DIELECTRIC NANOCOMPOSITE SURFACE-RELIEF GRATING COUPLERS AND THEIR VERTICAL INPUT COUPLING PROPERTIES

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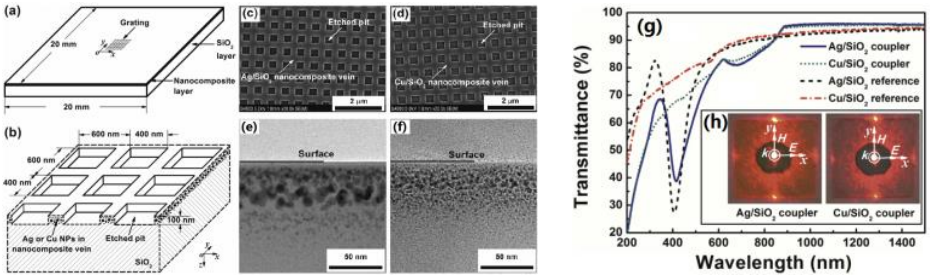
It is well known that optical waveguides of glass materials are widely used in the fabrication of PICs due to their inexpensive materials, good transparency and high optical damage threshold. However, due to the low refractive index of the optical waveguide of the glass material, the optical coupling efficiency of the grating coupler manufactured by it is low. So a two-dimensional composite grating coupler was fabricated by implanted low-energy metal ions like 90 keV Ag ions or 60 keV Cu ions at the same dose of 6×10^{16} cm^{-2} into the SiO_2 substrate to make sure the implanted depth is around 100 nm. Then electron beam etching was implemented. The prepared composite two-dimensional nano-grating has a period of 600 nm in a submicron periodicity and a depth of 100 nm. The experimental results show that the composite plate coupler can convert 620 - 880 nm light into guided wave of internal waveguide with different efficiencies, especially metal nanoparticles (NPs) play an special important role in it. Further research proves that the periodical phase modification of the transmitted beam is strongly enhanced due to the introduction of periodically distributed metal nanoparticles, and on the other hand the nanocomposite veins could be used as an effective light scatterers. It can be clearly get the result that the coupling efficiency of the prepared composite coupler is much larger than that of the coupler without nanoparticles when it has the same morphological parameters. By optimizing the parameters and improving the metal nanoparticles in volume fraction and size, it is possible to produce a more efficient metal/insulated composite surface relief type two-dimensional planar coupled grating. This preparation method can provide a new method for preparing an efficient micro surface relief grating coupler on a glass material optical waveguide.



(a) Appearance of expected metal/SiO_2 nanocomposite surface-relief grating coupler sample.
(b) Schematic drawing of local feature of grating zone.
(c-d) SEM micrographs of the gratings inAg/SiO_2 and Cu/SiO_2 coupler samples.
(e-f) Cross-sectional TEM images of Ag/SiO_2 samples and Cu/SiO_2 samples.
(g) Experimental transmission spectra of two coupler and two reference samples.
(h) Photos of two coupler samples vertically illuminated by a 650 nm-wavelength linearly polarized laser beam.

SESSION 8

SEMICONDUCTORS

Chair: T Som

O24 ION-INDUCED SURFACE NANOSTRUCTURES OF GERMANIUM(001)

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It is well known that ion beam irradiation can lead to various self-organized surface nanostructures depending on the irradiation conditions and the sample material. If the ion-irradiated sample is a semiconductor, its surface becomes amorphous if the bulk vacancies and interstitials produced by ion impacts cannot diffuse fast enough to reach the surface or recombine until the next ion impinges on the surface. However, if the sample is heated above the recrystallization temperature, the diffusion is enhanced and the surface remains crystalline during ion irradiation. This results in a further surface instability: the diffusion of adatoms and surface vacancies is biased by an additional energy barrier (Ehrlich-Schwoebel (ES) barrier) at the step edges of the crystal surface, which causes an effective uphill current for adatoms and a downhill current for surface vacancies. This instability is identified as a main process for the growth of surface structures in molecular beam epitaxy and was adopted as a possible source for roughening during ion sputtering [1].

In recent experiments it was found that periodic surface patterns develop during normal-incidence ion irradiation of Ge(001) above recrystallization temperature. These patterns consist of a checkerboard of inward and outward oriented pyramids. Their bases are square and oriented along the <100> crystal direction [2]. Pyramidal nanostructures were also found in homoepitaxy on Ge(001) [3].

