# TUESDAY POSTER PRESENTATIONS

# ICACS-25

# Experimental determinations of the energy straggling of slow ions in thin foils: the effects of foil roughness and projectile slowing down.

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Different theoretical models on the energy loss of ions in solids predict that the energy loss straggling $\Omega$ in metallic targets should be proportional to the ion velocity $v$ in the limit $v << v_F$, where $v_F$ is the Fermi velocity of the target electrons. This is a common prediction of linear [1,2] and non-linear [3] theories (such as Lindhard´s dielectric model in the first case or the Density Functional Theory (DFT) in the second). Previous comparisons of the theoretical DFT predictions with experimental values [4] showed a fair general agreement. However, in a recent publication [5] an apparent deviation from the predictions of the theoretical models was reported.

The problem of determining the so-called intrinsic straggling from experiments in the low energy range is a complex problem, due to the combined effects of slowing down in a thin foil and roughness effects at the incident and emerging surfaces. The total straggling that can be measured after ion-beam transmission through a thin foil is a convolution of the intrinsic straggling (arising from the statistical nature of the energy loss phenomenon) and the surface roughness straggling which depends on the stopping power.

We report here the results of experimental and theoretical analysis of this problem. The theoretical analysis includes a study of the influence of foil roughness and energy decrease in a thin foil. The experimental analysis includes determinations of the energy loss straggling of proton beams in thin self-supported foils of C, Si, Ag, Cu, Au and Bi. We show that a quantitative analysis requires a careful evaluation of the intrinsic straggling and foil roughness, as well as consideration of the decrease of ion energy within the foil. We show that failure to consider all these effects in a precise way may lead to erroneous values of the intrinsic straggling.

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# Computer-simulation study of the angular dependence of the energy loss of light ions in solids

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The interaction of ions with solids in the range of low energies is a subject of great current interest in relation with theoretical studies and experimental determinations of the energy loss and straggling coefficients for different ions and materials. Several recent publications have reported interesting effects that become particularly relevant at low energies, such as band structure effects (threshold effects), isotopic effects in the angular dependence of the energy loss, and non-linear effects in the screening and transport coefficients of ions in solids.

In this work we perform a computer simulation study of the energy loss of ions in solids and compare the results with experiments. The simulation code is based on the Monte Carlo method to represent the probability of ion collisions and deflections within the solid as well as fluctuations in the inelastic energy loss. The electronic energy loss is represented using the results of the density functional theory [1] as well as our own non-linear model, which includes band structure effects [2-4]. To represent realistic targets we also include in the simulations the effects of foil roughness. Using this approach we analyze the angular dependence of the energy loss and the associated energy straggling of protons, deuterons and helium ions transmitted through thin foils of different elements. Using different simulation options we are able to assess the contributions of elastic energy losses, path-length enlargement, foil roughness, and isotopic differences between protons and deuterons, as a function of the emergence angle. The results of these simulations are compared with those obtained from the SRIM code and with various experimental results.

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# Evolution of Nanostructures in a Graded Multi-trilayer System upon Ion Irradiation

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Periodic multilayers are used as efficient reflectors of extreme ultraviolet radiation to hard x-rays. They are also used in x-ray telescopes for applications in x-ray astronomy. More recently graded (depth-graded, laterally-graded, and double graded) multilayers have found increasing applications [1]. Double-graded multilayers are used for broad band focusing. Stability of multilayers against heating and charged particle irradiation is an important aspect. Pt/C multilayers have been used for making x-ray telescopes. However, for detection of x-rays above 80 keV there is strong absorption of x-rays in the Pt layers (Pt K-absorption edge is at ~ 79 keV). Suitable alternatives, such as Ni/C or Pt/Ni/C multilayers are being explored. We have earlier investigated ion irradiation effects in Pt/C multilayers [2-4]. In these multilayers individual layer thickness is about a couple of nanometers. Ion irradiation was found to form nanoparticles with pseudo-ordering at new length scales. Here we present ion irradiation effects in a double-graded Pt/Ni/C multi-trilayer system with 15 tri-layers or repeat units with a total thickness of ~ 100 nm, grown on a float glass substrate by ion-beam sputtering technique. Irradiation was carried out with 2 MeV Au ions at five different fluences between $1 \times 10^{14}$ and $2 \times 10^{15}$ ions/cm$^2$. The samples were investigated by x-ray reflectivity (XRR), x-ray standing wave (XSW) and cross sectional transmission electron microscopy (XTEM) measurements. A 4-10% expansion of the multilayer thickness along with an increase of interface roughness has been observed. At the highest fluence complete mixing between Pt and Ni layers and nanoscale grain growth of Pt-Ni alloys have been observed. Additionally Pt-Ni alloy nanoclusters encapsulated within the C layers have been found. The results are understood in the light of positive heat of mixing between Pt and C, and Ni and C, and negative heat of mixing between Pt and Ni. The effect of heat of mixing is dominant at high fluences in irradiation

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# Hydrogen negative ion formation on a graphite HOPG surface.

