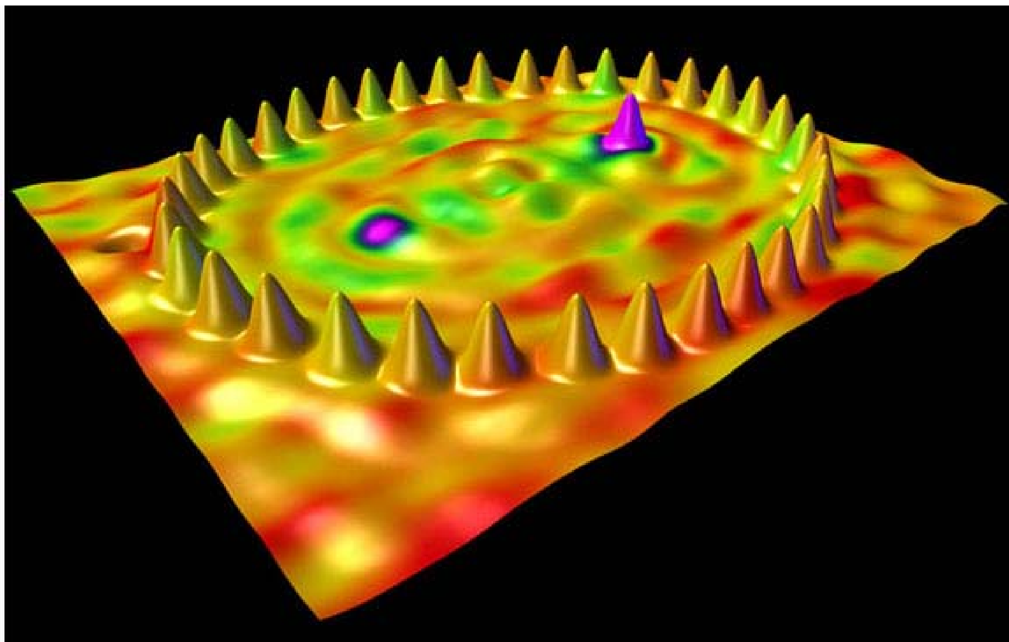
RUSSIAN ACADEMY OF SCIENCES
INSTITUTE OF MICROELECTRONICS AND INFORMATICS
RUSSIAN FOUNDATION FOR BASIC RESEARCH
HELSINKI INSTITUTE OF PHYSICS AND LABORATORY OF PHYSICS
HELSINKI UNIVERSITY OF TECHNOLOGY

**INTERNATIONAL WORKSHOP
ON**

MODERN PROBLEMS IN THE PHYSICS OF SURFACES AND NANOSTRUCTURES



BOOK OF ABSTRACTS

**YAROSLAVL, RUSSIA
18-21 JUNE 2001**

INTERNATIONAL PROGRAM COMMITTEE

T. Ala-Nissila	**Helsinki University of Technology, Helsinki, Finland**
Z. Chvoj	**Institute of physics CAS, Prague, Czech Republic**
F. Buatier de Mongeot	**University of Genova, Genova, Italy**
O. Trushin	**Institute of microelectronics and informatics RAS, Yaroslavl, Russia**

ORGANIZING COMMITTEE

O.S. Trushin	**head of the committee, IMI RAS, Yaroslavl, Russia**
A.E. Berdnikov	**IMI RAS, Yaroslavl, Russia**
V.F. Bochkarev	**IMI RAS, Yaroslavl, Russia**
V.V. Naumov	**IMI RAS, Yaroslavl, Russia**

Contents

Z.Chvoj SURFACE DIFFUSION OF ADSORBATES ON A SURFACE WITH TWO NON-EQUIVALENT ADSORPTION SITES……………… **5**

F.Buatier de Mongeot NANOSTRUCTURING SURFACES BY ION ETCHING AND MULTILAYER HOMOEPITAXY……………………... **6**

Rudakov V.I.ATOMIC MODEL OF THERMODIFFUSION…………… **7**

Zhuravlev I.V., Kibalov D.S., Smirnova G.F., Smirnov V.K. ACTION OF TEMPERATURE ON THE MORPHOLOGY OF THE WAVE-LIKE NANORELIEF ON SILICON SURFACE UNDER NITROGEN ION BOMBARDMENT………………………………………………………… **10**

Amirov I.I., Morozov O.V., Izumov M.O., Dubonos S. STEP FORMATION EFFECT ON THE BOTTOM OF DEEP TRENCH SiO_2 AT THE ETCHING IN HIGH DENSITY FLUOROCARBON PLASMAS……………………………………………………………… **13**

Tapio Ala-Nissila PHASE FIELD MODELS OF WETTING FRONT DYNAMICS……………………………………………………………….. **15**

O. Trushin, P. Salo, M. Alatalo and T. Ala-Nissila NEW MECHANISMS OF CLUSTER DIFFUSION ON METAL FCC(100) SURFACES……………………………………………………………... **16**

M. Karttunen CASE STUDIES OF THE APPLICABILITY AND VALIDITY OF THE DISSIPATIVE PARTICLE DYNAMICS METHOD IN MOLECULAR SIMULATIONS………………………………………. **17**

S.M. Klescheeva, P.V. Paschenko, M.I. Samoilovich, A.F. Belyanin NANOSTRUCTURE OPAL MATRIX-ZnS-3D SOLID STATE PHOTON CRYSTAL………………………………………………………… **18**

E. Kuusela, J. Lahtinen, T. Ala-Nissila, and S. Schwarzer ORIENTATIONAL ORDERING OF SPHEROIDS IN SEDIMENTATION…………………………………………………….. **19**

J.M. Lahtinen, T. Hjelt, T. Ala-Nissila, Z. Chvoj DIFFUSION OF HARD SPHERICAL AND RODLIKE MOLECULES ON SURFACES… **20**

V. V. Kostyuchenko and A. K. Zvezdin FIELD INDUCED PHASE TRANSITIONS IN A PRUSSIAN BLUE ANALOG MAGNET EXHIBITING TWO COMPENSATION TEMPERATURES……………. **21**

V.V. Kostyuchenko STRUCTURE OF THE SURFACE SPIN-FLOP PHASE IN MAGNETIC MULTILAYERS…………………………….. **23**

Kuznetsov V.S., *Prokaznikov A.V. GENERATION-RECOMBINATION INSTABILITY AND PORE FORMATION PROCESSES BY SILICON ANODIZATION IN *HF*………………………….. **25**

M.V. Lokhanin and V. B. Svetovoy MEASUREMENT OF LARGE DISPLACEMENT WITH ANGSTRöM RESOLUTION INTERFEROMETER………………………………………………………… **27**

M.N.Gerasimenko, M.I.Makoviychuk FLICKER NOISE PROCESSES IN ION-IMPLANTED SILICON STRUCTURES: STUDY OF DEFECTS…………………………………………………………………….. **28**

Kononenko O.V., Koval Yu.I., Borzenko T.B., Dubonos S.V., Matveev V.N., Field D.P. SELF-ION ASSISTED DEPOSITION TECHNIQUE FOR PREPARATION OF COPPER METALLIZATION… **31**

V. M. Mordvintsev, S. E. Kudryavtsev CONDITIONS OF SINGLE CONDUCTING NANOSTRUCTURE FORMATION IN AN INSULATING SLIT BY ELECTROFORMING………………………….. **33**

B.Budaguan, M.Meytin, R.Morozov, M.Frolova and A.Berdnikov THE AFM STUDY OF SURFACE MORPHOLOGY OF a-Si:H THIN FILMSPREPARED BY LOW_FREQUENCY PECVD………………….. **35**

Laptev A.N., * Prokaznikov A.V., Rud N.A.AUTO-OSCILLATING PROCESSES BY ADSORPTION IN STRUCTURES ON THE BASE OF POROUS SILICON…………………………………………………………... **36**

V.I.Rudakov, V.V.Ovcharov ANALYTICAL SOLUTION OF THE DIFFUSION EQUATION FOR GAUSSIAN SOURCE AT CONSTANT TEMPERATURE GRADIENT…………………………………………… **37**

Rudakov V.I.ATOMIC MODEL OF THERMODIFFUSION…………… **40**

Kibalov D.S., Smirnova G.F., Zhuravlev I.V., Smirnov V.K.FACTORS AFFECTING THE KINETICS OF THE WAVE-LIKE NANORELIEF FORMATION ON SILICON SURFACE UNDER NITROGEN ION BOMBARDMENT…………………………………………………………… **43**

A. Karim, A. Kara, T. Rahman ADATOM DESCENT FROM 2-DIMENSIONAL AG ISLANDS ON AG(111)…………………………… **45**

O. Trushin, S-C. Ying, E. Granato and T. Ala-Nissila LARGE MISFIT DISLOCATION NUCLEATION IN HETEROEPITAXY………………... **46**

V.F. Bochkarev, V.V. Naumov, A.A. Gorjachev, O.S. Trushin, A.A. Lebedev, A.S. Kunitsin EFFECT OF ION BOMBARDMENT DURING DEPOSITION PROCESS ON PROPERTIES OF NI FILMS….. **47**

A.-P. Hynninen, O. Trushin and T. Ala-Nissila HYPER-MOLECULAR DYNAMICS CALCULATIONS OF DIFFUSION OF A CU ADATOM ON THE CU(111) SURFACE…………………………….. **49**

M. Rusanen, I. Koponen, J. Heinonen, and T. Ala-Nissila STABILITY AND WAVELENGTH SELECTION DURING STEP FLOW GROWTH OF METAL SURFACES VICINAL TO FCC(001)………………………. **50**

B. G. Budaguan, A. A. Sherchenkov, A. E. Berdnikov*, E. I. Artemov THE INVESTIGATION OF HOMOGENEITY OF a-SiC:H THIN FILMS WITH USING OF CHEMICAL INDUCTION MODEL…………………. **51**

P.V. Paschenko, S.M. Klescheeva, M.I. Samoilovich, A.F. Belyanin FABRICATION OF 3D ARRAYS OF MGO NANOCLUSTERS IN UNDERSURFACE LAYERS OF OPAL MATRIX………………………. **53**

Chandana Ghosh, Abdelkader Kara, Talat S. Rahman VERTICAL AND LATERAL MANIPULATION OF ADATOM ON SURFACES…... **54**

Popov A.A., Berdnikov A.E., Chernomordick V.D., Budaguan B.G. SURFACE MORPHOLOGY FORMATION ON A-SI:H, DEPOSITED AT LOW FREQUENCY DISCHARGE…………………………………... **55**

E. Falck, I. Vattulainen, and T. Ala-Nissila MESOSCOPIC SIMULATION STUDIES OF AMPHIPHILIC SYSTEMS………………. **56**

S.A. Krivelevich, M.I. Makoviichuk, Y.I. Denisenko, E.O.Parshin, V.A. Gusev SYNTHESIS OF SILICATE GLASS LAYERS…………….. **57**

Budaguan B.G. Sherchenkov A.A Mazurov A.V.Chernomordick V.D. ELECTROPHYSICAL PROPERTIES OF A-SIC:H/C-SI HETEROJUNCTIONS………………………………………………….. **60**

V.I.Rudakov, V.V.Ovcharov CONCENTRATION PROFILE FOR AN EXTENDED SOURCE OF INFINITE EXTENT AND AN INSTANTANEOUS PLANE SOURCE DURING NON-ISOTHERMAL DIFFUSION…………………………………………………………... **61**

V.I.Rudakov, V.V.Ovcharov,V.P.Babarykina SURFACE SEMICONDUCTOR IRREGULARITIES CONTROL METHOD………. **63**

B.G. Budaguan, A.A. Sherchenkov, V.D. Chernomordik*, A.B. Grabov, A.V. Sizov.**SOLAR CELLS FABRICATED WITH HIGH RATE DEPOSITION METHOD………………………………………….. **66**

Abdelkader Kara and Talat S. Rahman AB INITIO CALCULATIONS OF MULTILAYER RELAXATIONS OF CU(331), CU(511) AND CU(211)}……………………………………………………………... **68**

Kononenko O.V. , Matveev V.N. , Field D.P. THE EFFECT OF LOW ENERGY GRAIN BOUNDARIES ON ELECTROMIGRATION BEHAVIOUR OF MULTIGRAIN ALUMINUM THIN FILM CONDUCTORS………………………………………………………… **69**

M.A. Gosalvez, R.M. Nieminen,P. Kilpinen, E. Haimi, V. Lindroos ANISOTROPIC WET CHEMICAL ETCHING OF CRYSTALLINE SILICON: ATOMISTIC MONTE-CARLO SIMULATIONS AND EXPERIMENTS………………………………………………………… **70**

G.P. Vyatkin, T.P. Privalova, A.E. Chudakov, S.I. Morozov AG AND SN SURFACE PHASES IN COPPER-BASED ALLOYS………………... **71**

S. Majaniemi PROPERTIES OF EFFECTIVE NOISE FOR SYSTEMS WITH QUENCHED RANDOMNESS……………………………………. **73**

P. Salo, M. Alatalo, K. Honkala and K. Laasonen FIRST-PRINCIPLES CALCULATIONS FOR THE CO OXIDATION ON PD(111) SURFACES…………………………………………………………... **74**

SURFACE DIFFUSION OF ADSORBATES ON A SURFACE WITH TWO NON-EQUIVALENT ADSORPTION SITES.

Z.Chvoj

Institute of Physics AVCR, Prague, Czech Republic

The space and time correlation of mass density fluctuations of adsorbed atoms play a decisive role in surface diffusion. Such correlation is determined by both the interaction of atoms and their potential energy on surface, which determine the distribution of atoms on surface. We focus on the interrelation between surface symmetry, formation of ordered phases and diffusion of adsorbed atoms. The surface diffusion coefficient D is calculated for a lattice-gas where diffusion proceeds through two non-equivalent sites, the numbers of which in elementary cell are different. Also different are the energy barriers for individual jumps and the adsorption energy. We studied two basic models, the fcc(100) and fcc(111) surface. Renormalization group formalism is than applied to obtain the phase diagrams of the system with additional lateral interaction δE between adjacent atoms. The phase diagram of the system for the case of repulsive interaction and fcc(100) surface differs considerably from the phase diagram of an ordinary lattice gas with equivalent sites and shows non-monotonic dependence of the critical temperature T_C on adparticle surface coverage Θ. For large values of ΔE, the sites with higher adsorption energy are predominantly occupied and the existence range of the ordered phase shifts to lower Θ. For a square lattice, D exhibits for a particular parameter set a step-like increase at a critical coverage, e.g. Θ_C=0.33 for δE=0 or Θ_C=0.5 for ΔE=0. We correlate the positions of these coverages Θ_C with the corresponding phase diagrams. We also observed the diffusion coefficient to considerably deviate from an Arrhenius behaviour for high differences in the diffusion energy barriers.

On the other hand, on the fcc(111) surface only the local maximum in coverage dependence of collective diffusion coefficient were observed at Θ=0.5. Diffusion slows down if the barrier for deep positions is increased.

NANOSTRUCTURING SURFACES BY ION ETCHING AND MULTILAYER HOMOEPITAXY

F.Buatier de Mongeot
INFM-Unità di Genova and Dipartimento di Fisica, Università di Genova
Via Dodecaneso 33, I-16146 Genova, Italy
e-mail: buatier@fisica.unige.it

Self-organized structures on metal surfaces have been obtained by molecular beam epitaxy (MBE) and ion sputtering. Besides producing equilibrium-oriented patterns similar to those obtained during epitaxy, ion sputtering can also be used to pattern the surface along non-equilibrium orientations. By tuning the competition between erosion and diffusion induced surface re-organisation, it is for example possible to pattern a substrate characterized by square symmetry with a well ordered ripple structure running parallel to the ion beam. Such phenomena have been investigated by several techniques like STM, SPA-LEED and X-Ray diffraction [1], demonstrating that sputter etching is a powerful method which permits the in-situ production of substrates with well defined vertical roughness, lateral periodicity in the nanometer range and with a controlled step size and orientation.