The changing patterns during ion irradiation experiments with varying ion incidence angles between 0° and 80° and two different azimuthal angles allow for an investigation of the associated change of kinetic and diffusive mechanisms. For off-normal ion incidence with a <110> azimuthal direction the checkerboard pit-and-mound patterns develop to mound patterns for incidence angles greater than 20°. Furthermore, the bases of the pyramids deform into more pronounced rhombohedral shapes along the ion beam projection. This may be attributed to the momentum transfer from the ions to the near surface atoms of the sample in the direction of the beam. In case of incoming ions with an azimuthal direction along <100>, the pyramidal mounds also tend to elongate along the projected ion beam. However, an exception has to be made for an incidence angle of 40°, where the pyramids surprisingly tend to elongate along the perpendicular direction of the incoming ions - the <110> direction. This phenomenon could be associated with an enhanced ion channeling at this incidence angle.

All these surface patterns can be described by a continuum equation which combines the ballistic effects of ion irradiation and the effective diffusion currents due to the ES barrier on the crystalline surface. The performed simulations indicate that, at least for a <100> azimuthal ion beam direction, the surface gradient dependent sputter erosion seems to be the leading process during pattern formation.

[1] Chey SJ, Van Nostrand JE, Cahill DG, Physical Review B, 52 (1995) 16696.
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[3] Van Nostrand JE, Chey SJ, Cahill DG, Physical Review B, 57 (1998) 12536.

O25 CONTROLLED NANOPOROSITY INDUCED BY ION IRRADIATION OF Ge THIN FILMS

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Irradiation of germanium with large fluences (>1 × 10^{15} ions/cm^2) of low/medium (10 - 10^2 keV) energy ions with mass similar or higher than the Ge one results in completely decomposed structures with variety of shapes [1-3]. The typical structures are columnar nanovoids with diameters of several tens of nm, depths going from 10 to ~10^2 nm and separated by Ge walls of ~15 nm of thickness. The final nanostructures depend on a number of irradiation parameters (ion species, energy, incidence angle and fluence) and on substrate temperature and crystallographic structure. Though, a lot of effort has been already devoted to understanding the formation mechanisms in the case of bulk Ge, there are new intriguing aspects for the formation of these nanostructures in case of deposited thin (~10^2 nm) films [4,5]. Furthermore, the possibility to fabricate nanoporous semiconductor films on insulator or transparent substrates would allow applications in technologically appealing fields like sensing, thermoelectric energy harvesting, optical devices.

In this work, we report on the investigation about the ion induced nanostructuration of Ge thin films (either 100 or 200 nm thickness) deposited by several processes on ~10^2 nm SiO_2/Si substrates, aiming to create nanoporous semiconductor thin films on insulator. The ion irradiation was carried out with either As or Ge ions with energy ranging from 140 to 190 keV and ion fluence of ~1 × 10^{16}. Several strategies were adopted to control the geometry of nanovoids, using pre-implantation annealing or depositing controlled thin cap layers. Morphological characterizations of the films were performed by high resolution scanning electron microscopy in plan as well as in cross-sectional mode. It has been observed that the presence of protective cap layer is affecting the nano-structuration mechanism allowing more ordered nanovoid arrays along with preventing the erosion of nanostructures.

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[5] Romano L, Impellizzeri G, Bosco L, Ruffino F, Miritello M, Grimaldi MG, Journal of Applied Physics, 111 (2012) 113515.

O26 COMPARISON OF Si AND Ge SURFACE PATTERNS PRODUCED BY ION IRRADIATION IN THE REVERSE EPITAXY REGIME

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In addition to sputtering, ion irradiation is often also leading to restructuring of the surface and a plethora of surface patterns can appear. At irradiation temperatures high enough to dynamically anneal defects induced by the collision cascades the surface remains crystalline. Still, a high density of ion-induced surface vacancies and adatoms remains and their diffusion is affected by the Ehrlich-Schwoebel (ES) barrier, i.e. an additional diffusion barrier to cross terrace steps. These defects are therefore trapped on terraces, nucleate and form pits or mounds [1]. In this way three-dimensional, faceted nanostructures are formed, reflecting the underlying crystal lattice. Due to the similarity to growth of three-dimensional structures in molecular beam epitaxy this mechanism is called reverse epitaxy.