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In past years scattering of hydrogen ions on graphite surfaces has attracted considerable attention in relation with the development of plasma confinement devices, negative ion sources, the understanding of plasma/wall interactions and divertor physics [1-6]. Some experiments have shown that in scattering of atomic and molecular hydrogen ions on polycrystalline graphite and diamond surfaces at low energies (below a few keV) high negative ion fractions of have been observed. Because of the high workfunctions of these surfaces the observation of high negative ion yields were surprising. Some discrepancies amongst different experiments were noted. We therefore performed and report here a study of hydrogen negative ion formation on highly oriented pyrolitic graphite (HOPG), for grazing scattering conditions previously used for various metallic and dielectric surfaces [7-9]. Inspite of the large workfunction of the surface the negative ion fractions were found to be quite large: significantly larger than for metal surfaces such as Mg or Al. The dependence of the anion fraction on the exit angle with respect to the surface resembles that of metals as predicted by recent calculations of Goldberg et al [5,6]. However the magnitude is much larger.

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Tu-005

# Secondary Electron Emission from a Thin Carbon Foil by $H^+$, $He^{2+}$ and $Li^{3+}$ of 1 MeV/u

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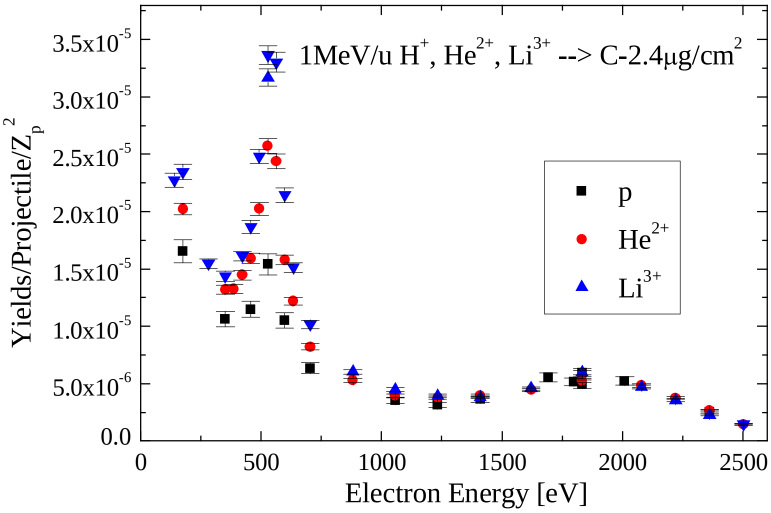
The statistical distributions of the number of simultaneously emitted secondary electrons (SEs) from a thin carbon foil have been measured with $H^+$, $^4He^{2+}$, and $^6Li^{3+}$ ions of 1 MeV/u. In this experiment, the forward- and backward-emitted SE's have been measured simultaneously in coincidence with foil-transmitted ions in order to investigate their correlation. As a result, it is found that the forward- or backward-emitted SE yields, that is, the mean numbers of the forward- or backward-emitted electrons per projectile decreases gradually with increasing the number of SEs in the opposite direction irrespective of projectile species. This trend is quite understandable assuming that the amount of the internal secondary electrons produced by the projectiles can be scaled with the square of the projectile atomic number, $Z_p$, over the entire electron velocity. On the other hand, the inclusive SE yields divided by $Z_p^2$ become smaller with increasing $Z_p$ both in the forward and backward directions. To look into further details, we have measured the energy spectra of the emitted electrons from a carbon foil of a similar thickness to that employed in the number distribution measurement. Figure 1 shows the result. As is clear from the figure, the $Z_p^2$-scaling holds at the energy region of the binary electron. The observed reduction of SE yields from the $Z_p^2$-scaling seems to be due to the collective electric field along the projectiles path[1-3].