In the case of Molecular Beam Epitaxy it was possible to obtain the growth of well ordered ripples in the multilayer thickness regime, by choosing an anisotropic substrate such as Ag(110). Spot Profile Analysis LEED [1] and Variable Temperature STM indicate that after deposition of 30 ML of Ag at a temperature greater than 210 K a ripple-like surface instability is produced and the ridges of the ripples are found to be parallel to the <1 1 0> direction which is

the thermodynamically favored orientation. Unexpectedly, as the deposition temperature is decreased to 130 K, a 90° switch of the ripple orientation is observed. The ridges of the ripples and the steps are in this case parallel to <100>. In the intermediate temperature range a checkerboard of rectangular mounds results. We interpret our results in terms of the peculiar hierarchy of inter- and intra-layer diffusion barriers present on the anisotropic Ag(110) surface. In general, the nanostructures grown by MBE have a symmetry which is forced by the preferential diffusion directions, so that on a substrate endowed with a square symmetry such as Ag(001) the formation of a checkerboard of square mounds is observed [3].

References

[1] S.Rusponi, G.Costantini, F.Buatier de Mongeot, C.Boragno and U.Valbusa, Appl. Phys. Lett.v.75, p.3318 (1999)

[2] F.Buatier de Mongeot, G.Costantini, C.Boragno and U.Valbusa, Phys. Rev. Lett. v.84, p.2445 (2000)

[3] G. Costantini, F. Buatier de Mongeot, C. Boragno and U. Valbusa, Phys. Rev. Lett. v.86, p.838 (2001)

ATOMIC MODEL OF THERMODIFFUSION

Rudakov V.I.
Institute of Microelectronics and Informatics RAS
Universitetskaya 21, Yaroslavl 150007, Russia

Introduction. A fundamental problem in the case of thermodiffusion in solids is identification of physical meaning of the heat of transport Q^*_{mi} and development of a method for calculating its [1]. One of the approaches to this problem involves adoption of atomic model of diffusion under a temperature gradient and derivation of an expression for Q^*_{mi} on the basis of this model. The

purpose of this work is to obtain the expression for heat of transport in impurity solids with used approach [2].

Model. We shall consider a simple cubic lattice of the dilute substitutional solution in which impurity atom jumps to all the adjacent lattice sites are equiprobable and the probabilities of jumps to other sites is low. We shall assume that the temperature gradient acts along the x axis of the crystal lattice (crystallographic direction [100]) and we shall identify two adjacent planes 1 and 2 (crystallographic planes {100}) perpendicular to the x axis. We have x and $x+\Delta x$ are the coordinates, T and $T+\Delta T$ are the temperatures, c_v and $c_v+\Delta c_v$ are the concentrations of vacancies of the planes 1 and 2, respectively. We shall consider the impurity atom jumps between these planes.

If the impurity atom diffuses by means of vacancy migration then the probability that the atom can jump in adjacent site is equal the probability of finding a vacancy in this site multiplied by the probability that an impurity atom occupies this site. Thus, we can write down the frequency of impurity atom jumps in an adjacent site as

$$\Gamma=\omega_i c_v, \tag{1}$$

where ω_i is the frequency of impurity atom jumps i at an adjacent vacancy and c_v is the concentration of vacancies, expressed in atomic fractions. The frequencies of impurity atom jumps in the planes 1 and 2 are ω_i and $\omega_i+\Delta\omega_i$, respectively. We can represent frequencies of impurity atom jumps moving from the plane 1 to the plane 2 and back as $\Gamma_{12}=(\omega_i+\Delta\omega_i)c_v$ and $\Gamma_{21}=\omega_i(c_v+\Delta c_v)$, respectively. The flux of impurity atoms from the plane 1 to the plane 2 is $J_{12}=c_i\Gamma_{12}$. Similarly, we have $J_{21}=(c_i+\Delta c_i)\Gamma_{21}$, where c_i and $c_i+\Delta c_i$ are the concentration of impurity atoms in the planes 1

and 2, respectively, expressed in atomic fractions. Under steady-state conditions the equality $J_{12} = J_{21}$ is obeyed and the heat of transport of atoms is

$$Q_{mi}^{*} = kT^{2} \frac{\partial}{\partial T}\left(\ln \frac{\omega_i}{c_v} \right). \qquad (2)$$

It is evident from eq.2 that the heat of transport is the energy carried by a jump. This energy is due to a change in the ratio of the frequency ω_i of jumps of an atom to the concentration of vacancies c_v when temperature T is varied. In its turn the ratio ω_i / c_v represents the number of jumps of an atom per one vacancy. The value of this ratio can be used to determine the direction of motion of atoms in a solid under of a temperature gradient. If $\omega_i / c_v > 1$ then $Q_{mi}^{*} > 1$, and atoms move in the direction of lower temperatures. If $\omega_i / c_v = 1$, then $Q_{mi}^{*} = 0$ and an atom moves independently of the temperature gradient direction. If $\omega_i / c_v < 1$, then $Q_{mi}^{*} < 1$ and atoms travel in the direction of higher temperatures. We shall now consider the influence of equilibrium and non-equilibrium vacancies on the processes of heat of transport in impurity solids.

We have for vacancy equilibrium condition

$$Q_{mi}^{*} = E_i^m - E_v^f + E_{vi}^b. \qquad (3)$$

Similarly, we have for deviation from a local equilibrium of vacancies

$$Q_{mi}^{*} = E_i^m - \gamma E_v^f + E_{vi}^b, \qquad (4)$$

where E_i^m, E_v^f and E_{vi}^b are the migration energy of impurity atoms, the vacancy formation energy and the vacancy-impurity binding energy, respectively. A quantity γ is a function of the coordinate x which has to be determined. The values of γ lie between 0 and 1.

Conclusion. The thermodynamic definition of the heat of transport can by given a kinetic explanation. This heat represents the resultant net energy transported by an atom in a jump. Two competing processes contribute to the net energy: one of them is due to a change in the frequency of jumps of the diffusing atoms with temperature and the other is due to a change in the concentration of vacancies with temperature. The value of the ratio of the frequency of the jumps of an atom to vacancy concentration can be used to find the direction of motion of an atom in a crystal in the presence of a temperature gradient. The heat of transport depends on the binding energy of complexes of point defects, in particular, the impurity-vacancy complexes. Therefore the value of the heat of transport can be larger of the value of the atom activation energy. Moreover, the heat of transport depends strongly on the state of vacancies in a crystalline solid. Deviation of vacancies from an equilibrium gives rise to a difference between the heats of transport in single crystals and in polycrystalline samples.

References

1. R.A.Oriani, *J.Phys. Chem. Solids*. 1969. V.40. P.339.
2. V.I.Rudakov, *Sov. Phys. Solid State*. 1992. V.34. P.1965.

ACTION OF TEMPERATURE ON THE MORPHOLOGY OF THE WAVE-LIKE NANORELIEF ON SILICON SURFACE UNDER NITROGEN ION BOMBARDMENT

Zhuravlev I.V., Kibalov D.S., Smirnova G.F., Smirnov V.K.
Institute of Microelectronics and Informatics of RAS, 150051 Yaroslavl, Krasnoborskaya 3, tel (0852) 11-53-46, e-mail: beam@yarteleport.ru

Generation of wave-ordered structure (WOS) as the manifestation of self-formation process on silicon surface under the action of a beam of nitrogen ions is of scientific and practical interest. The accumulation of the body of knowledge in this branch of investigations is an actual problem.

The purpose of carried out experiments was the study of influence of temperature on the development and morphology of WOS for N_2^+-Si system.

Along with the ion energy (E) and angle of ion incidence (θ) the temperature action renders essential influence on the processes of WOS formation on silicon surface under the irradiation with low-energy ions. Dynamic characteristic of WOS formation process is the formation depth of WOS (D_m), and morphology characteristic of WOS formed is the wavelength (λ). From a practical point of view reaching minimum values of λ and D_m is of interest. It is known, that in a O_2^+-Si system sample heating results in the deceleration of WOS formation process and even to full suppression of WOS development. We found that for N_2^+-Si system the increase in sample temperature induces the decrease in λ and D_m. Thus, dependences $D_m(T)$ for systems O_2^+-Si and N_2^+-Si are essentially differ one from another. On the graph of dependence $D_m(T)$ for N_2^+-Si system it is possible to allocate two parts. In an interval of temperatures from room up to 550 K D_m does not depend on sample temperature and is determined only by E and θ. This clearly demonstrates that WOS formation process is stable to a variation of temperature in the specified range. The further heating up to 1000 K results in fall in D_m and λ. Such a behaviour of $D_m(T)$ and the existence of a stable WOS make N_2^+-Si system attractive for reaching minimum λ and D_m.

The action of temperature differs for λ and D_m. For E ranging from 1.6 to 8 keV and θ ranging from 38 to 55? referred to the surface normal our data show that the influence of temperature is reduced with lowering the ion energy and increasing the ion incidence angle. So for a WOS formed at 1000 K by N_2^+ ion beam of 8 keV and θ=38?, both λ and D_m decrease two- and six-fold respectively. At the same time, a WOS formed at 1000 K by N_2^+ ion beam of 1,6 keV and θ=55? does not exhibit any change in λ and D_m under the heating up to 1000 K.

The heat of a sample up to 1000 K results in the shift of the lower boundary of the domain of WOS existence (determined by E and θ) towards smaller angles. Depending on experimental conditions the shift can be of about 10°. At this temperature the wavelength of WOS formed ceases to depend on an angle of ion incidence and is determined only by ion energy.

Temperature acts essentially on the morphology of WOS formed. With a raise of temperature the number of WOS defects is increased. The extension of the waves decreases. The specific feature of the morphology of WOS formed at temperatures exceeding 900 K is found out. WOS formation at E = 8 keV, θ=55° is accompanied by the formation of 30-nm spherical structures on the wave slopes, which are directed backwards to the ion beam. With decrease in the angle of bombardment down to 46° the formations of such structures is not observed.

Thus, it is found out that for a N_2^+-Si system temperature influences on WOS formation dynamics, morphology and wavelength. The sample heating results in the acceleration of WOS growth and reduces the wavelength. Effectiveness of this action is determined by the experimental conditions. With lowering ion energy and increase in ion incidence angle the influence of temperature on the wavelength and WOS formation depth is reduced. The growth of sample temperature affects WOS morphology resulting in the magnification of the number of WOS defects.

This work was performed under the contracts №5-99/7И and №40-2001/7И signed between Institute of Microelectronics and Informatics of RAS and Agency for marketing of scientific products Ltd.

STEP FORMATION EFFECT ON THE BOTTOM OF DEEP TRENCH SiO_2 AT THE ETCHING IN HIGH DENSITY FLUOROCARBON PLASMAS

Amirov I.I., Morozov O.V., Izumov M.O., *Dubonos S.
Institute of microelectronics and information of RAS, Universitetskaya st., Yaroslavl, 15007, Russia, Tel.:+7(0852)116552, Fax: +7(0852)116552, E-mail: ildamirov@chat.ru
***Institute problems of microelectronics of RAS, Chernogolovka, Russia. 142432. Tel.: (095) 9628080. E-mail:dubonos@ipmt-hpm.ac.ru**

Step formation effect on the bottom of deep trench SiO_2 at the etching in high density fluorocarbon C_4F_8+H_2 rf inductive plasmas are presented. This is due to the effect of the ion shadowing near the vertical wall of resist mask are believed. The negligible microstep and microtrench on the bottom of trench at the definite of plasma parameters and experimental conditions are observed.

Etching of deep contact holes and trenches into SiO_2 layer is one of the most frequently and promising processes in the fabrication of integrated circuits. In order to provide the high etching selectivity SiO_2 to Si process perform in a fluorocarbon plasmas. However, in this plasmas arise different negative effects, which make formation ideal vertical feature profile difficult. There are aperture, “stop-etch” effects, and effect of microtrench formation on the edge of bottom trenches [1]. In this study we are show that at the deep trench etching in fluorocarbon plasma not only microtrench but also microstep simultaneously formation are observed. Its generation by ion shadowing are believed.

Experiment carry out in inductive coupled plasmas etcher described in [2]. Briefly, coil (7 lopes) supplied with 2000 W power at 13,56 MHz generated plasma in the discharge camera in the magnetic field of two solenoids. From the discharge camera plasma spread to reactor camera, where on the 30 cm distance from the discharge range the holder of samples is situated. The energy at which ion bombard the substrate is controlled by applying a rf bias power to the holder.

In order to study feature size dependent etching effect we used the samples with two layers mask. Sample consisted of 2μm thick SiO_2 film deposited on a silicon wafer, covered with a 400 nm thick photoresist layer and 50 nm poly-Si. On the poly-Si was deposited layer of electron resist (200 nm). Trench pattern into resist layer created by direct electron writer using REM JEOL 840 and PROXY program. Trench line and space size were 0,2, 0,4, 0,8, 1,6 μm. This pattern was transfer into Si layer and resist layer in fluorine and O_2+Ar plasmas.

The etching of the samples performed in CHF_3+40%H_2 plasma at 0,45 Pa operating pressure, 1500 W inductive power and 125 W rf bias power. At the this conditions self-bias voltage was –75 V. Etch rate of SiO_2 was 0.26 μm/min, selectivity SiO_2 to Si – 25, selectivity SiO_2 to resist – 10. Deep trenches was 1,6 μm. Aperture effect was not observed.

Cross-sectional scanning electron micrograf of samples after exposure to the process showed that on the wall on edges of the bottom trench observed microsteps width 120 nm and high 600 nm. Microsteps of equal size observed on the wall of all trenches 200 – 1600 nm. Besides microsteps in 0.3 μm structure observed and microtrenches.

Microsteps and microternches were and at the –150 V self-bias (Fig.1). They didn't observed at the more ion flux and lower pressure - 0,14 Pa (Fig.2).

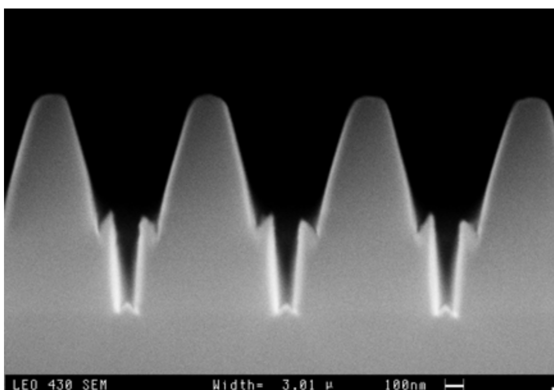


Fig.1

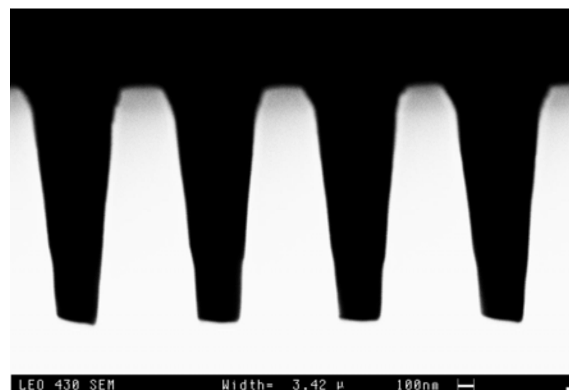


Fig.2

The decreasing etching rate of SiO_2 on the sidewall of the trenches are due to ion-shadowing effect [3]. Because etch rate of trench bottom surface near the corner is controlled ion bombardment the decreasing number of incident ions on sidewall and increasing shadowing of the bottom surface from ion contribute to reduce etch rate. Microstep formation can be explain by fluorocarbon film deposition near sidewall of the trench also.

References

1. Schaepkence M., Oehrlein G.S., Cook J.M. Effect of radio frequency bias on SiO_2 feature etching in inductively coupled fluorocarbon plasmas.//J.Vac.Sci.Technol.2000.V.B.18.P. 848.
2. Amirov I.I., Morozov O.V. SiO_2 film deposition in SiH_4 +O_2 rf inductive low pressure plasma. // Microelectronics. 2000. V.29.N3. C.170.
3. Lee G-R., Cho B-O., Hwang S-W., Moon S.H. Side wall-angle effect on the bottom etch profile in SiO_2 etching using a CF_4 plasma. // J.Vac.Sci.Technol.2001.V.B.19. N1. P. 172

PHASE FIELD MODELS OF WETTING FRONT DYNAMICS

Tapio Ala-Nissila
Helsinki Institute of Physics and Laboratory of Physics,
Helsinki University of Technology, P.O. Box 1100, FIN-02015 HUT,
Espoo, Finland.
E-mail: alanissi@csc.fi

I will describe recent results on the phase-field modeling of the dynamics of wetting fronts. I will concentrate on the dynamics and kinetic roughening of fronts in disordered media. For the dynamics of imbibition fronts driven by capillarity as in the case of paper wetting, I will describe a new model where liquid conservation is taken into account explicitly [1]. This leads to a slowing down of the wetting front as described by Washburn's law, with the emergence of an intrinsic length scale due to the competition between capillary driving and

the conservation of liquid. The kinetic roughening of the front becomes nonlocal, with unusual roughening behaviour. I will also consider the effects of gravity and evaporation [2]. As an extension of the model, I will discuss the dynamics of capillary rise in a 3D system, with disorder along the walls where the liquid rises [3]. Some other applications of the model are also considered.