We will present patterns on Si and Ge surface induced by low energy, normal incidence, high fluence ion irradiation at temperatures above the recrystallization temperature. Patterns with very different symmetry can result, depending on the surface orientation: pyramidal structures with four-fold symmetry on the (001) surface, with three-fold and six-fold symmetry on the (111) surface and elongated structures with two-fold symmetry on the (011) surface [2].

Although Si and Ge have the same diamond crystal lattice, the resulting patterns and facets are different: on Ge(001) predominantly (105) facets are formed, whereas (115) facets are found on Si(001). Similarly, on Si(111) the pattern exhibits a six-fold symmetry with (123) facets, whereas on Ge(111) the patterns are formed by (356) facets and exhibit a three-fold symmetry. The formation mechanism and possible effects leading to these differences on Ge and Si surfaces will be presented and discussed.

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POSTERS

P01 MORPHOLOGY, DENSITY, AND TEMPORAL EVOLUTION OF TOPOLOGICAL DEFECTS IN REVERSE EPITAXY

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Low-energy ion-irradiation of semiconductors above their recrystallization temperature has been shown to induce regular nanoscale patterning of the crystalline surface. The mechanism is called reverse epitaxy in analogy to epitaxy in growth: ion-induced mobile vacancies and ad-atoms on the crystalline surface encounter the Ehrlich-Schwoebel energy barrier for crossing terrace steps and exhibit preferential diffusion along specific in-plane directions. This can lead to the formation of well-defined faceted surface structures with morphologies strongly dependent on crystalline structure and surface orientation. For instance, GaAs(001) and InAs(001) develop periodic ripple structures with a saw tooth profile.

We have studied the topological defects in ion-induced patterns on GaAs(001) and InAs(001), i.e. ripple junctions, and present results from both experiments and simulations on the following aspects:

- defect morphology and the influence of polar and azimuthal ion incidence angles thereon;
- dependence of the defect density on sample temperature and ion energy;
- temporal evolution of the defect density;
- defect motion and annihilation processes.

We find strong dependencies on the easily controllable external process parameters, which is crucial information when preparing ion-induced surface patterns for specific applications.

P02 PRODUCTION OF HOMOGENEOUS PLASMONIC GALLIUM NANOPARTICLES USING HEXAGONAL PIT TEMPLATES

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Metallic nanoparticles (NPs) have attracted a lot of attention in the last decade due to their application in plasmonics [1]. Together with the traditional metals (silver and gold), the III-group metals such as Al, Ga and In exhibit interesting properties due to the possibility to tune the localized surface plasmon resonance (LSPR) in different ranges of the electromagnetic spectrum, including the ultraviolet regime [2]. Indeed, these Ga NPs have been already used for waveguiding, surface-enhanced Raman spectroscopy and fluorescence and biosensing [3]. However, the production of homogenous and spherical Ga NPs is complex because of the coalescence mechanisms that occur during the growth by Joule-effect thermal evaporation, leading to broad size distributions and affecting the and FWHM of the LSPR [2].

Herein, we present a novel method to order Ga NPs by using a nanopatterned Al pit array obtained from porous anodic alumina in three simple steps [4]. The first step is the anodization of Al foils to form the alumina (Al_2O_3) membrane formed is constituted of hexagonal cylindrical pores. The second step is the etching (in chromic oxide and phosphoric acid) of this oxide to produce an Al template formed by nanometric pit arrays. The last step is the deposition of the Ga NP.

Using three different pit sizes, we produced a unimodal distribution of Ga NPs with a diameter of 40, 80 and 300 nm respectively. Interestingly, due to the selective coalescence induced by the pit geometry and the surface tension of the Ga droplets, these NPs show a pseudo-spherical shape with excellent plasmonic characteristics and a range that cover the UV (40 nm diameter), the visible (80 nm diameter) and the IR (300 nm diameter) regions. These optical properties were measured by spectroscopic ellipsometry and compared with the theoretically calculated resonances using DDA simulations. The LSPR satisfies the plasmon ruler equation, demonstrating the universal scaling behavior of these NPs.

In conclusion, our work presents a novel method to obtain highly hexagonal ordered arrays of Ga NPs using three-step process. This method improves the optical performance (both FWHM and intensity) in a wide spectroscopic range from the UV to the IR. This procedure paves the way to fabricate better sensing platforms.