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# Translational Energy induced Oxidation of Ni(111) Surface at Room Temperature by Supersonic $O_2$ Molecular Beam

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Although the Ni(111) surface reacts with $O_2$ molecules to form a thin oxide layer on the surface at 147 K showing a Langmuir-type oxygen uptake curve, a plateau appears in an intermediate region of the oxygen uptake curve at higher temperatures [1]. This behaviour was explained by a two-dimensional (2D) oxide island growth model [2, 3]. Generally speaking, the surface chemical reaction rate of incident molecules depends also on their translational kinetic energy. Indeed, the oxygen uptake curve for the Ni(111) oxidation by an $O_2$ beam with a hyperthermal energy of 0.6 eV at 300 K indicated a kinetics change from the 2D model to the Langmuir type [4]. Translational energy effects have been also shown for the initial sticking coefficients [5].

The incident energy of $O_2$ molecules was increased up to 2.3 eV by using our supersonic molecular beam (SSMB) technique. Using this technique, the effects of $O_2$ incident energy have been widely studied by soft x-ray photoemission spectroscopic surface analysis with high brilliance and high energy-resolution synchrotron radiation. Both an $O_2$ SSMB and the monochromatic synchrotron radiation were irradiated on a sample surface simultaneously. Real-time in-situ photoemission spectroscopy of chemical bonding states for the oxidized surface was conducted during SSMB irradiation.

Oxygen uptake on the surface has been observed at various $O_2$ incident energies higher than those of previous reports. The first plateau, which appears at an intermediate region of the oxygen uptake curve, was found to disappear with increasing $O_2$ incident energy. Furthermore, an oxygen content at saturation of 5.5 ML was observed for an incident energy of 2.3 eV. This is 1.8 times larger than that observed at a low energy region of 0.06 eV to 0.6 eV (3 ML). These observations can be attributed to the influence of activated adsorption mechanisms. The initial sticking rate continued to increase as incident energy increased up to 1.0 eV, and a remarkable re-increase was observed in the region around 2.3 eV. The first increase is due to the activated dissociative adsorption of $O_2$ molecules through a potential energy barrier of 1.0-eV height, and the second increase around 2.3 eV implies that another potential energy barrier exists with a height larger than 2.3 eV. Higher $O_2$ incident energy leads to higher formation rates and higher contents at saturation for the NiO component.

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Tu-007

# The Positron Spur, Diffusion, and the Effective Interaction in the Liquid Phase

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Since fluctuation from the equilibrium medium is preferable in liquid phase, localization of charged particles like positrons is highly induced. Free energy density functional theories provide self-trapping as a solution of the charged particle in a given host liquid. Gramsch et al.[1,2] have observed very different behavior of the diffusion length $L_+$ of positrons in liquid and solid metals by means of a slow positron beam. That is, on melting $L_+$ decreases remarkably, and the liquid phase $L_+$ increases with temperature. Kanazawa and coworkers [3-6] proposed a qualitative explanation for the increase of the positron diffusion length with temperature in the liquid phase, by using the theoretical formula, which is based on the gauge-invariant effective Lagrangian with spontaneously broken density (the hedgehog-like fluctuation) and the massive internal gauge fields. In this study, extending the theoretical formula [3-6], we shall discuss the positron energy loss mechanism and the effective interactions in the liquid phase.

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# Materials modifications using MeV ion beams obtained from small/medium sized accelerator facilities

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Materials modifications using swift heavy ion beams provided by large scale accelerators have been used for many years in a wide variety of ways, e.g. to produce ion tracks or to modify shape of nanoparticles. In all this applications the most relevant parameter for materials modification is electronic stopping power and not the ion total kinetic energy. For many materials, ions delivered from the medium and small size accelerators have sufficiently high values of electronic stopping power to modify materials in different ways. In the present contribution, we review recent experimental and theoretical achievements of the Zagreb group in this field. These include swift heavy ion tracks in $SrTiO_3$ [1], [2], development of single ion irradiation setup [3] and ion beam assisted formation of ordered QD arrays [4]. In all cases, ion beams delivered from the 6 MV Tandem Van de Graaff accelerator based at RBI, Zagreb have been used. Together with experimental work, we present thermal spike model, which was applied to describe obtained features. Recent description of highly charged ion tracks using an extension of the thermal spike model is also presented [5].

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Tu-009

# Electronic stopping of slow light ions: Some experimental aspects

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Many experiments have shown that in contrast to common expectation, electronic stopping of slow light ions, $S_e$, may depend on the ion velocity in a quite complex way, due to band structure effects [1, 2]. There are various possibilities to determine $S_e$, but in any case it is a demanding task to measure $S_e$ for ion energies below 1 keV. Let us consider this situation in detail. Obviously, any direct measurement of Se has to determine two types of information, typically sample thickness and energy loss of the ions.