References

1. M. Dube, M. Rost, K. R. Elder, M. Alava, S. Majaniemi and T. Ala-Nissila, Phys. Rev. Lett. v83, p.1628 (1999); Eur. Phys. J. B v15, p.701 (2000)
2. M. Dube et al., to be published
3. M. Kuittu et al., unpublished.

NEW MECHANISMS OF CLUSTER DIFFUSION ON METAL FCC(100) SURFACES

O. Trushin[1], P. Salo[2], M. Alatalo[2] and T. Ala-Nissila[2]
[1]Institute of microelectronics and information of RAS, Universitetskaya st. 21, Yaroslavl, 15007, Russia, Tel.:+7(0852)116552, Fax: +7(0852)116552
[2]Helsinki Institute of Physics and Laboratory of Physics,
Helsinki University of Technology,
P.O. Box 1100, FIN-02015 HUT, Finland
email ole@fyslab.hut.fi

We have studied atomic mechanisms of small clusters diffusion on the fcc(001) metal surfaces using semi-empirical and ab-initio molecular static calculations. Primary goal of these studies was to investigate possible many-body mechanisms of cluster motion which can contribute to low temperature crystal growth. We used EAM [1] and Glue [2] potentials in semi-empirical simulations of Cu and Al. Combination of Nudged Elastic Band [3] and Eigenvector Following [4] methods allowed us to find all the possible transition paths for cluster movements on flat terrace. In case of Cu(001) we have found several new mechanisms for diffusion of clusters, including mechanisms called

row-shearing and dimer-rotating in which a whole row inside an island moves according to a concerted jump and a dimer rotates at the periphery of an island, respectively. In some cases these mechanisms yield a lower energy barrier than the standard mechanisms [5].

References

1. S. M. Foiles, M. I. Baskes, and M. S. Daw, Phys. Rev. B v33, p.7983 (1986).
2. F. Ercolessi and J.B. Adams, Europhys.Lett. v26, pp. 583-588 (1994).
3. H. Jonsson, G. Mills and K. W. Jacobsen in "Classical and Quantum Dynamics in Condensed Phase Simulations", ed. by B. J. Berne, G. Ciccotti, and D. F. Coker (World Scientific, Singapore, 1998).
4. L. J. Munro and D. J. Wales, Phys. Rev. B v59, p.3969 (1999), and Referencess therein.
5. O. S. Trushin, P. Salo, T. Ala-Nissila, Phys. Rev. B ,v62, p.1611 (2000).

CASE STUDIES OF THE APPLICABILITY AND VALIDITY OF THE DISSIPATIVE PARTICLE DYNAMICS METHOD IN MOLECULAR SIMULATIONS

Mikko Karttunen
Biophysics and Statistical Mechanics Group
Laboratory of Computational Engineering
Helsinki University of Technology, Finland
Email: mikko.karttunen@hut.fi

Dissipative Particle Dynamics (DPD) is a mesoscopic simulation technique particularly well suited for studies of soft condensed matter systems. It is characterized by coarse-graining in particle representation, which leads to a simplified description of interparticle interactions in terms of conservative, dissipative, and random forces. This formulation leads to momentum conservation, which implies that hydrodynamic flow effects are properly taken into account. However, it has been observed recently that, due to the presence of stochastic and velocity-dependent dissipative forces, integration schemes

often used in molecular dynamics simulations may give rise to artifacts when applied as such in DPD simulations.

We assess the quality of various integrators through DPD model studies for a number of physical observables such as temperature, radial distribution function, compressibility, and tracer diffusion. Our results show that certain integration schemes may indeed lead to pronounced artifacts in often studied physical observables such as response functions and transport coefficients. Clearly, this fact may constitute a serious problem for large-scale studies of soft systems via DPD. However, we demonstrate that such artifacts can be sufficiently suppressed by using schemes in which the velocity dependence of the dissipative forces is taken into account.

Finally, we discuss the applicability of the DPD method in lipid bilayer simulations and the possibility of combining DPD with classical molecular dynamics via systematic coarse-graining.

NANOSTRUCTURE OPAL MATRIX-ZnS-3D SOLID STATE PHOTON CRYSTAL

S.M. Klescheeva[1], P.V. Paschenko[1], M.I. Samoilovich[2], A.F. Belyanin[1]
[1]Central research technological institute "TECHNOMASH",
Iv. Franko str. 4, Moscow 121108, Russia,
Tel. (095) 146-10-95
[2]AOZT "Almaztechnocrystal" , Fabrika Kalinina str. 14a,
Alexandrov, Vladimir region, Russia,
Tel. (095) 584-58-19

We developed the method for fabrication of highly ordered arrays of single crystal particles of SiO_2 , analogous to natural opal matrix. At sizes of SiO_2 particles of 200-600 nm, such arrays contain structural empty zones with sizes of 60-200 nm, which partially filled by different materials. It allows to create new type of materials – 3D superstructures, including so-called "photon crystals". Photon crystals represent new class of materials for applications in

micro- and optoelectronics, which properties being determined by periodic changing of dielectric constant (ε). It leads at definite conditions (for example in ideal cubic structures) to creation of photonic zones and finally to prohibited zones in the inverse space.

Deposition of ZnS was performed by magnetron RF-sputtering of powder ZnS target in Ar plasma. We consider different variants of the design of experimental set-up for ZnS deposition. Experimental conditions for the deposition were as follows: Ar pressure of 0.5-2 Pa, RF discharge voltage of 300-650 V, RF discharge power of 40-100 W, temperature of opal matrix of 373-473 K.

We studied the effect of the change of Ar pressure and RF discharge power on the depth of ZnS penetration inside opal matrix, and also on the extent of crystal ordering, crystal structure and electric properties of as-deposited Zn-S.

ORIENTATIONAL ORDERING OF SPHEROIDS IN SEDIMENTATION

E. Kuusela[1], J. Lahtinen[1], T. Ala-Nissila[1,2], and S. Schwarzer[3]
[1]Helsinki Institute of Physics and Laboratory of Physics, Helsinki University of Technology, P.O. Box 1100, FIN--02015 HUT, Espoo, Finland
[2]Department of Physics, Brown University, Providence, R.I. 02912--1843, U.S.A.
[3]Institute for Computer Applications I, Stuttgart University, Pfaffenwaldring 27, 70569 Stuttgart, Germany. email ehk@hugo.hut.fi

We study the sedimentation of non-Brownian spheroids using a computational model that is based on the immersed-boundary method[1]. In small but non-zero Reynolds numbers we observe a change in the orientation distribution when the particle density is increased. In the dilute systems the spheroids favors horizontal alignment but tends to orientate vertically when the volume fraction is increased. In the case of very small Reynolds number, the

tendency for vertical alignment during sedimentation has been observed in the experiments by B. Herzhaft and E. Guazzelli [2] as well as in numerical simulations by M. Mackaplow and E. Shaqfeh [3].

We show also the effect of aspect ratio and Reynolds number on the orientation distribution and examine the importance of the orientation distribution as the explanation to the non-monotonic behaviour of mean settling speed.

References

1. K. Hofler, and S. Schwarzer, Phys.Rev. E, v.61 (2000), p.7146.

2. B. Herzhaft, and E. Guazzelli, J. Fluid Mech v.384 (1999) p.133.

3. M. Mackaplow, and E. Shaqfeh, J. Fluid Mech v.376 (1998) p.149.

DIFFUSION OF HARD SPHERICAL AND RODLIKE MOLECULES ON SURFACES

J.M. Lahtinen[1], T. Hjelt[1], T. Ala-Nissila[1,2], Z. Chvoj[3]
[1] Helsinki Institute of Physics and Laboratory of Physics Helsinki University of technology, Espoo, Finland.
[2] Brown University, Dept of Physics, Providence, RI
[3] Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic

We have studied the diffusion and spreading of hard spherical and rigid rodlike molecules on surfaces using Molecular Dynamics simulations. The molecules are interacting via a repulsive $1/r^{12}$ potential and the surface is taken to be smooth and structureless. We compute the behaviour of the tracer and collective diffusion coefficients $D_T(\rho)$ and $D_C(\rho)$, respectively, as a function of the density ρ. [1]

For the case of hard spherical particles we have compared the existing analytic theories for the compressibility with numerical simulations, and calculated the mobility numerically to obtain $D_C(\rho)$. We also used the mode

coupling approximation [2] to estimate $D_T(\rho)$ self-consistently. In the case of rods we have also evaluated the rotational diffusion coefficient.

References

[1] J. M. Lahtinen, T. Hjelt and T. Ala-Nissila, Surf. Sci. v. 454-456, p.598 (2000).

[2] A. V. Indrani and S. Ramaswamy, Phys. Rev. Lett. v.73, p.360 (1994).

FIELD INDUCED PHASE TRANSITIONS IN A PRUSSIAN BLUE ANALOG MAGNET EXHIBITING TWO COMPENSATION TEMPERATURES.

V. V. Kostyuchenko[1] and A. K. Zvezdin[2]
1 Institute of Microelectronics and Informatics, Russian Academy of Sciences, Universitetskaya 21, Yaroslavl, 150007, Russia
2 Institute of General physics, Russian Academy of Sciences, Vavilov 38, Moscow, 117942, Russia

L. Neel for the first time established the possibility of existence of the compensation point in 1948. By the present time a large number of various ferrimagnetic compounds with compensation points was experimentally investigated. There are many theoretical studies of ferrimagnets with compensation point too (see e.g. [1] and References therein). But as late as 1999 the compounds with two compensation points were found [2]. The prototypes of these materials are Prussian blue analogs [3, 4]. The Prussian blue analogs are very sensitive to the acting of various factors (temperature, light etc.). It makes them a very promise compounds for applications. But field-induced transitions in these compounds have not been studied. This is the subject of present work. It is considered four-sublattice ferrimagnets with the formula $(Ni_{x2}Mn_{x3}Fe_{x4})_{1.5}[Cr(CN)_6]$ zH_2O and $x_2+x_3+x_4=1$. Among these compounds don't all have a two compensation points, but the possibility of theoretical prediction of their properties are very helpful. The ease of theoretical predictions of magnetic properties is based on two assumptions [2, 4]. At first, only

exchange interactions between nearest neighbors are taking into account, and, at second, the character of such interaction is known. It makes possible the prediction of magnetic properties of these materials on the base of molecular field theory [2, 4]. According to the molecular field method the interaction between spins is approximated by the effective magnetic fields. As far as the exchange interaction between sublattices is greater than exchange interaction within sublattices the necessary condition of molecular field applicability is satisfied. In present work we extended this model to have an opportunity of noncollinear phase investigation. In present work the field-induced phase transitions in a blue Pruss analogs with two compensation temperatures are theoretically investigated. The strong dependence of compensation temperatures from chemical compound are established. The H-T phase diagram for compounds with two compensation points are presented. As expected the value of critical field for transition from collinear to angle phase is tends to zero near the compensation points. The magnetization of some compounds is very small in the temperature region between two compensation points. As far as we know this phenomenon have not observed earlier. This work was supported by Ministry of Industry, Science, and Technology Grant No. 204-13(00), Russian Fund Basic Research grant N 99-02-17830, and INTAS grant N 97-705.

References

[1] A. K. Zvezdin, in K. H. J. Buschow, ed., Handbook of magnetic materials (Elsevier Science, 1995), vol. 9, p. 405.

[2] S. Ohkoshi, Y. Abe, A. Fujishima, and K. Hashimoto, Phys. Rev. Lett. 82, (1999), p. 1285.

[3] A. Ludi and H. U. Geudel, in J. D. Dunitz, P. Hemmerich, J. A. Ibers, C. K. Jorgensen, J. B. Neilands, R. S. Neiholm, and R. J. P. W. D. Reinen, eds., Structure and Bonding (Springer-Verlag, Berlin, Heidelberg, New York, 1973), vol. 14, p. 1.

[4] S. Ohkoshi, T. Iyoda, A. Fujishima, and K. Hashimoto, Phys. Rev. B 56, (1997), p. 11642.

STRUCTURE OF THE SURFACE SPIN-FLOP PHASE IN MAGNETIC MULTILAYERS

V.V. Kostyuchenko
Institute of Microelectronics and Informatics,
Universitetskaya 21, Yaroslavl, 150007, Russia.

The influence of the surface on phase transitions is an important problem of physics of magnetism. The existence of surface spin-flop transition was theoretically predicted in 1967 [1] (see also [2]). But for a long time it was impossible to gain experimental verification of this prediction due to the technological problems. For the first time the surface spin-flop transition has been found experimentally in Fe=Cr magnetic superlattices [3]. It simulates the further theoretical [4--10] and experimental [11] investigations in this field. It is common knowledge that at bulk spin-flop transition an external magnetic field induces the transition from antiferromagnetic phase to angle phase over all volume. At surface spin-flop transition the changing of magnetization orientation is localized near the surface. For magnetic superlattices with even layers number the critical field of surface spin-flop transition is significantly lower than the critical field of bulk spin-flop transition. Thus the existence of surface spin-flop transition has effect on phase diagrams of magnetic superlattices and respectively on their magnetoresistive characteristics. So it is important not only for fundamental science but for practical applications as well. The changing of surface spin-flop phase structure under the changing of anisotropy energy is investigated in present paper. The surface spin-flop phase can be treated as inhomogeneous state such that domain wall separates the spin-flop phase near the surface from antiferromagnet phase in bulk. The characteristics of this domain wall have not been considered before. In present work the dependence of wall width and coordinate of wall center are investigated. It is shown that the dependence of wall width on anisotropy energy has unusual for magnetic materials linear character. The dependence of

coordinate of wall center has stepwise character due to the Peierls-Nabarro barrier. This work was supported by Ministry of Industry, Science, and Technology Grant No. 204-13(00).

Refernce

[1] D. L. Mills, Phys. Rev. Lett. v.20 (1968) p.18.

[2] F. Keffer, H. Chow, Phys. Rev. Lett. v.31 (1973) p.1061.

[3] R. W. Wang, D. L. Mills, E. E. Fullerton, J. E. Mattson, S. D. Bader, Phys. Rev. Lett. v.72 (1994) p.920.

[4] R. W. Wang, D. L. Mills, Phys. Rev. B v.50 (1994) p.3931.

[5] N. S. Almeida, D. L. Mills, Phys. Rev. B v.52 (1995) p.13504.

[6] L. Trallori, P. Politi, A. Rettori, M. G. Pini, J. Villain, Phys. Rev. Lett. v.72 (1994) p.1925.

[7] L. Trallori, P. Politi, A. Rettori, M. G. Pini, J. Villain, J. Phys.: Cond. Mat. v.7 (1995) p.L451.

[8] N. Papanicolaou, J. Phys.: Cond. Mat. v.10 (1998) p.L131.

[9] L. Trallori, Phys. Rev. B v.57 (1998) p.5923.

[10] C. Micheletti, R. B. Griffiths, J. M. Yeomans, Phys. Rev. B v.59 (1999) p.6239.

[11] S. L. Gnatchenko, A. B. Chizhik, D. N. Merenkov, V. V. Eremenko, H. Szymczak, R. Szymczak, K. Fronc, R. Zuberek, J. Magn. Magn. Mater. v.186 (1998) p.139.

GENERATION-RECOMBINATION INSTABILITY AND PORE FORMATION PROCESSES BY SILICON ANODIZATION IN *HF*

Kuznetsov V.S., *Prokaznikov A.V.
Yaroslavl State University named after P.G. Demidov, 150000, Yaroslavl, Sovetskaya, 14, vk@univ.uniyar.ac.ru
***Institute of Microelectronics and Informatics RAS, 150007, Yaroslavl, Universitetskaya, 21, prok@univ.uniyar.ac.ru**

Porous silicon attracts an interest either from scientific or practical point of view. During silicon anodization in hydrofluoric acid solution the processes of self-organization take place that are characterized by complex *I-V* characteristic. A number of publications on porous silicon are devoted to the investigations of properties of this material and in last time some works were published about pore formation mechanism. In our work [1] on the base of general approach the theoretical model of the processes, that describe the pore formation phenomenon, was considered. We suppose that the electrolyte/semiconductor system is united, non-linear one, the multistage processes in which cause the temporal and spatial self-organization in charge transfer processes and anodization. There were considered the processes of generation and recombination of charge carriers in silicon at strong electric field as well as chemical reactions on the electrolyte/silicon border.