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P03 REALIZATION OF WAFER-SCALE GRATINGS WITH SUB-50 nm PERIOD THROUGH VACANCY EPITAXY

Stefan Facsko[1], Xin Ou[1,2], Qi Jia[2,5], Jiangtao Feng[3], Hao Huang[2,7], Xiaowei Yang[3,7], Joerg Grenzer[1], Kai Huang[2,4], Shibing Zhang[2,4], Jiajie Lin[2,4], Hongyan Zhou[2,4], Tangui You[2], Wenjie Yu[2], Philippe Jonnard[5], Meiyi Wu[5], Angelo Giglia[6], Zhong Zhang[3], Zhi Liu[2,7], Zhanshan Wang[3] and Xi Wang[2]

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Gratings, one of the most important energy dispersive devices, are the fundamental building blocks for the majority of optical and optoelectronic systems. In photon spectroscopy and other diffraction instruments, the period of the grating is the key parameter that determines and limits the dispersion and resolution of the system, especially in the short wavelength region. With the rapid development of large photon science facilities, high quality gratings with periodicities below 50 nm are in urgent need for the development of ultrahigh-resolution X-ray spectroscopy. However, the wafer-scale fabrication of uniform nanogratings through conventional patterning methods is difficult.

Here, we report on a maskless and high-throughput method to generate wafer-scale, multilayer gratings with period in the sub-50 nm range (line density above 20,000 lines/mm). The grating structure is fabricated by low-energy ion irradiation at elevated temperature on GaAs (001) surfaces and then coated with X-ray multilayers.

A diffraction efficiency of 11% was demonstrated at 87.5 eV and the extremely large angular dispersion is consistent with theoretical predictions. A 2 inches size nanograting with a line density of 24,500 lines/mm was fabricated which showed relatively uniform diffraction properties over a large area.

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P04 TEXTURIZATION OF POLYCRYSTALLINE Ti-BASED SURFACES BY LOW-ENERGY ION-BEAM IRRADIATION: IMPLICATIONS IN BIOMEDICAL IMPLANTS

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Titanium (Ti) and Ti-alloys (e.g. TiAlV) are relevant materials for biomedical implants [1], where surface morphology can play a crucial role in their performance [2]. Our study focuses on surface morphology changes on Ti-based targets induced by ion-bombardment and their eventual biomedical implication. For this work, polycrystalline Ti and TiAlV disks (1 cm in diameter) were irradiated with a low-energy (≤1 keV) broad-beam of argon or xenon ions and the morphology was imaged with scanning electron microscopy (SEM) while the surface roughness analysis was performed with a mechanical profiler. Irradiations at various incidence angles with respect to the surface normal and temperatures were performed. The irradiated surfaces display a variety of irregular mixed structures from the nanometer to micrometer range scale. In general, a transition from patches of ripples to elongated pillars occurs as the ion incidence angle is increased from 60° to 75°. The rippled domains are randomly oriented on the surface as attributed to the polycrystalline nature of the targets. Such nature is even revealed at high-temperature (>500°C) irradiations, since grain boundaries can be visually identified. On the contrary, elongated pillars produced at 75° are found to be preferentially oriented along the ion beam projection on the surface. Preliminary tests of cell adhesion and proliferation on these ion-induced surfaces is also presented.

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P05 ADSORPTION OF FULLERENE ON SURFACE AND EDGES OF GRAPHENE

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The unique possibilities of fullerene are broadened when fullerene is combined with other atoms and molecules, and endofullerenes are of special interest when additional atoms, for example, alkali metal ones, are in the inner cavity of fullerene. However, the practical application of fullerenes and endofullerenes in nanoengineering is due to the question what substrate will be used for fullerene structures. Such substrates can be the surfaces of silicon carbide crystals, silicon, diamond and graphene that, in view of miniaturization, is more successful since its thickness is one atomic layer.