In a transmission experiment a thin self-supporting foil is required; in backscattering a thin supported film may be used. In both cases, the request of the energy loss $\Delta E$ to be small compared to the ion energy, E, leads to a very low thickness of 10 nm or even less. Thus, quantitative thickness determination is demanding, with RBS being one of the most promising techniques, at a level of accuracy of better 5 %. What is also common to both experimental approaches is that due to the large scattering cross section at low ion energies the assumption of a straight trajectory is not justified anymore. Consequently, influences of multiple scattering and atomic collisions have to be taken into account when deducing Se from the measured energy loss. This requires non-trivial treatment, since not all impact parameters will contribute to the atomic collisions. In addition, surface contaminations may represent a major source of systematic error in a transmission experiment, as pointed out by Mertens, since surface impurities contribute to the energy loss of the ions [3]. In backscattering, surface impurities hardly lead to a systematic error [4]. Finally, also thickness inhomogeneity would lead to erroneous energy loss data, since thinner parts of a foil will lead to a narrower angular distribution than the thicker ones [5].

In backscattering, the use of thin layers can be avoided, by comparing the height of backscattering spectrum of the sample of interest to that of a material of known stopping. When the spectrum height ratio is also determined in a Monte-Carlo simulation which allows for multiple scattering and electronic energy loss, $S_e$ for the material of interest may be deduced from the known $S_e$ of the reference material. In this way, all possible systematic errors may be eliminated, the main source of uncertainty being the amount of primary ion charge impinging on the samples, which may introduce a possible error of 5 %. Thus, overall accuracy for $S_e$ better 10% should be achievable even in this regime.

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# The effect of conductivity on ion guiding through insulating capillaries

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First experiments on guiding of highly charged ions through straight insulator nano-capillaries showed a remarkable effect: after an initial charge up phase, the ion beam could be steered by tilting the capillary axis while remaining in the initial charge state indicating that the transmitted ions never touched the inner walls [1]. Subsequent experiments confirmed this guiding effect also for macroscopic glass capillaries, both straight [2, 3] and tapered ones [4]. Microscopic simulations revealed that a self-organized charge up of the capillary walls due to preceding HCI impacts leads to an electric guiding field, which steers the incoming projectile ions along the capillary axes [5]. Ion guiding ensues as soon as a dynamical equilibrium of charge-up by the ion beam and charge relaxation by bulk or surface conductivity is established. In this contribution we show that a key control parameter for guiding is the small residual electric conductivity of the highly insulating capillary material whose dependence of temperature $\sigma(T)$ is nearly exponential.

We use a single straight macroscopic glass capillary (inner diameter: 160 $\mu$m; length: 11.4 mm) made of Borosilicate (Duran) for which the guiding effect has been previously established [2]. The current experimental set-up allows for a controlled and uniform temperature variation of the glass capillary between -30°C and +90°C [6]. Within such a moderate variation of the temperature the conductivity changes by almost five orders of magnitude. Our experiments [7] show that increasing the temperature of a glass capillary and therefore its conductivity leads to a reduction of guiding and, eventually, to a complete disappearance of the guiding effect. This strong temperature dependence can be employed to stabilize guiding against Coulomb blocking due to a high incident ion flux [8].

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Tu-011

# Detection of Cu Vacancies During the Phase Transition of the 0.5 ML Sn/Cu(001) Surface Alloy by Direct Recoil Spectroscopy

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Atoms deposited on metal surfaces may form islands siting above the top substrate layer or they may substitute some atoms to form a surface alloy. Formation of a surface alloy implies the movement of many atoms, often leading to surface reconstruction and or vacancy creation. Direct detection of vacancies is important to understand the surface behavior but usually it represents a difficult task for most surface techniques. This is not the case in ion scattering at surfaces since a missing atom implies an extension of the interatomic distances and therefore a reduction in either the shadowing or the blocking critical angle, so by tuning the azimuthal and incidence angles appropriately one can obtain a backscattering signal or a recoiling signal that appears only if a vacancy has been created (Figure 1). In this work we use these effects to characterize the line of vacancies formed by the adsorption of Sn on the Cu(100) surface. In addition, we follow the evolution of these vacancies during the reversible crystallographic phase transition of the 0.5 ML Sn/Cu(100) taking place around 360 K ((3√2x√2)R45°→(√2x√2)R45°). Combining this technique with MC simulations, we conclude that the high-temperature phase is disordered. The phase transition can therefore be characterized as an order-disorder transition driven by the Cu vacancies entropy.