In this work the idea is put forward concerning explanation of part of peculiarities in behaviour for complex interacting system: electrolyte/border/semiconductor in the presence of current and illumination by collective processes in space charge region (SCR) near the surface. At a strong field in SCR the generation-recombination instability, bistability, threestability of homogeneous stable states of charge carriers, the phenomena of threshold switching, the current filament formation can take place. SCR region is considered for the n-type semiconductor with donor type recombination and capture centers (the nature of which is not defined: it can be dislocations, vacancies, dopant atoms with deep levels *etc*.) under applied electric field which

attracts free holes to the surface. The conditions of bistability, threestability of homogeneous stable states are analyzed as well as the stability of these stages. The influence of positive charge in SCR is investigated. In the region of low electric field one state of charge carrier is stable. Creation of two or three stable states can take place by increasing of electric field strength and illumination. The stability of these stages depends on electric field strength and illumination. Theoretical model considered make it possible to explain a complex behaviour of *I-V* characteristic, which consists of different regions, what is caused by influence of different mechanisms depending on system parameters. The current filament formation can take place in space charge region at avalanche breakdown. As a consequence the silicon oxidation and following etching in hydrofluoric acid will occur more intensive in the regions of current filament localization near the surface. It should be mentioned here that filament localization can be connected with defects in SCR: dislocations, vacancies, dopant atoms, surface profile *etc*. Because the electric field in SCR is not homogeneous, the electric field strength is maximal near the surface. The avalanche breakdown near the surface begins earlier than in space charge region. It can explain formation of two scales of pores (micro- and macropores).

References

[1] Kuznetsov V.S., Prokaznikov A.V. Investigared in Russia, 1991, N 1,
http://zhurnal.ape.relarn/articles/1999/027.pdf

MEASUREMENT OF LARGE DISPLACEMENT WITH ANGSTRöM RESOLUTION INTERFEROMETER

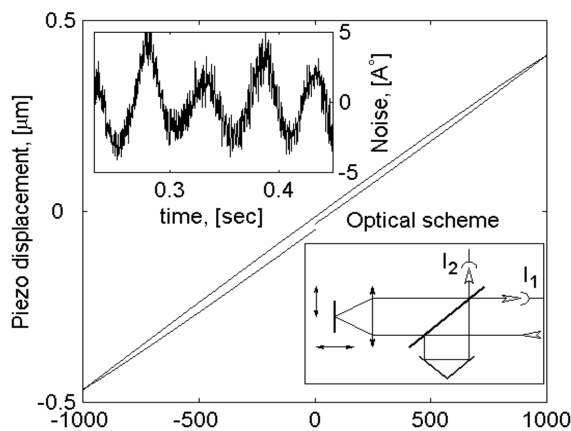
M.V. Lokhanin and V. B. Svetovoy
Institute of Microelectronics, RAS

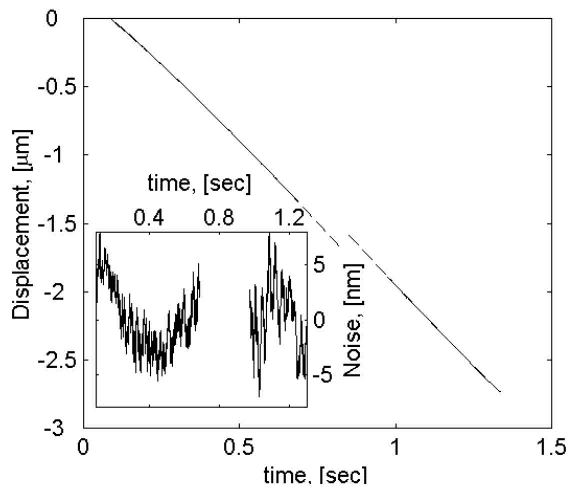
The necessity to register small deviations against a background of large displacement appears in many physical problems. The best solution is the Michelson-type interferometer with a computer on-line. In the device the beamsplitter introduces the phase shift between the References and measurement arms (see the bottom onset in Fig. 1). The output signal of photodiods can be written as follows:

$$I_1 = A_1 + B_1 \cos\xi, \quad I_2 = A_2 + B_2 \cos(\xi + \varphi), \quad \xi(t) = 4\pi x(t) / \lambda. \qquad (1)$$

Here $x(t)$ is the displacement, λ is the laser wavelength, A_1, A_2, B_1, B_2, φ are the parameters which can drift slowly compared with $\xi(t)$ due to variation of optical properties of investigated surface. In the plane I_1 - I_2 the signal is wound around the current ellipse. The movement low $x(t)$ can be restored choosing the time buffer of sufficient length $t_m : t_{m+n}$ and fitting the signals using (1) to find the current ellipse parameters.

This technique was used to register movement of bimorphous piezo and to measure the thickness of deposited step-like layer. Fig. 1 shows the hysteresis loop of the piezo with overall displacement along the laser beam of about 0.8 μm. The movement was fitted with cubic polynomial. The difference between the fit and restored displacement is shown in the top onset. The rms noise is estimated as 3 Å but it can be reduced further to 0.7 Å by filtering the low-frequency noise. Significantly larger noise (3 nm) has been found when the beam scanned the surface to detect the deposited film. The results are shown in Fig. 2.





. Figure 1 Figure 2

The substrate displacement above and below the transition region has been restored. The step height of 156 nm was found by extrapolation to the transition region. The noise is mostly due to vibration of the transducer.

FLICKER NOISE PROCESSES IN ION-IMPLANTED SILICON STRUCTURES: STUDY OF DEFECTS.

M.N.Gerasimenko[1) , M.I.Makoviychuk[2)

[1)Moscow Institute of Electronics Engineering, 103408 Moscow, Zelenograd, K-498, RUSSIA.

E-mail: nik@techcen.zgrad.su

[2)Institute of Microelectronics & Informatics, Russian Academy of Sciences, Universistetskaya str., 21, Yaroslavl, 150007, Russian Federation

The special place among new electrophysical methods takes a method of a joint control of a sheet resistance and flicker-noise characteristics of researched semiconductor structures.

The high sensitivity of flicker current fluctuations to structural defects and high selfdescriptiveness of results, obtained on the basis of flicker -noise measurements, have allowed to offer and experimentally to realize a new research method for diagnostics the structure disordered semiconductors - flicker -noise spectroscopy (FNS).

Instrument implementation of a method of a sheet resistance measurement ρ_s and its spectral density of fluctuations $S_{\rho_s}(f)$ on Si wafer is realized by a two-combinative four-point probe method (TCFPPM), random error of which much below than error a conventional four-point probe method. TCFPPM much simplifies the procedure of measurements, as the registration of the geometrical factor does not require definition the coordinates of probes position on a surface of a sample. This advantage of a method has allowed to create on its basis an automated complex (AMC) for a control of ρ_s, $S_{\rho_s}(f)$ and their distribution over a surface of a wafer.

The power spectral analysis was done in the frequency range 10 Hz – 20 kHz.

We express the flicker noise intensity as a parameter α defined by relation due to Hooge, which we write in the form :

$$S(f) \equiv \frac{S_R(f)}{R^2} = \frac{\alpha}{f^{\gamma} N}, \quad 0.8 < \gamma < 1.2 \qquad (1)$$

Here R is the resistance of a homogeneous silicon sample that fluctuates with a spectral power density $S_R(f)$, N is the total number of electrons, f is the frequency.

In order to compare experimental and theoretical results, we shall express the flicker noise of ion-implanted sample as a parameter β_s, defined by the relation:

$$\beta_s(f) = \frac{S(f) WL}{q\rho_s} \qquad (2)$$

where q is the electron charge, L and W are the length and width of the sample respectively.

(1) Dependence on the implantation dose.

Maximum on doze dependence of spectral density of fluctuations $S(\Phi)$ is experimentally detected at a doze $\Phi = 5\times10^{14}$ cm^{-2} for silicon, implanted by ions of an argon. Comparing experimental results (on measurement of a signal EPR) about accumulation of defects in layers $^{40}Ar^{+}/Si$ with obtained results, it is

possible to assume, that the observable maximum at $\Phi=5\times10^{14}$ cm^{-2} is stipulated by presence in a layer of defects as tetravacancies, amount of which at this doze is maximum. At further increase of a doze ($\Phi>5\times10^{14}$ cm^{-2}) concentration of tetravacancies the gradually decreases, and at $\Phi>1\times10^{15}$ cm^{-2} intensive growth of concentration of noise centers, identified as VV-centers is observed.

Presence of four regions of slow and fast accumulation of radiation damages is determined on dependence S (Φ) for boron implanted silicon ($^{11}B^+$/Si) in a range Φ from 5×10^{10} cm^{-2} up to 1×10^{16} cm^{-2} . The nonmonotone character of change S(Φ) testifies to presence in a $^{11}B^+$/Si layer of different type defects, the structure and amount of which varies with rise of Φ. At an isochronous annealing of $^{11}B^+$/Si layers regions of slow accumulation are annealed more actively, than regions of fast accumulation of defects. On an initial region I (range of dozes $\Phi = 5\times10^{10} \div 5\times10^{11}$ cm^{-2}) the ion implantation process is accompanied by accumulation of point defects, which are annealed completely at T=600 °C. On regions II-IV (5×10^{11} cm^{-2} < Φ < 1×10^{16} cm^{-2}) it is possible to select at least defects of three types, the structure of which much becomes complicated with rise of Φ.

(2) Dependence on implantation energy.

The form of dependence β(E) indicates presence in ion-doped layer ($^{11}B^+$/Si: $\Phi_1=8\times10^{12}$ cm^{-2} , $\Phi_2=8\times10^{13}$ cm^{-2} for energy range $20\le E\le 200$ keV) two sources of a flicker-noise:

(i) the surface noise source predominate for $20\le E\le 100$ keV;

(ii) the bulk noise source — for $E\ge 100$ keV.

The similar results are obtained for ion-implanted layers $^{27}Al^+$/Si: $\Phi_1=1\times10^{13}$ cm^{-2} , $\Phi_2=1\times10^{14}$ cm^{-2} , $\Phi_3=1\times10^{15}$ cm^{-2} for a large range of implantation energies $10\le E\le 500$ keV.

(3) Dependence on ion-beam current density

The range of ion-beam current density is somewhat limited, 0.08-4 μA/cm^2. The sharp increase of a noise level with rise j_b is explained by rise of speed of point defect generation. Implantation at high beam current density causes two competing effects (i) sample heating, which will lead to partial annealing of radiation damage and (ii) higher defect densities.

The significance of the received results consists in development of a system approach to the problems of fluctuation analysis, enveloping all stages of the ion-doped structures creation and permitting to realize an operating feedback between parameters of quality and technological conditions. We consider the perspectives of the fluctuation analysis for nondestructive test purposes (method of flicker noise spectroscopy), path of its perfecting for obtaining complete information about quality of semiconductor structures in microelectronics.

SELF-ION ASSISTED DEPOSITION TECHNIQUE FOR PREPARATION OF COPPER METALLIZATION

Kononenko O.V. †, Koval' Yu.I., Borzenko T.B., Dubonos S.V., Matveev V.N. †, Field D.P. ‡
† Institute of Microelectronics Technology and High Purity Materials, RAS, 143432 Chernogolovka, Moscow district, Russian Federation.
E-mail: oleg@ipmt-hpm.ac.ru
‡ School of Mechanical and Materials Engineering, Washington State University, Pullman, WA 99164-2920 USA.

Copper films were deposited onto oxidized silicon wafers by the partially ionized deposition technique [1]. A 0 or 6 kV bias was applied to the substrate during deposition. The films were patterned into parallel line arrays of 20 lines of 0.5 mm length and 0.8 μm width, using electron lithography and dry etching. After patterning, the lines were covered by silicon oxide and annealed in vacuum for 1 hour at 450°C. Electromigration testing was performed in air in the temperature range from 280° to 350°C and at the current density 3×10^6

A/cm^2. Resistivities of the films deposited at the 6 kV bias and without bias were 1.7 and 2.0 μΩ·cm, respectively. Median times to failure were 400 and 240 hours for 6 and 0 kV lines, respectively.

Microstructural analysis of the copper films was performed by orientation imaging microscopy. Inherent in the imaging technique is complete crystallographic information which describes texture and microtexture including grain boundary structure as defined by crystallite lattice orientation on either side of the grain boundary plane. The through thickness tilt of the boundary is unknown, but is assumed to be normal to the specimen surface in this investigation.

Metallization of trenches and vias with small feature sizes and high aspect ratios processed in a polyaimide layer was prepared by the partially ionized deposition technique at the different bias conditions. It was found that trenches and vias can be filled with void-free copper after copper deposition at the high bias.

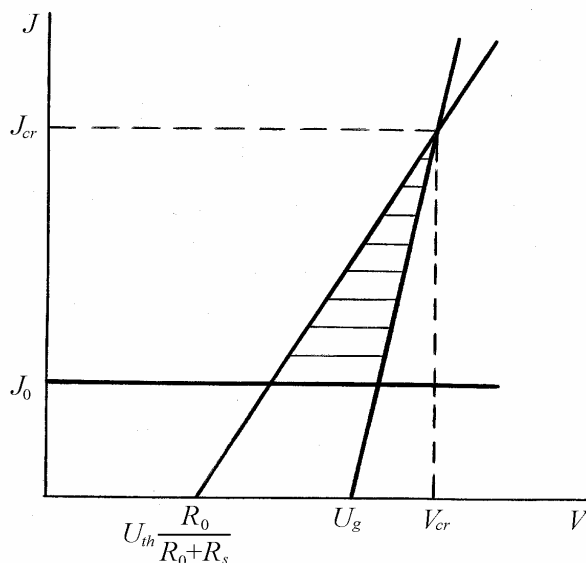
References

1. Kononenko O.V., Matveev V.N., Kasumov A.Yu., Kislov N.A. and Khodos I.I. The effect of self-ion bombardment on the properties of thin metal films. Vacuum **46** (1995) 685.

CONDITIONS OF SINGLE CONDUCTING NANOSTRUCTURE FORMATION IN AN INSULATING SLIT BY ELECTROFORMING

V. M. Mordvintsev, S. E. Kudryavtsev
Institute of Microelectronics and Informatics of RAS. 21 Universitetskaya st. Yaroslavl Russia 150007. Tel/fax 0852-11-53-53. E-mail: mvm@imras.yar.ru

On the basis of analysis of many results earlier was established [1], that the electroforming can be considered as a self-forming process of an insulating gap having essentially nanometer width in the carbonaceous conductive medium being originated in an open insulating slit between metal electrodes of structure metal-insulator-metal (MIM). The carbonaceous medium is derived from external organic matter (from a gas phase or from a film, for example of photoresist, marked on structure), which conductivity varies because of organic molecules destruction at electron impact as a result of a current passing through it. Experiments on the electroforming in opened "sandwich" structures Al-Al_2O_3-W with oxide thickness 20 - 40 нм (it defines an insulating slit width) have shown [2], that in defined conditions, in particular at presence of high "ballast" resistance R_b series MIM-structure, the formation of a carbonaceous conducting medium happens only in one place of perimeter of the opened dielectric film butt-end on length compared to width of an insulating slit. It has allowed to speak about origin of a single conducting nanostructure.



The research of electroforming in opened "sandwich" structures Si-SiO_2-W has shown, that the formation of single conducting nanostructures in them is complicated, the carbonaceous conducting medium

arises more often on many sites of perimeter at once. Basic factors leading to such result, are high material specific resistance of a silicon electrode, that means appearance of noticeable local resistance R_s series originating nanostructure, and presence of significant initial conductivity on a surface of an insulating slit (appropriate resistance - R_0).