In the present work the adsorption of fullerene C_{60} onto the surface and edges of defect-free graphene was studied by computer simulation within the framework of classical molecular dynamics. The computer model of a single defect-free C_{60} fullerene was built by the energy minimization method using the second-generation Brenner potential (REBO) and the cohesive energy of each carbon atom in the fullerene was determined. For consideration of fullerene adsorption on graphene surface the computer model of “infinite” defect-free graphene with the distance between its nearest atoms 1.4 Å and cohesion energy E_g of each atom 7.4 eV was obtained by the same method with a glance of periodic conditions for boundary atoms. For fullerene adsorption on graphene edges to be considered, a computer model of defect-free nano-graphene was constructed. This model was constructed in the same way as that of “infinite” defect-free graphene model but without imposing the boundary conditions on the edge atoms. As a result, nano-graphene with the distance between its nearest atoms approximately 1.4 Å was obtained. It was obtained that the C_{60} fullerene adsorption on graphene surface can be realized by different ways: (1) interaction of one atom of fullerene with one atom of graphene; (2) interaction of fullerene hexagons and graphene; (3) interaction of two neighboring atoms of fullerene and two neighboring atoms of graphene; (4) interaction when the center of fullerene hexagon is located over the graphene atom, and (5) interaction of two nearest non-neighboring atoms of fullerene and two nearest non-neighboring atoms of graphene. It should be noted that from all the ways of adsorption the first one I is the best because the fullerene C_{60} has the highest energy of binding with graphene and the adsorbed fullerene is less deformed as a result of its interaction with graphene. The geometrical characteristics of fullerene C_{60} adsorbed on graphene surface were obtained. It was established that the fullerene is better adsorbed on the armchair edge of nanographene and worst on the “corner” atom of nanographene. The binding energy for adsorption on the nanographene edge can be almost twice as large as the highest binding energy of adsorption on the graphene surface and stronger deformation of the fullerene shape is observed. The results are in good agreement with experimental data and results obtained from first principles.

P06 CARBON ATOM HYDROGENATION INFLUENCE ON GRAPHENE DEPOSITION

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The defect-free graphene by being a two-dimensional hexagonal carbonic crystal lattice with the distance between the nearest atoms of 1.42 Å represents a one-of-a-kind object. At the same time, attachment of additional atoms or molecules to the defect-free graphene changes and extends the properties of a free graphene. A graphene with such additional objects is referred to as functionalized.

This paper discusses a possibility of functionalization of graphene using computer simulation in molecular dynamics approximation by virtue of deposition of carbon atoms with different degree of hydrogenation and hydrogenation influence on deposition probability. We have built computer models of a free carbon atom with different degree of its hydrogenation: methine CH, methylene CH_2, methyl CH_3 and methane CH_4. The computer model of the defect-free graphene of squared shape, which was composed of 112 carbon atoms, was also built by using energy minimization method with Brenner potential. Additionally, we have imposed periodic conditions on boundary atoms of graphene along the structure plane. After damping and thermalization processes we have obtained a two-dimensional hexagonal crystal lattice with distance between nearest neighbor atoms of 1.42 Å and cohesion energy of each carbon atom equal to 7.395 eV. After we have built computer models of the free hydrogenated carbon atoms CH, CH_2, CH_3, CH_4 and defect-free graphene heated up to 300 K, deposition processes of hydrogenated and dehydrogenated carbon atoms with kinetic energies of 1.0, 1.2, 1.5, 2.3 and 3.1 eV on graphene surface were investigated. For the purposes of data set generation a place of vertical fall of the deposited particle on graphene at every deposition energy was assigned 100 times in a random manner. For CH, CH_2, CH_3, CH_4 particles additionally their orientation relative to graphene was assigned in a random manner. It was established that the deposition processes of dehydrogenated and hydrogenated carbon atoms on defect-free graphene are dependent on the degree of carbon atom hydrogenation. It was shown that the more the hydrogenation degree of the carbon atom the smaller its chemisorption probability on graphene. Methane as a fully hydrogenated carbon atom does not undergo chemisorption on graphene at deposition energies from 1 to 3.1 eV. It is also established that in the cases when the deposited particles formed the bound state with graphene, then these particles are situated near the characteristic points: A, B, C and D. Besides, a varying probability exists for bound particle to be situated in these points above the graphene. Point A is one of the graphene atoms, point B is the exact middle between two nearest-neighbor graphene atoms, point C is the hexagonal geometric middle, point D is situated between A and C points. It was shown that the maximum probability of chemisorption of C, CH, CH_2 and CH_3 on graphene should be observed at the energy of their deposition of about 2.3 eV.

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