The simple model of a process of the electroforming in terms of the equivalent electrical circuit taking into account balance of the factors both promoting to and precluding from to forming of a single conducting nanostructure is constructed. The results of simulation are shown in the figure as the diagram in coordinates current J through MIM-structure - voltage V of power supplies, on which the area of existence of a single conducting element is shaded. The slope of straight lines bounding this area at the right is equal $1/R_b$, and at the left is

$$\frac{1}{R_b + \dfrac{R_s R_0}{R_s + R_0}}.$$

The value of $J_0 = U_g/R_0$, where U_g is voltage of a conducting nanostructure origin, which is easily defined experimentally on a current jump at a smooth voltage growth. U_{th} is a threshold voltage of a beginning of a carbonaceous conducting medium formation from organic molecules. It is defined by a process of destruction of molecules at electronic impact and lies about 3 V.

The maximum size, up to which the nanostructure can grow remaining single, defines its minimum resistance r_{cr}, appropriate to critical point of intersection of straight lines on the diagram:

$$r_{cr} = \frac{U_{th} + U_g \dfrac{R_s}{R_0}}{U_g - U_{th}} R_s .$$

References

1. Valiev K. A., Levin V. L., Mordvintsev V. M. Z. Tek. Fiz. 1997. V. 67. №11. P. 39-44.

2. Mordvintsev V. M., Kudryavtsev S. E., Levin V. L. Russian Microelectronics. 1998. V. 27. № 1. P. 40-46.

THE AFM STUDY OF SURFACE MORPHOLOGY OF a-Si:H THIN FILMSPREPARED BY LOW_FREQUENCY PECVD

B.Budaguan[1], M.Meytin[1], R.Morozov[1], M.Frolova[1] and A.Berdnikov[2]
[1]Depatment of Materials Science and Physical Chemistry, Moscow Institute of Electronic Technology, Moscow 103498 Russia,
[2]Institute of microelectronics of RAS, Yaroslavl 150007 Russia

We observed that the films surface have the complex structure consisting of islands of different size, and their average size and surface allocation significantly varies from sample to sample. With help of special software acquired data was preprocessed by convolution-based filtering to omit influence of different image defects and then island diameters was measured. The histograms of diameter distribution were approximated using log-normal distribution and average diameter was recalculated to take into consideration the distribution specifics.

Comparing our results with IR spectroscopy data we found that the dependencies of islands average diameter and hydrogen content on substrate temperature have the similar behaviour with temperature changes. These dependencies have maximum at T_s=170 °C. Thus, in our case the a-Si:H surface morphology was controlled by hydrogen content. According to the proposed model the increase of hydrogen content, N_H, up to T_s=170 °C is connected with ion treatment of the growing surface in LF plasma, while N_H decrease is controlled by the hydrogen effusion at T_s>170 °C.

AUTO-OSCILLATING PROCESSES BY ADSORPTION IN STRUCTURES ON THE BASE OF POROUS SILICON

Laptev A.N., * Prokaznikov A.V., Rud N.A.
Yaroslavl State University named after P.G. Demidov, 150000, Yaroslavl, Sovetskaya, 14, rud@univ.uniyar.ac.ru
Institute of Microelectronics and Informatics RAS, 150007, Yaroslavl, Universitetskaya, 21, prok@univ.uniyar.ac.ru

In the present time a particular interest is expressed in investigations of low-dimensional structures, which exhibit a number of unusual properties. These properties are not inherent to an initial semiconductor material. In low-dimensional structures the contribution of surface effects increases, that enhances theirs influence on the background of the processes in the bulk of the nanocrystallites. All that make it possible to observe a number of new, unusual phenomena. Porous silicon, which is obtained by anodization of silicon wafers in hydrofluoric acid solutions, is one of such substances, which contains objects with low dimension.

In this work on the base of investigations of specially created structures *Me-porSi-Si-Al* the negative differential conductivity was discovered for dynamical *I-V* chracteristics in the atmosphere of polar molecules. The position of region with negative differential conductivity depends on the sort of concrete substance with polar molecules (ether *etc*). By fulfilled investigations the appearance of oscillations on both *I-V* characteristics and relaxation dependencies of reverse current with respect to time was discovered. Keeping for a long time (more than one week) the structures in the atmosphere of ether results in disappearance of the region with negative differential conductivity and widening of hysteresis on *I-V* characteristics. Keeping in vacuum the structures investigated results in recovering of behaviour of dynamical *I-V* characteristics. Repeating of the influence of vapors of substances with polar molecules gave rise to appearance of mentioned above effects.

Suggested theoretical model is based on kinetic equations which describe the surface processes with participation of polar molecules. These equations were investigated for non-stationary case. Non-linearity in presented equations due to the presence of the region with negative differential conductivity make it possible to reduce the investigation of dynamics of the system to the Van-der-Pol equation, which describes the bifurcation of passing to the limiting circle, i.e. to the appearance of oscillations. The typical dynamics of development of the processes is connected with adsorption/desorption of polar molecules phenomena on semiconductor surface with charging of surface states.

ANALYTICAL SOLUTION OF THE DIFFUSION EQUATION FOR GAUSSIAN SOURCE AT CONSTANT TEMPERATURE GRADIENT

V.I.Rudakov, V.V.Ovcharov
Institute of Microelectronics and Informatics RAS
Universitetskaya 21, Yaroslavl 150007, Russia

Introduction. In the processing of VLSI ion implantation is widely used for formation shallow p-n junctions. Dopant activation by heating results in undesirable spreading of an initial profile. For decreasing this effect a dopant activation can be carried out in a inhomogeneous temperature field. In this case for evolution description of the profile the thermodiffusion equation should be solved.

Diffusion model. In the one-dimensional case as shown in the works [1,2] the thermodiffusion substance flux

$$J_k = -D(\nabla C + C\frac{Q^*}{kT}\frac{\nabla T}{T}) \tag{1}$$

can be reduced to

$$J_k = D_1\frac{\partial U}{\partial x}\ , \tag{3}$$

by substitution

$$U(x,t) = C(x,t)\,\mathbf{exp}\left(-\frac{Q^*}{kT(x)}\right) \tag{2}$$

where,

$$D_1 = D_0\,\mathbf{exp}\left(-\frac{E-Q^*}{kT}\right); \tag{4}$$

C(x,t) is the concentration of impurity for the time moment *t* and the point *x*; *T* is the absolute temperature; ∇T is the temperature gradient; $D = D_0 \exp(E/kT)$ is the diffusion coefficient; Q^* is the heat of transport; *E* is the activation energy; *k* is the Boltzmann's constant.

By expression the argument of the exponential factor in the expression (4) as the Macloren series in *x*

$$-\frac{E-Q^*}{kT(x)} = -\frac{E-Q^*}{kT_0}\left(1-\frac{\nabla T}{T^2}x+...\right) \tag{5}$$

and neglecting of all terms except unity we can write the substance flux at near-surface region in the form

$$J_k = -D_1 \nabla U \tag{6}$$

The equation corresponding to the flux (6) has the form

$$\frac{\partial U}{\partial x} = D(0)\frac{\partial^2 U}{\partial x^2}. \tag{7}$$

Results. Let consider the case when an initial concentration is described by gaussian function (gaussian source)

$$C(x,0) = \frac{M}{\sqrt{2\pi}\Delta R_p}\,\mathbf{exp}\left(-\frac{x^2}{2\Delta R_p^2}\right), \tag{8}$$

where ΔR_p is the straggling; *M* is the total amount of a substance in the layer referred to unit of its area.

It can be shown from the equation (7) the expression for the relative concentration of an impurity

$$C_r = \frac{2\Delta L\sqrt{\pi}C}{M} \quad (9)$$

for the dimensionless coordinates

$$X = x/\Delta L,\ G = (\nabla T/T_0)\Delta L,\ q = Q^*/(kT_0),\ e = E/(kT_0),\ \Theta = \frac{D(0)t}{\Delta L^2},$$

$$\Delta L = \Delta R_p/\sqrt{2}$$

has the form

$$C_r(X,\Theta) = \mathbf{exp}\left[q\left(\frac{1}{1+GX}-1\right)+\frac{\Theta(qG/2)^2}{\Theta+1}\right]WC_{isoth} \quad (10)$$

where

$$W(X,\Theta) = \mathbf{cosh}\left(\frac{qGX}{\Theta+1}\right)+$$

$$\frac{1}{2}\left[\mathbf{exp}\left(-\frac{qGX}{\Theta+1}\right)\mathbf{erf}\left(\frac{(1/2)qG - X/\sqrt{\Theta}}{\Theta+1}\right)+\mathbf{exp}\left(\frac{qGX}{\Theta+1}\right)\mathbf{erf}\left(\frac{(1/2)qG + X/\sqrt{\Theta}}{\Theta+1}\right)\right],$$

$$C_{isoth}(X,\Theta) = \frac{\mathbf{exp}\left(-\frac{X^2}{\Theta+1}\right)}{\sqrt{\Theta+1}}.$$

Conclusion. It can be shown the solution for a gaussian source describes the thermodiffusion process at the near-surface region for $X \le 1.5$ (i.e. $X \le \Delta R_p$) with good accuracy. Thus it can be used for description of thermodiffusion in the process of dopant annealing in Si plate after ion implantation for creation shallow p-n junctions.

Referencess.

[1] V.I.Rudakov and V.V.Ovcharov, *Analytical solution of the diffusion equation for an extended source of infinite extent at constant temperature gradient*, International Journal of Heat and Mass Transfer v.40, N9, 1997, p.2231- 2234.

[2] V.I.Rudakov and V.V.Ovcharov, *Analytical solution of the diffusion equation for an instantaneous plane source at constant temperature gradient*, International communications in Heat and Mass Transfer v.24 ,N4, 1997, p.579 – 585.

ATOMIC MODEL OF THERMODIFFUSION

Rudakov V.I.
Institute of Microelectronics and Informatics RAS
Universitetskaya 21, Yaroslavl 150007, Russia

Introduction. A fundamental problem in the case of thermodiffusion in solids is identification of physical meaning of the heat of transport Q_{mi}^{*} and development of a method for calculating its [1]. One of the approaches to this problem involves adoption of atomic model of diffusion under a temperature gradient and derivation of an expression for Q_{mi}^{*} on the basis of this model. The purpose of this work is to obtain the expression for heat of transport in impurity solids with used approach [2].

Model. We shall consider a simple cubic lattice of the dilute substitutional solution in which impurity atom jumps to all the adjacent lattice sites are equiprobable and the probabilities of jumps to other sites is low. We shall assume that the temperature gradient acts along the x axis of the crystal lattice (crystallographic direction [100]) and we shall identify two adjacent planes 1 and 2 (crystallographic planes {100}) perpendicular to the x axis. We have x and $x+\Delta x$ are the coordinates, T and $T+\Delta T$ are the temperatures, c_v and $c_v+\Delta c_v$ are the concentrations of vacancies of the planes 1 and 2, respectively. We shall consider the impurity atom jumps between these planes.

If the impurity atom diffuses by means of vacancy migration then the probability that the atom can jump in adjacent site is equal the probability of

finding a vacancy in this site multiplied by the probability that an impurity atom occupies this site. Thus, we can write down the frequency of impurity atom jumps in an adjacent site as

$$\Gamma = \omega_i c_v, \qquad (1)$$

where ω_i is the frequency of impurity atom jumps i at an adjacent vacancy and c_v is the concentration of vacancies, expressed in atomic fractions. The frequencies of impurity atom jumps in the planes 1 and 2 are ω_i and $\omega_i + \Delta\omega_i$, respectively. We can represent frequencies of impurity atom jumps moving from the plane 1 to the plane 2 and back as $\Gamma_{12} = (\omega_i + \Delta\omega_i)c_v$ and $\Gamma_{21} = \omega_i(c_v + \Delta c_v)$, respectively. The flux of impurity atoms from the plane 1 to the plane 2 is $J_{12} = c_i\Gamma_{12}$. Similarly, we have $J_{21} = (c_i + \Delta c_i)\Gamma_{21}$, where c_i and $c_i + \Delta c_i$ are the concentration of impurity atoms in the planes 1 and 2, respectively, expressed in atomic fractions. Under steady-state conditions the equality $J_{12} = J_{21}$ is obeyed and the heat of transport of atoms is

$$Q^*_{mi} = kT^2 \frac{\partial}{\partial T}\left(\ln \frac{\omega_i}{c_v}\right). \qquad (2)$$

It is evident from eq.2 that the heat of transport is the energy carried by a jump. This energy is due to a change in the ratio of the frequency ω_i of jumps of an atom to the concentration of vacancies c_v when temperature T is varied. In its turn the ratio ω_i / c_v represents the number of jumps of an atom per one vacancy. The value of this ratio can be used to determine the direction of motion of atoms in a solid under of a temperature gradient. If $\omega_i / c_v > 1$ then $Q^*_{mi} > 1$, and atoms move in the direction of lower temperatures. If $\omega_i / c_v = 1$,

then $Q^*_{mi} = 0$ and an atom moves independently of the temperature gradient direction. If $\omega_i / c_v < 1$, then $Q^*_{mi} < 1$ and atoms travel in the direction of higher temperatures. We shall now consider the influence of equilibrium and non-equilibrium vacancies on the processes of heat of transport in impurity solids.

We have for vacancy equilibrium condition

$$Q^*_{mi} = E^m_i - E^f_v + E^b_{vi}. \tag{3}$$

Similarly, we have for deviation from a local equilibrium of vacancies

$$Q^*_{mi} = E^m_i - \gamma E^f_v + E^b_{vi}, \tag{4}$$

where E^m_i, E^f_v and E^b_{vi} are the migration energy of impurity atoms, the vacancy formation energy and the vacancy-impurity binding energy, respectively. A quantity γ is a function of the coordinate x which has to be determined. The values of γ lie between 0 and 1.

Conclusion. The thermodynamic definition of the heat of transport can by given a kinetic explanation. This heat represents the resultant net energy transported by an atom in a jump. Two competing processes contribute to the net energy: one of them is due to a change in the frequency of jumps of the diffusing atoms with temperature and the other is due to a change in the concentration of vacancies with temperature. The value of the ratio of the frequency of the jumps of an atom to vacancy concentration can be used to find the direction of motion of an atom in a crystal in the presence of a temperature gradient. The heat of transport depends on the binding energy of complexes of point defects, in particular, the impurity-vacancy complexes. Therefore the value of the heat of transport can be larger of the value of the atom activation energy. Moreover, the heat of transport depends strongly on the state of vacancies in a crystalline solid. Deviation of vacancies from an equilibrium gives rise to a

difference between the heats of transport in single crystals and in polycrystalline samples.

Referencess.

1.R.A.Oriani, *J.Phys. Chem. Solids*. 1969. V.40. P.339.

2.V.I.Rudakov, *Sov. Phys. Solid State*. 1992. V.34. P.1965.

FACTORS AFFECTING THE KINETICS OF THE WAVE-LIKE NANORELIEF FORMATION ON SILICON SURFACE UNDER NITROGEN ION BOMBARDMENT

Kibalov D.S., Smirnova G.F., Zhuravlev I.V., Smirnov V.K.
Institute of Microelectronics and Informatics of RAS, 150051 Yaroslavl, Krasnoborskaya 3, tel (0852) 11-53-46, e-mail: beam@yarteleport.ru

The wave-ordered structure (WOS) is of interest as a phenomenon of self-formation of an anisotropic periodic structure expressed in the generation of "waves" on a surface of a rigid body under the ion bombardment. For practice the phenomenon deserves attention as a nonlithographic process for creation of patterns with submicrometer and nanometer scale features on a silicon surface.

The development and morphology of WOS on silicon surface under the action of a beam of nitrogen ions N_2^+ is determined by the energy of primary ions (E), angle of ion incidence (θ), sample temperature (T) and is characterized by the formation depth of WOS (D_m) and WOS wavelength (λ). The study of the additional factors affecting WOS formation is of interest. It will give new possibilities of the effective control of WOS formation process and WOS properties, and also will promote the better understanding of processes of WOS evolution.

The purpose of the carried out researches was the establishment of the factors effectively influencing the process of WOS formation. Considered are the effects of oxygen flooding, irradiation with electrons, and metal films on

WOS formation process. The basic regular trends of development and morphology of WOS generated under the action of these factors are investigated.

As is known for O_2^+-Si system oxygen flooding results in the acceleration of WOS formation. Our investigations established that for N_2^+-Si system oxygen flooding retards the development of WOS. This influence has a threshold character and is exhibited in a range of oxygen pressure $P=10^{-6}\div10^{-5}$ Torr. At $P=10^{-5}$ Torr the development of WOS is completely suppressed. The analysis of SEM images of WOS formed allows us to make a conclusion about a lack of influence of oxygen flooding on WOS morphology. The influence of oxygen flooding on sputtering yield of silicon by N_2^+ ions in a range of oxygen pressure $10^{-8}\div5\cdot10^{-6}$ Torr is not revealed essential.

The research of influence of electron irradiation was carried out in a wide range of energies and current densities of an electron probe. During experiments the part of a raster, formed by an ion beam, was exposed to an electron irradiation. Then the comparison of a developed WOS with SEM was made. Electron irradiation results in stunted growth of WOS. Influence of the electron irradiation on the morphology and on λ is not revealed. The similar data were obtained in experiments on study of joint action of oxygen flooding and electron irradiation of silicon surface during WOS formation.

For study of influence of metal films on WOS formation process the films of Au, Pt, Ti, and W of a various thickness were deposited on silicon surface. It was found that the presence on silicon surface of a golden film resulted in significant acceleration of WOS formation dynamics. A 20-nm thick golden film reduces by an order of magnitude a value of D_m. Films of Pt, Ti, and W have similar effect on WOS formation dynamics as well as pre-implantation of gold into silicon.

Influence of metal films on WOS wavelength was not revealed. There are differences in morphology of WOS generated at the same conditions on silicon

surface covered with metal and without a covering. The presence of films on silicon surface results in increasing the number of WOS defects like the branching of waves and their widening. Note that a film of W induces the significant perturbation of WOS. In the experiments with golden films the development of pits due to sputtering was observed to be suppressed.

Thus, carried out research is established that oxygen flooding and electron irradiation decelerate WOS formation process, not rendering essential influence on the morphology of WOS. The presence on silicon surface of metal films of Au, Pt, Ti and W results in the acceleration of WOS formation and renders influence on the morphology of WOS formed.

This work was performed under the contracts №5-99/7И and №40-2001/7И signed between Institute of Microelectronics and Informatics of RAS and Agency for marketing of scientific products Ltd.

ADATOM DESCENT FROM 2-DIMENSIONAL AG ISLANDS ON AG(111)

A. Karim, A. Kara, T. Rahman
Kansas State University, USA

Diffusion mechanisms, paths, barriers, and prefactors for adatoms at the edges and corners of four-atom island on Ag(111) are examined using a combination of theoretical techniques with embedded atom method interaction potentials.

The activation barriers and reaction paths determined from contour plots of the potential energy surface favor concerted exchange mechanism involving a corner atom and a path leading to the creation of a (100)-facetted (A-type) step face with an overall energy barrier of 86 meV in comparison with 240 meV for the process leading to the seeds of a (111)-facetted (B-type) step.

Assuming the same prefactors for both mechanisms, extrapolation of these results from 0 K-energetics predicts the probability to form A-type step to be 0.99 at 300K, 0.95 at 500K and 0.89 at 700K.

Accompanying molecular dynamics simulations, however, show these quantities to be 0.94 at 300K, 0.47 at 500K and 0.42 at 700K.

These results suggest that the assumption of same prefactor for the two processes may not be correct and that results at 0K cannot be extrapolated easily to predict happenings at finite temperatures.

LARGE MISFIT DISLOCATION NUCLEATION IN HETEROEPITAXY

O. Trushin[1], S-C. Ying, E. Granato and T. Ala-Nissila[2]
Institute of Microelectronics, RAS
[2]Helsinki Institute of Physics and Laboratory of Physics,
Helsinki University of Technology, P.O. Box 1100, FIN-02015 HUT, Finland
email ole@fyslab.hut.fi

We have studied atomic mechanisms of misfit dislocation nucleation in heteroepitaxy with semiempirical potentials. Many-body mechanisms of stress relaxation are systematically investigated with Lennard-Jones potential in 2D and 3D cases. Energy barriers for dislocation nucleation are estimated using modern methods for saddle point search (Nudged Elastic Band [1], Eigenvector Following [2] and others). Moreover, new simple and effective method for transition paths searching is proposed. Based on the data the critical thickness of film is estimated as a function of film-substrate lattice misfit. Moreover, to make the study more realistic we used EAM [3] potentials in simulations of Pd/Cu and Cu/Pd systems.

We show that the dislocations nucleate more easily in compressive than tensile strained films, and in fcc(111) orientation rather than in fcc(100). These findings are in agreement with recent experimental and theoretical works. This

work was partially supported by Ministry of Industry, Science, and Technology Grant No. 204-13(00).

Referencess

1. H. Jonsson, G. Mills and K. W. Jacobsen, in “Classical and Quantum Dynamics in Condensed Phase Simulations”, ed. by B. J. Berne, G. Ciccotti, and D. F. Coker (World Scientific, Singapore, 1998).

2. L. J. Munro and D. J. Wales, Phys. Rev. B v59, p.3969 (1999), and Referencess therein.

3. S. M. Foiles, M. I. Baskes, and M. S. Daw, Phys. Rev. B v.33, p.7983 (1986).

EFFECT OF ION BOMBARDMENT DURING DEPOSITION PROCESS ON PROPERTIES OF NI FILMS

V.F. Bochkarev, V.V. Naumov, A.A. Gorjachev, O.S. Trushin, A.A. Lebedev, A.S. Kunitsin
Institute of microelectronics and informatics,
150007 Yaroslavl, Universitetskaja 21, Tel. (0852) 11-16-32.
Fax: (0852) 11-65-52
e-mail: trushin@tornado.yars.free.net

We present the results of a study of the effect of low energy ion bombardment (1-100 eV) during deposition process on growth mode and properties of thin Ni films. The films of Ni were deposited by RF sputtering in Ar at pressure of 1 Pa. During the deposition process RF bias with the same frequency was applied on the substrate. In such a way the series of samples were fabricated at different values of DC component of substrate bias changing in the range from 0 V up to -180 V with step of 30 V. The density of as deposited films was determined based on the date of X-ray fluorescent spectroscopy and measurements of the thickness with STM [1]. Dependence of the thickness and density of the films on the value of substrate bias presented on fig.1. The density is normalized to the density of bulk Ni. From the fig.1 one can see that maximal

density is achieved at substrate bias of –60 V. It is equal to bulk Ni density within experimental error bar.

We also investigated crystal structure of as deposited films with X-ray diffractometer DRON-3M. The films deposited at bias in the range from 0 V up to –30 V had typical polycrystal structure. At all other conditions the films had axial texture (111) perpendicular to the surface of film. Maximum of intensity of Ni (111) reflex corresponds to the substrate bias of –90 V. It demonstrates high content of crystal phase in the sample.

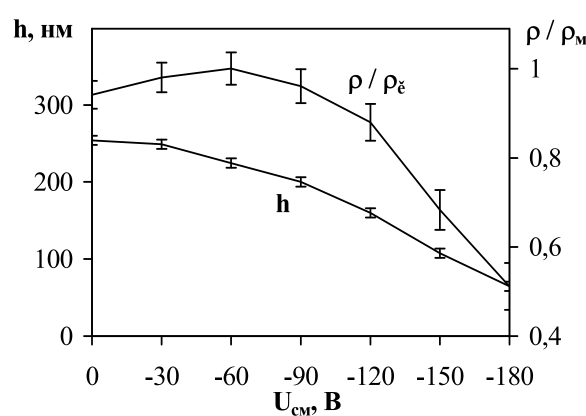


Fig.1. Dependence of the density and the thickness of Ni films on DC component of substrate bias.

However the quality of crystal ordering (minimum of microstress and maximum of the size of coherently scattering blocks) is higher for the films deposited at substrate bias of –60 V.. It correlates with maximum of the density of film. Our studies demonstrate that at definite experimental conditions it is possible to obtain more dense films than bulk substance. We also measured electric resistance of as-deposited films. It has been shown that the most dense films have the lowest resistance of 8.5 10^{-6} Ohm (resistance of bulk Ni - 6.14 10^{-6} Ohm).

Referencess

1.O.S. Trushin, V.F. Bochkarev, A.A. Goryachev, V.V. Naumov, A.A. Lebedev Determination of mean density of thin films based on the date of X-ray fluorescent spectroscopy// Industrial laboratory (in rus), 2000. № 10. p.39-40.

HYPER-MOLECULAR DYNAMICS CALCULATIONS OF DIFFUSION OF A Cu ADATOM ON THE Cu(111) SURFACE

A.-P. Hynninen[1], O. Trushin[2] and T. Ala-Nissila[1]
[1] Laboratorio of Physics, Helsinki University of Technology, P.O.B. 1100, FIN-02015 HUT, Finland
[2] Institute of Microelectronics, Universitetskaga 21, Yaroslavl 15007, Russia
email aphy@cc.hut.fi

The main limitation of using molecular dynamics (MD) simulations in the study of surface diffusion is the length of the time scale achieved: with a reasonable amount of computing power only processes in time scale of nanoseconds can be observed. For example, studying the diffusion of clusters with MD would require a microsecond time scale. Recently, a time accelerated variant of MD has been proposed [1] which makes it possible to extend the MD time scale by many orders of magnitude and therefore, reach time scales of microseconds and even more. Because of the extended time scale, this so called ``hyper-MD'' could be used, for example, to follow the motion of large clusters and to detect new rare processes. Or, when taken to its extreme, it could be used to perform materials simulations on macroscopic length and time scales. Hyper-MD is based on the transition state theory (TST) [2] and is therefore applicable especially at low temperatures, where the observation of rare events with regular MD becomes prohibitively difficult. Of course, the acceleration in time does not come without a cost, and therefore the question rises, how much of the physics is lost when using hyper-MD. The purpose of our study is to answer this question in part, by checking whether or not hyper-MD can be used to accurately determine the adatom diffusion coefficients. We calculate the diffusion coefficients with hyper-MD for a single Cu adatom on a Cu(111) surface at low temperatures, where regular MD cannot be used. Combining this data with regular MD results at higher temperatures we obtain a common Arrhenius plot. The embedded-atom method (EAM) [3] is used to describe the

potential energy between the Cu atoms. From the Arrhenius plot we observed that hyper-MD gives the correct Arrhenius behaviour and therefore we conclude that hyper-MD can be used to calculate diffusion coefficients. The microsecond time scale was achieved with hyper-MD simulations.

Referencess

1. A. F. Voter, Phys. Rev. Lett. v78 (1997) p.3908.

2. Hanggi, Talkner and Borkovec, Rev. Mod. Phys. v62 (1990) p251.

3.S. M. Foiles, M. I. Baskes, and M. S. Daw, Phys. Rev. B v32 (1986) p7983.

INSTABILITY AND WAVELENGTH SELECTION DURING STEP FLOW GROWTH OF METAL SURFACES VICINAL TO FCC(001)

M. Rusanen, I. Koponen, J. Heinonen, and T. Ala-Nissila:

We study the onset and development of ledge instabilities during growth of vicinal metal surfaces using kinetic Monte Carlo simulations. We observe the formation of periodic patterns at [110] close packed step edges on surfaces vicinal to fcc(001) under realistic molecular beam epitaxy conditions. The corresponding wavelength and its temperature dependence are studied by monitoring the autocorrelation function for step edge position. Simulations suggest that the ledge instability on fcc(1,1,m) vicinal surfaces is controlled by the strong kink Ehrlich-Schwoebel barrier, with the wavelength determined by dimer nucleation at the step edge. Our results are in agreement with recent continuum theoretical predictions, and experiments on Cu(1,1,17) vicinal surfaces.

THE INVESTIGATION OF HOMOGENEITY OF a-SiC:H THIN FILMS WITH USING OF CHEMICAL INDUCTION MODEL

B. G. Budaguan, A. A. Sherchenkov, A. E. Berdnikov*, E. I. Artemov.
Department of Materials Science and Physical Chemistry, Institute of Electronic Technology, k-498, Moscow, 103498, Russia.
e-mail: ms@ms.miee.ru
***Institute of Microelectronics and Informatics of RAS, Yaroslavl, 150007, Russia**

Thin films of hydrogenated amorphous silicon-carbon alloy (a-SiC:H) are widely used for device applications because of the possibility to control different properties like the optical band gap and the electrical conductivity by changing the carbon concentration. The physical properties and stability of a-SiC:H thin films as well as device quality strongly depend on material's structural properties and, particularly, on its structural homogeneity. A number of structural carbon-containing configurations such as diamond-like or graphite-like particles present in a-SiC:H are influenced the device parameters.

In this paper we determine the local chemical environment of the Si-H bond and the forms of carbon incorporation by analyzing the dependence of the Si-H stretching frequency shift on the alloy composition r=[C]/[Si]. Our films were prepared by decomposition in the low frequency (55 kHz) glow-discharge plasma the gas mixtures of silane and methane with varying methane fraction. The deposition was carried out on c-Si wafers at constant substrate temperature of 320^0C.

There are four possible combinations of Si and C atoms as the nearest neighbours of Si-H bond in the form of $HSiSi_{3-n}C_n$ configuration with n=0÷3. In a-SiC:H alloy matrix, up to three carbon atoms can be backbonded to Si-H bond. So we analysed the shape of the IR absorption band between 1840 and 2300 cm^{-1} attributed to the Si-H stretching vibrations by decomposing this band into four subbands with Gaussian distribution where it was possible. Using the chemical induction model we calculated the dependencies of the frequencies for each of

the four peaks both on the local environments of the Si-H group, and on the medium. Then mismatch between calculated values and real observed frequencies was determined. In order to estimate the validity of frequency evaluations we calculated the probabilities of $HSiSi_{3-n}C_n$ structures as the functions of carbon content r. The probabilities were calculated assuming the homogeneous film and random bonding.

There are two slopes in the peak position of the Si-H stretching mode vs r dependence. At $r<0.16$ only two structural configurations $HSiSi_3$ and $HSiSi_2C$ dominate in a-SiC:H. For $r>0.16$ the inhomogeneity in medium due to carbon clustering in the forms of $HSiSiC_2$ and $HSiC_3$ plays the main role and shifts the frequency of Si-H stretching mode to higher values. The same dependencies with the point of inflection at $r=0.16$ are observed in the dependence of optical band gap on r.

So it can be concluded that: 1) our films, prepared at non-equilibrium conditions, show significant inhomogeneity in carbon distribution; 2) there is correlation between the dependencies of optical band gap and the type of inhomogeneities as functions of film composition, but the influence of the structural inhomogeneities on thin films optical properties will be discussed further.

FABRICATION OF 3D ARRAYS OF MGO NANOCLUSTERS IN UNDERSURFACE LAYERS OF OPAL MATRIX

P.V. Paschenko[1], S.M. Klescheeva[1], M.I. Samoilovich[2], A.F. Belyanin[1]
[1]Central research technological institute "TECHNOMASH",
Iv. Franko str. 4, Moscow 121108, Russia,
Tel. (095) 146-10-95
[2]AOZT "Almaztechnocrystal" , Fabrika Kalinina str. 14a,
Alexandrov, Vladimir region, Russia,
Tel. (095) 584-58-19

Opal matrix represent 3D optical lattice, inside which single crystal SiO_2 particles are packed according to cubic law. We develop the method for fabrication of artificial opal matrixes with controled size of SiO_2 particles and structural empty zones, partially filled by different materials. In such a way the material to be filled in creates own sublattice with 3D periodicity. This way was used for first syntesis of nanocomposit materials with unique physical properties determined by quantum size effects.

To obtain such nanocomposit we deposited MgO film on opal substrate by RF magnetron sputtering of Mg in gas mixture of Ar and O_2 . We studied the effect of different experimental parameters on the rate of film growth and its crystal structure. Optimal conditions for MgO deposition are as follows:

Composition of gas mixture Ar+90% O_2

Pressure 0.5-2 Pa,

RF discharge voltage 130-250 V

RF discharge power 150-200 W

Temperature of opal matrix 373-473 K,

It was shown that MgO deposition begins at O_2 concentration > 85% and RF discharge power > 100 W.

VERTICAL AND LATERAL MANIPULATION OF ADATOM ON SURFACES

Chandana Ghosh, Abdelkader Kara, Talat S. Rahman (Kansas State University, Manhattan, Kansas 66506),

We have carried out calculations of vertical and lateral manipulations of adatoms on flat, stepped and kinked (111) surfaces of several fcc metals to understand the dependence of the process on the cohesive energy, local atomic coordination and tip geometry. Vertical manipulation was found to be most effective on flat surfaces, while on stepped surface a "floating" region was found at which the adatom was equally attracted to the tip and the surface (for a blunt Cu(111) tip on (100)-microfacetted step edge at a height of 3.6Å). With a Cu(100) sharp tip on the same stepped surface, for heights ranging from 2.75Å-3.5Å the total energy of the system is found to be minimum when the adatom is very close to the surface. As the adatom is pulled the total energy of the system first rises and then reaches another minimum when the adatom touches the tip. Thus to pull an adatom vertically, the tip should be brought close to the adatom and then quickly pulled to a higher height. In the case of lateral manipulation it was found that Au had the lowest barrier to diffuse from one hollow site to the next (37 meV) at a tip height of 2.75Å and a lateral separation of 2.5Å. In this systematic study on six metal surfaces the effect of kinks and local step edge geometry is examined and results are rationalized on the basis of bond-length/bond-order correlation.

References

1 G. Dujardin, A. Mayne, O. Robert, F. Rose, C. Joachim, and H. Tang, Phys. Rev. Lett. v.80, p.3085 (1998).

2. U. Kürpick and T.S. Rahman, Phys. Rev. Lett. v.83, p.2765 (1999).

SURFACE MORPHOLOGY FORMATION ON A-SI:H, DEPOSITED AT LOW FREQUENCY DISCHARGE.

Popov A.A., Berdnikov A.E., Chernomordick V.D., Budaguan B.G.

Institute of Microelectronics and Informatics RAS
Universitetskaya 21, Yaroslavl 150007, Russia

Micro structure appear on a-Si:H surface during deposition from gas phase in low frequency glow discharge. Structures is a spherical hills with high 1 – 10 nm and diameter 5 – 500 nm. Analogy shape of surface exist on a-Si:H, deposited same other methods.

For an explanation of surface structure formation on a-Si:H the hypothesis was offered, that hills appears from conformal deposition of a film on clusters, which generated and besieged from a gas phase. Necessary requirements of a conformal deposition is the overflow of a free path of molecules in a gas phase above a References feature dimension of a surface structure at absence of the chosen direction of a stream of particles, overflow of the size of surface inhomogeneities above of radicals drift length on a surface, absence of elements with high aspect ratio. This requirements is present in our deposition system.

The definition of interrelation of diameter d of a built in a film cluster, its depth from a surface R, height h and diameter D of hill, formed on a surface was spent from geometrical reasons under the next formulas:

H=d (1) and $R = \frac{(D/2)^2 + h^2}{2h}$ (2) if D>>h

On available AFM the images of a-Si:H surface the diameters and their height all hills were measured. The depths from surface were calculated for each cluster by the formula (2). The main part of calculated depths uniformly deposited on of a film thickness. Approximation line of dependence of a cluster diameter from depth of cluster position practically is horizontal. It means, that dependents of cluster diameter distribution from time of deposition is absent.

The distribution of quantity of built-in clusters from their diameter carries character of a decadent exponential curve, that corresponds them formation in gas phase. All results confirms the offered hypothesis of shaping formation on a surface.

MESOSCOPIC SIMULATION STUDIES OF AMPHIPHILIC SYSTEMS

E. Falck[1], I. Vattulainen[1], and T. Ala-Nissila[1,2]
[1] Laboratory of Physics and Helsinki Institute for Physics, Helsinki University of Technology, P.O. Box 1100, 02015 HUT, Finland
email: emma.falck@hut.fi
[2] Department of Physics, Box 1843, Brown University, Providence, R.I. 02912--1843, U.S.A.

Computational methods in physics are traditionally atomistic or macroscopic. Due to limitations of theoretical knowledge and computing power, the time and length scales between atomistic and macroscopic regimes have received little attention until recently. The mesoscale regime, however, is of interest to many fields of science and technology, such as polymer science, chemical engineering, and life sciences. As examples of processes at mesoscopic scales one may think of morphological properties of copolymers and polymer blends, flow through porous media, and the formation of micelles and liposomes. We are developing a mesoscopic model for amphiphilic systems. Our model is essentially a hybrid molecular dynamics scheme. The amphiphiles are treated microscopically, while the solvent is described in terms of coarse grained particles obeying a multiparticle collision dynamics algorithm. This efficient hybrid model is based on the scheme suggested by Malevanets et al. [1,2], and our aim is to use it for investigating the diffusion of micellar and liposome structures.

In this work, we present the model and discuss the results obtained for simple amphiphilic systems.

Referencess

[1] A. Malevanets and R. Kapral, J. Chem. Phys. 110, 8605 (1999).

[2] A. Malevanets and R. Kapral, J. Chem. Phys. 112, 7260 (2000).

SYNTHESIS OF SILICATE GLASS LAYERS

S.A. Krivelevich, M.I. Makoviichuk, Y.I. Denisenko,
E.O. Parshin, V.A. Gusev
Institute of Microelectronics and Information Science, Russian Academy of Sciences, Yaroslavl 150007, Universitetskaya 21,
e-mail: ksa@imras.yar.ru, ph.: 0852 115346, Fax: 0852 116552

Now there are some technologies, in which the ionic synthesis is used for creation of the buried layers of silicon dioxide. It's widely known, for example, SIMOX process, including an ionic implantation of oxygen and subsequent high-temperature (> 1300°C) annealing within several hours. The existing tendencies on an increase of quality SOI/SIMOX of structures and decrease of complexity of process are implemented in practice in a known means of ionic synthesis - ITOX process.

However, classic variant of SIMOX process, which is widely spread nowadays, has some drawbacks. The first one is that it's impossible to solve the problem concerning maintenance of the functional layer quality on condition of reduction of a dose of implantation (homogeneous continuous oxydic layer will not be formed, the dislocation density in the upper working layer is increased). The second drawback consists in the absence of the possibility to reduce the thermal budget of postimplantation treatments. The third one is that the processes of degradation at the interface between working layer and layer of the oxide take place. The fourth drawback is that there is high level of thermal voltages in the upper working layer. The fifth one is that it is impossible to

provide an effective guidance by the electro-physical characteristics of the buried layer and by its optical thickness particularly. The sixth drawback is an increase of thermal silicon dioxide on a surface of a working layer resulting in the considerable expenditure of silicon.

In the present paper in order to solve all the problems mentioned above it's suggested to implant the ions of another substance, with close disposed or coinciding comparatively implanted oxygen by maximum of a profile of concentration, alongside with ions of oxygen into the work material. As ions of other material one should use components including atoms, which with SiO_2 form a glass together (for example - boron, phosphorum or lead), and the depth of an implantation of these atoms coincides or is located further from a surface of a substrate, than for implanted oxygen. The subsequent heat treatment will be carried out at a certain temperature. It must be greater than softening point but smaller than vitrification point of the forming glass. The time of heat treatment does not exceed the time of migration of atoms of the indicated elements towards the profile of concentration of oxygen, where their essential shares of the total amount will derivate new compounds with silicon. Besides it, the process presented in this paper is characterized by the fact that if the inserted atoms of devices are the donors or acceptors in an active area of the upper instrument layer of silicon, the time of heat treatment can exceed time of their migration in formed glass. This time is restricted by reaching of indispensable concentration of free charge carriers in the given active area.

The variant of the technology offered here has the following advantages. The first one is that at a minimum dose of implantation it's possible to achieve practically complete absence of the disruptive bonds in the buried layer. The second advantage is that the thermal budget of the process is sharply reduced, since varying a composition of a synthesized glass makes it possible to drive effectively the temperature of its emolliating, which, as a rule, does not exceed 1000°C in a wide range of compositions. The third one is that changing of a

composition of glass gives the possibility for smooth governing by the constants of thermal expansion, the optical thickness of the buried layer and its other physical and mechanical characteristics. The fourth advantage is that the alloying properties and dielectric parameters known on application in microelectronics of glasses can be utilized at a select of a material of the buried layer:

a) Glass with a small value of inductivity — for shaping rapid SOI of structures with minimum spurious capacitances in relation to a substrate,

b) Glass with high insulant properties and thermal conductivities — for shaping SOI of structures of power devices,

c) Glass — radiants alloying silicon of impurities (for example, — of boron or phosphorum) — for overlapping heat treatment on a final stage of ionic synthesis with a doping of the upper instrument layer SOI of structures.

Both experiments and theory are necessary for more detailed study of the process. Therefore authors suggests a variant of theoretical model, based on the theory of phase changes Hinzburg – Landau.

The present work is carried out within the framework of the Federal scientific and technical program for special purpose "Examinations and developments on priority directions of science and technique progress for civil purposes" and at a financial support of INTAS (Ref. [1] 99-01872).

ELECTROPHYSICAL PROPERTIES OF A-SIC:H/C-SI HETEROJUNCTIONS

Budaguan B.G.[1], Sherchenkov A.A[1], Mazurov A.V.[1], Chernomordick V.D.[2]
[1]Depatment of Materials Science and Physical Chemistry, Moscow Institute of Electronic Technology, Moscow 103498 Russia
[2]Institute of microelectronics and informatics of RAS, Yaroslavl 150007 Russia.

Amorphous/crystalline materials heterojunctions are widely used in nanostructures. However the physics of such heterojunctions is not clear yet. The aim of this work was to understand the carrier transport mechanism dominating in heterojunction a-SiC:H/c-Si, and investigate the hetrojunction interface.

The I-V characteristics were studied under light and the dark conditions. The a-SiC:H films were deposited in low frequency glow discharge plasma at different concentrations of methane in the gas mixture. Boron doped crystalline silicon wafers were used as substrates.

The results of I-V characteristic simulation showed that forward current was determined by the multistep tunneling capture emission. Modeling of I-V characteristics allowed to determine trapping level (Et) position in the a-SiC:H mobility gap. It was found that the spectral characteristics of relative quantum efficiency of a-SiC:H/c-Si heterojunction is wideband which is due to the presence of some maxima. Such spectral characteristic indicates on the high quality of the interface between two different materials a-SiC:H and c-Si.

Trapping level (Et) position in the a-SiC:H mobility gap moves from Fermi level to the valence band edge with increasing methane fraction. At 0% CH_4 fraction trapping level is equal to Et=0.84 eV, while at 60% CH_4 fraction it increases to 1.45eV. As we specified, this behaviour of Et is due to the hydrogen atom rerrangement from Si-H to C-H bonds with defect creation. This behaviour of Et is confirmed by increasing density of defect states with methane fraction.

CONCENTRATION PROFILE FOR AN EXTENDED SOURCE OF INFINITE EXTENT AND AN INSTANTANEOUS PLANE SOURCE DURING NON-ISOTHERMAL DIFFUSION

V.I.Rudakov, V.V.Ovcharov
Institute of Microelectronics and Informatics RAS
Universitetskaya 21, Yaroslavl 150007, Russia

Introduction. Consider a system with two fluxes: a solvent substance J_1 and a heat flux J_2. The isotropic balance equations for a solvent substance concentration C and the temperature T are [1]

$$\frac{\partial C}{\partial t}=\frac{\partial}{\partial x}\left[D\left(\frac{\partial C}{\partial x}+\frac{Q^*}{kT}\frac{\nabla T}{T}C\right)\right], \tag{1}$$

$$\frac{\partial T}{\partial t}=-\mathbf{div}\,J_2\ , \tag{2}$$

where $D = D_0\exp(E/kT)$ is the diffusion coefficient; E is the activation energy; k is the Boltzmann's constant; ∇T is the temperature gradient; Q^* is the heat of transport.

Suppose the system is a thin plate, that has fixed surface temperatures. If the heat transform is realized by conductance only from the hot to cold surface and the conductance rate K does not depend on the temperature and the impurity concentration in a plate, for one-dimensional case T will be the linear function of x [2] in the steady state (the x-axis is directed to normal towards the plate surface). Then

$$J_2=-K\nabla T=const\ , \tag{3}$$

and hence in the equation (1) the $\nabla T = const$.

Diffusion model. The thermodiffusion equation (1) for one-dimensional case and $\nabla T = const$ can be solved by the substitution

$$\xi(x)=\int_0^x \mathbf{exp}\left(\frac{Q^*}{kT(\nu)}\right)d\nu \tag{4}$$

in linear approximation of expanding of the function *1/T(x)* into Macloren's series [3,4]. The solutions [3,4] for an extended source of infinite extent and an instantaneous plane source are represented as asimptotic series and are inconvenient for an analysis of the thermodiffusion process in this form. By expressing $1/T[\xi(x)]$ as the Macloren series in ξ and introducing dimensionless variables

$$X = x/\Delta L,\; G = (\nabla T / T_0)\Delta L,\; q = Q^*/(kT_0),\; e = E/(kT_0),\; \Theta = \frac{D(0)t}{\Delta L^2},$$

in a linear case, we have:

$$\Psi(X) = -\frac{\exp q}{qG}\left[\exp(-qGX) - 1\right],$$

where $D(0) = D_0\exp(E/kT_0)$ is diffusion coefficient for the $T = T(0) = T_0$; ΔL is characteristic length.

Results. . Denoting

$$A = \frac{(e-2q)}{\Delta L} G \exp(-q),\; B = \left(\sqrt{\pi}/4\right) A \exp q,\; C_r = \frac{C(X,\Theta)}{C_0},$$

$$K(\Psi) = \exp\left[q\left(\frac{1}{T(\Psi)} - \frac{1}{T_0}\right) - A\Psi/4\right],\; W(\Psi,\Theta) = \frac{1-\exp(-A\Psi/2)}{A\Theta\exp q},$$

and neglecting all terms containing higher than first degrees of the parameter A we obtain the solutions of the equation (4) in a compact form at $A\Psi \ll 1$:

for an extended source of infinite extent ($C_0 = C(0)$)

$$C_r = K \operatorname{erfc} W; \tag{6}$$

for an instantaneous plane source ($C_0 = \frac{M}{\Delta L\sqrt{\pi}}$, M is total amount of a substance in the layer referred to unit of its area)

$$C_r = K\left[\frac{\exp(-W^2)}{\sqrt{\Theta}} - B \operatorname{erfc} W\right]. \tag{7}$$

Conclusion. For diffusion from an extended source of infinite extent and an instantaneous plane source the compact forms of the thermodiffusion equation solution taking into account the diffusion coefficient *D*[*T(x)*] and thermodiffusion factor's $Q^{*}/[kT(x)]$ temperature dependence are obtained. In the form this solutions are convenient for an analysis and a graphical interpretation.

Referencess.

[1] I.Gyarmati, *Non-Equalibrium Thermodynamics*. Springer, Berlin, 1970.

[2] H.S.Carslow and J.C.Jaeger, *Conduction of Heat in Solids*. Clarendon Press, Oxford, 1959.

[3] V.I.Rudakov and V.V.Ovcharov, *Analytical solution of the diffusion equation for an extended source of infinite extent at constant temperature gradient*, International Journal of Heat and Mass Transfer v.40, N9, 1997, p.2231-2234.

[4] V.I.Rudakov and V.V.Ovcharov, *Analytical solution of the diffusion equation for an instantaneous plane source at constant temperature gradient*, International communications in Heat and Mass Transfer v.24 , N4, 1997, p.579 – 585.

SURFACE SEMICONDUCTOR IRREGULARITIES CONTROL METHOD

V.I.Rudakov, V.V.Ovcharov, V.P.Babarykina
Institute of Microelectronics and Informatics RAS
Universitetskaya 21, Yaroslavl 150007, Russia

Introduction. For every standard microelectronic process it is desired that undestructional control of semiconductor surface properties is carried out. It is known that absorption coefficient $\varepsilon(\lambda,T)$ is depended on surface roughness, composition and structure of interface layer. With steady dependence of heat flux density q between heater and surface being studied (absorber) from it

(absorbtion surface) temperature T_a one can propose the undestructional method to control the surface properties..

M**odel of set for taking q(T_a) characteristics.** A model of set comprises three plane-parallel plates close together: heater(H), absorber (A) or investigated surface and screen (S) disposed between them. The heater temperature T_h is fixed and known, the temperature of investigated surface T_a is changed under control, and with it the screen temperature T_s.

Consider the fluxes between the plates at steady state. Density of heat flux between heater and screen (q_{hs}) is defined as

$$q_{hs} = \varepsilon_{r1}(T_h^4 - T_s^4), \qquad (1)$$

where

$$\varepsilon_{r1} = \left(\frac{1}{\varepsilon_h} + \frac{1}{\varepsilon_s(T_s)} - 1\right)^{-1}$$

is the reduced emittance of heater and screen; and ε_h is the emittance of heater, ε_s is the emittance of screen. Here, ε_h is fixed, and dependence of $\varepsilon_s(T_s)$ is proposed to be known.

The flux between investigated surface (absorber) and screen (q_{sa}) is given by formula:

$$q_{sa} = \varepsilon_{r2}(T_s^4 - T_a^4), \qquad (3)$$

where

$$\varepsilon_{r2} = \left(\frac{1}{\varepsilon_s(T_s)} + \frac{1}{\varepsilon_a(T_a)} - 1\right)^{-1}, \qquad (4)$$

ε_{r2} is reduced emittance of screen and absorber, and ε_a is emittance of absorber.

Here, $\varepsilon_a(T_a)$ is unknown and the temperature of T_a is measured as it is changed.

For the steady-state, the heat flux density between heater and screen equals the heat flux density between screen and absorber

$$q_{hs}=q_{sa}, \tag{5}$$

that the dependence of $q_{sa}(T_a)$ is known for every value of T_a. Thus, the flux in eq.(5) can entirely characterize the emissivity of the surface under study.

Technique for investigation of surface irregularities. Method is based on the comparison study of temperature dependence of absorptive coefficient of investigated sample surface before and after processing. The spectrum dependence of $\varepsilon(\lambda,T)$ is a specific radiative characteristic of composition and surface structure. One can always indicate one spectral interval (λ_1, λ_2) at least on which spectral dependence of absorption of investigated surface before and after processing differs. Also, one can argue that one can almost without exception find like difference in infrared spectral interval from 0,78 to 1000 mkm.

On the other hand, to Wien displacement law [2] the maximum emission of blackbody is corresponded to wavelength λ_{max},

where

$$\lambda_{\max} = \frac{2890}{T} \text{ (mkm)}, \tag{6}$$

depending from absolute temperature T of emitting (absorbing) body. If the value of λ_{max} is among the one of the specific intervals (λ_1, λ_2) in which spectrums of two comparing surfaces $\varepsilon_1(\lambda,T)$ and $\varepsilon_2(\lambda,T)$ are essentially distinct from each other, one can suggest that temperature dependence $\varepsilon_1(\lambda,T)$ and $\varepsilon_2(\lambda,T)$ at not-too-large temperature interval covering the value of $\lambda_{\max} = \frac{2890}{T}$ are appreciably distinguished.

The considerations are used as the basis for choosing the temperature interval for plotting the $q(T_a)$ characteristics of two surfaces being compared.

Conclusion. The surface semiconductor irregularities control method is suggested. The basis for the method is the sensitivity of absorption coefficient $\varepsilon(\lambda,T)$ to the surface roughness, chemical composition and structure of interface layer.

Referencess.

[1] Fan N.Y. Infra-red absorption in semiconductors; Reports on progress in physics, v.XIX, p.107-155 (1956)

[2] Siegel R., Howell J.R. Thermal radiation heat transfer, v.38 (1972).

SOLAR CELLS FABRICATED WITH HIGH RATE DEPOSITION METHOD

B.G. Budaguan, A.A. Sherchenkov, V.D. Chernomordik*, A.B. Grabov, A.V. Sizov.**
(Moscow Institute of Electronic Technology, Moscow, ms@ms.miee.ru;*Institute of Microelectronic and Informatics, Yaroslavl' 150007 Russia; **RSC "Energia" named after S. P. Korolev, Korolev, Moscow region, Lenina street 4a, 141070)

The efficiency of the photovoltaic devices is directly dependent on the layer deposition technology. In this paper a new deposition technology in low frequency glow discharge was used for the fabrication of a p-i-n structures, which allowed to increase the film grow rate.

For the preparation of the solar cells we used 50x50 cm2 wafers from Corning Glass 7059 with the TCO layer, which were fabricated by Asahi firm.

The developed fabrication process of solar cell includes following operations:

1.Cutting of a Corning Glass 7059 with the TCO layer by the diamond disk.

2.Cleaning of the wafers in acetone at room temperature with ultrasonic treatment. After that wafers were immersed in isopropil alcohol and dried.

3.Forming of the contacts to TCO layer. Thin Al films of 0.3 mcm thickness and of 5 mm in length were deposited through the mask on TCO layer. The forming of layer was carried out by magnetron sputtering at 150 0C.

4.Series depositing of i-, n-layers of a-Si:H [1] and p-layer of a-SiC:H [2] for the forming of p-i-n structure was used. After the depositing of each layer (p-type of a-SiC:H, i-type intrinsic a-Si:H, n-type a-Si:H with the thicknesses of 9 nm, 450 nm, 50 nm, respectively) the reaction cameras were changed. Different regimes of deposition were used for the formation of amorphous layers.

5.The forming of the back side contact of the p-i-n structure.

The measurements of an I-V characteristics of solar cells at room temperature showed that with the increasing of contact size the efficiency of solar cell decreases. This may be due to the increase of the series resistance of solar cell. It was found that for the thicknesses (0.317 and 0.670 mcm) for i-type a-Si:H the efficiency of solar cells are practically equal.

So, for the first time solar cells with efficiencies riching 7% were fabricated with using of high rate deposition technology in low frequency glow discharge. The received results showed perspectiveness of this technology for the fabrication of optoelectronic devices.

Referencess

1. B.G. Budaguan, A.A. Sherchenkov, A.E. Berdnikov, V.D. Chernomordik. The high-rate method of the deposition of amorphous silicon. "Microelectronics, 2000, v.29, No.6, p.442-448."

2.B.G. Budaguan, A.A. Sherchenkov, A.E. Berdnikov, J.W. Metselaar, A.A. Aivazov. The properties of a-SiC:H and a-SiGe:H films deposited by 55kHz PECVD. "Mat. Res. Soc. Symp. Proc. v.557, 1999 Materials Research Society."

AB INITIO CALCULATIONS OF MULTILAYER RELAXATIONS OF CU(331), CU(511) AND CU(211)}

Abdelkader Kara and Talat S. Rahman
Department of Physics, Kansas State University, Manhattan, Kansas 66506, USA.
Klaus Peter Bohnen and Rolf Heid
Institut fuer Festkorperphysik, Forschungszentrum Karlsruhe, Karlsruhe, Germany.

In order to understand the effect of local geometry and coordination surface structure and dynamics and to address several outstanding issues, we have carried out ab initio electronic structure calculations of the multilayer relaxation of three stepped Cu surfaces with similar terrace width but varying terrace and step-edge orientations. The calculations are based on density functional theory in the local density approximation with norm-conserving, non-local pseudopotentials in the mixed basis representation. On all three surfaces the outermost layer contracts inwards, in agreement with experimental findings and previous calculations. Interesting results are found for d_{23} (d_{ij} being the spacing between layers *i* and *j*) which for Cu(331) is different (-3.3%) from that obtained by EAM potentials (+1.7%) and LEED data (+0.4%). On Cu(511), d_{23}=-10.7% which is in favor of results from LEED (-6.1%) rather than those from X-ray scattering (+8.1%). The other calculated interlayer separations for Cu(511) are also in better agreement with the LEED data rather than those from X-ray measurements. In general, these calculations predict similar relaxation patterns for the three surfaces, while previous calculations with EAM potentials had found the relaxation and local vibrational properties of Cu(331) to be different from those of Cu(511) and Cu(211). We discuss the implications of the calculated relaxation patterns on the dynamical properties of these surfaces.

THE EFFECT OF LOW ENERGY GRAIN BOUNDARIES ON ELECTROMIGRATION BEHAVIOUR OF MULTIGRAIN ALUMINUM THIN FILM CONDUCTORS

Kononenko O.V. †, Matveev V.N. †, Field D.P. ‡
† Institute of Microelectronics Technology and High Purity Materials, RAS, 143432 Chernogolovka, Moscow district, Russian Federation.
E-mail: oleg@ipmt-hpm.ac.ru
‡ School of Mechanical and Materials Engineering, Washington State University, Pullman, WA 99164-2920 USA.

Electromigration rates in polycrystalline interconnect lines are controlled by grain boundary diffusion. As such, reliability of interconnects is a direct function of the grain boundary character distribution in the lines. In the present work, drift velocity experiments were performed on multi-crystalline lines of pure Al to determine the electromigration activation energy of the lines. Lines cut from films processed by partially ionized beam deposition techniques were analyzed. One set of lines was analyzed in the as-deposited condition, while the other film was annealed before testing. The measured drift velocities varied dramatically between these two types of films, as did the grain boundary character distributions measured by orientation imaging. The data were analyzed based on Borisov's equation to obtain mean grain boundary energies. Grain boundary energy of the film with poor electromigration performance was calculated to be that reported for random boundaries, while that for the more reliable film was calculated to be that reported for twin boundaries in Al. Percolation theory is used to aid in explaining the results based upon the fraction and connectedness of «special» boundaries in the films.

SEM observation of Al conductors showed that grain boundary structure strongly influences the morphology of electromigration damage formed on cathode and anode edges. In the films containing a high fraction of low angle grain boundary hillocks with flat tops are formed on the anode edge. Cathode edge drift occurs by collapse of grains nearest to the edge. It leads to the

expansion of the drifting front up to 2-6 μm. In the case of low fraction of low angle grain boundaries, long and narrow whiskers and tooth paste like hillocks grew on the anode edge. The cathode edge was quite sharp. Analysis of data was made on the basis of the model of creep affected electromigration advanced by Glickman [1].

Referencess

1. E. Glickman, M. Nathan, Microelectronic Engineering v.50 (2000) p.329.

ANISOTROPIC WET CHEMICAL ETCHING OF CRYSTALLINE SILICON: ATOMISTIC MONTE-CARLO SIMULATIONS AND EXPERIMENTS

M.A. Gosalvez[a], R.M. Nieminen[a],
P. Kilpinen[b], E. Haimi[b], V. Lindroos[b]
[a] Laboratory of Physics,
Helsinki University of Technology, 02015 Espoo, Finland
[b] Laboratory of Physical Metallurgy and Materials Science,
Helsinki University of Technology, 02015 Espoo, Finland
e-mail: mag@fyslab.hut.fi

An atomic-scale simulation model for anisotropic wet chemical etching of Si (100)-wafers covered with masks of arbitrary shape and a series of experiments for comparison are presented. The model assumes that the probability of removal of a surface atom depends on the number of first and second neighbors. A removal probability function is presented in order to describe the probabilities of removal corresponding to the different surface atoms having different numbers of first and second neighbors.

Etching experiments on Si(100)-wafers using 10 wt-% KOH solution at 75 C^{o} are presented and the performance of the model is evaluated against them. We compare the underetched structures obtained in the simulations and experiments using a mask pattern consisting of a wagon wheel and a set of

rectangular frame-like openings with varying orientation. The simulations show good agreement with the experiments. The model predicts the existence of fastest-etched planes in accordance with experiment, and describes accurately the evolution of under-etching below the masks for all mask orientations, including the slopes of the planes appearing below the mask.. The results show that the cooperative effects of atoms evolving according to a simple rule generate most features of the meso- and macroscopic etching patterns. They also show that the use of only first neighbors or a partial incorporation of the second neighbors in the modeling strategy is not sufficient in order to describe the under-etching processes and that the second neighbors must be fully incorporated into the model.

AG AND SN SURFACE PHASES IN COPPER-BASED ALLOYS

G.P. Vyatkin, T.P. Privalova, A.E. Chudakov, S.I. Morozov

Southern Ural State University, Lenin str, 76, Chelyabinsk, Russia, 454080

Surface composition and structure can be very different that in the bulk. Knowledge of the structure of alloy surfaces is very important for the understanding of many surface phenomena. Enrichment of the surface in Cu–Ag and Cu–Sn alloys is found by means of spectroscopic experiments and computer simulation, but in solid state and for low Ag and Sn bulk concentration only. Our spectroscopic and computer experiments confirm these results and show that surface segregation exists in the liquid state even. Moreover, this effect can be found up to about 15 at.% of Ag and Sn in bulk. Our experimental method is temperature-programmed desorption (TPD), computer simulation is based on Monte Carlo method with Embedded-Atom Method (EAM). EAM is powerful technique based on density-functional theory.

In $Cu_{1-x}Ag_x$ (x=0.005 .. 0.13) alloys both methods show the surface concentration of Ag as high as 60±10 at. % in polycrystalline state and 30-35 at.% Ag in liquid state. In these ranges surface concentration of Ag decreases with the increase of bulk concentration in crystalline state and it increases in liquid state. 300% change of bulk concentration corresponds 10% change in surface. This fact can be explained by presence of specific surface phases. Simulation shows a set of phases in solid state depending on surface index. In liquid state only p(1x1)Ag phase is found. The same phase is for (111)Ag surface. By the way, the structure of liquid copper surface is very similar to (111)Ag.

In $Cu_{1-x}Sn_x$ (x=0.005 .. 0.17) alloys character of tin segregation is the same as segregation of silver in Ag–Cu alloys. But surface concentrations of tin in the 1st atomic layer are two times lower both in solid and liquid state than in Ag–Cu alloys. Then surface segregation occupies more atomic layers than in Ag–Cu alloys. The most typical tin structure in surface is chain. For Ag–Cu alloys close-packed structures or islands are typical.

Initial TPD-experiments with ternary $Cu_{99}Ag_{0.5}Sn_{0.5}$ alloy show significant surface segregation both silver and tin in polycrystalline state. High surface concentration of tin and silver saves in liquid state too. Now the experimental researches and modeling are in progress.

This work is supported by Russian Ministry of Education T00–5.1–3007 and RBRF-Ural N01–03–96420.

PROPERTIES OF EFFECTIVE NOISE FOR SYSTEMS WITH QUENCHED RANDOMNESS

S. Majaniemi
Laboratory of Physics and Helsinki Institute of Physics, Helsinki University of Technology, FIN-02015 HUT, Finland
email majaniem@rock.helsinki.fi

The fluid-fluid phase boundary wandering in a disordered medium such as a Hele-Shaw cell filled with porous material experiences exotic correlations which are quite different from the static correlations characterizing the material properties of the medium. The equation of motion for the phase boundary is obtained by projecting out the bulk degrees of freedom. It is used to determine the noise properties of the nonlinear Langevin equation describing the dynamics of lower dimensional collective coordinates like interfaces and contact lines. Effect of local conservation law at the level of bulk dynamics changes the universal properties of the fluctuation of collective coordinates in a non-trivial way. As a particular example we use the refinements of the spontaneous imbibition model originally introduced for wetting of random medium [1].

Referencess

1. M. Dube, M. Rost, K.R. Elder, M. Alava, S. Majaniemi, T. Ala-Nissila, Eur. Phys. J. B v15 (2000) p. 701.

FIRST-PRINCIPLES CALCULATIONS FOR THE CO OXIDATION ON PD(111) SURFACES

P. Salo[1], M. Alatalo[1], K. Honkala[2] and K. Laasonen[2]
[1]Helsinki Institute of Physics and Laboratory of Physics, Helsinki University of Technology, P.O. Box 1100, FIN-02015 HUT, Finland
[2]Department of Chemistry, P.O. Box 3000, FIN-90014 University of Oulu, Finlandemail Petri.Salo@hut.fi

A fundamental aspect in the modeling of chemical reactions on metal surfaces is the study of the energetics and the electronic and structural properties of such surfaces. One catalytically interesting material is Pd. We perform first principles pseudopotential calculations for the energetics of the reactions between a CO molecule and an O atom on Pd surfaces using the density functional theory with a generalized gradient approximation. The reaction paths and transition states for the CO oxidation are systematically studied using the nudged elastic band method[1]. A low energy barrier for the oxidation is found for an initial state where the CO molecule and the O atom both are located at fcc sites. In the final state the linear CO_2 molecule lies down horizontally and it is bound very loosely on the Pd surface. The energy barrier and transition state found for this process are similar to those for the CO oxidation on Ru(0001) surfaces[2].

Another process with a low activation energy starts with an initial state where the CO molecule and the O atom is located at a top and fcc site, respectively, and the final state is similar to that mentioned above. This process is rather similar to that found for the CO oxidation on Pt(111) surfaces[3].

Referencess

[1] H. Jonsson, G. Mills and K. W. Jacobsen, in “Classical and Quantum Dynamics in Condensed Phase Simulations”, ed. by B. J. Berne, G. Ciccotti, and D. F. Coker (World Scientific, Singapore, 1998).

[2] C. Stampfl and M. Scheffler, Phys. Rev. Lett. v 78, 1500 (1997); Surf. Sci. v 433-435, 119 (1999).

[3] A. Alavi, P. Hu, T. Deutsch, P. L. Silvestrelli, and J. Hutter, Phys. Rev. Lett. v 80, 3650 (1998).