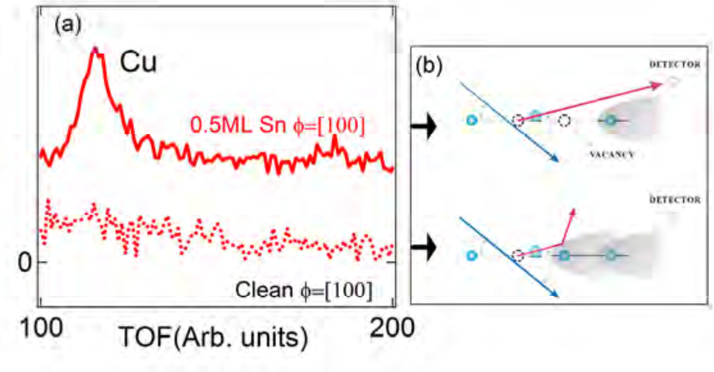

Figure 1 (a)TOF spectra for the clean surface and for Sn/Cu. The appearance of the Cu direct recoil peak is related to the formation of a vacancy line upon adsorption of Sn. (b) Schematics of the blocking effect.

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Tu-012

# Monitor for Detection and Analysis of Electrons and Ions in Geostationary Orbit Satellites

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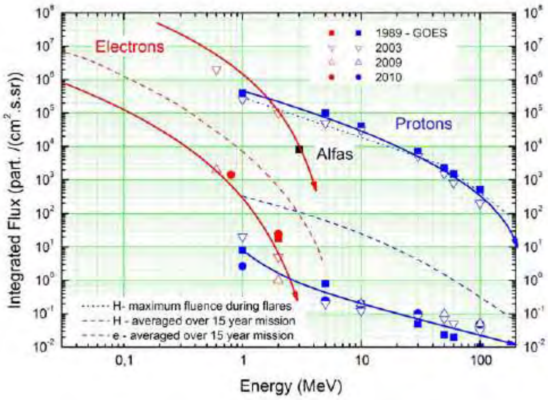
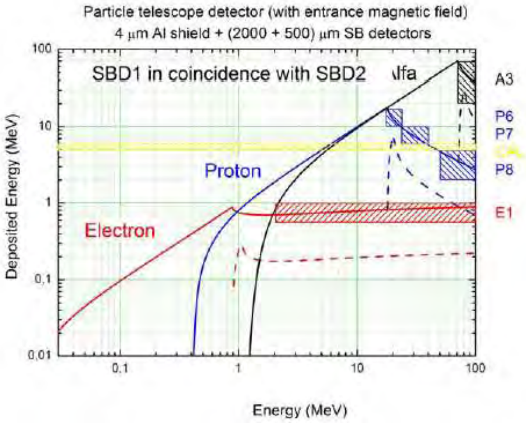
Commercial satellites in geostationary orbits are exposed to a strong environment (mainly electrons and protons) that generates a degradation of the satellite surfaces, materials, and electronic components, thus limiting the life of the satellite. In this context, monitoring the space weather to provide signals of warnings and to characterize the spectrum of both electrons and ions becomes a critical issue for the satellite itself, and can also be used to study the solar activity, particularly during solar flares. The requirements for such a monitor include 1) more than ten orders of magnitude in the variation of the fluence, 2) more than 5 orders of magnitude in the energy range of the particles to be detected, 3) expected life of more than 15 years unattended. In this report we present a design and preliminary tests of a simple instrument for monitoring the electrons and ions hitting the surface of an Argentinean commercial GEO satellite. First we present estimations of the space weather to be encountered by the monitor and of the expected effects (deep and surface charging, SEUs,) on its components. The detector design based on a combination of collimators, filters and surface barrier detectors is then discussed. Calculations of stopping and ion ranges in solids are used to choose the best materials for shielding the detectors according to the energy thresholds of operation. Some considerations about the analog and digital electronics, and about the thermal behavior of the detectors are finally provided.



Expected space environment during low and high solar activity.



Example of the estimation of the energy deposition of the particles on two surface barrier detectors after transmission through the entrance foil.

# Reactive MD Study of Hyperthermal Si-Oxidation Mechanisms in Ultrathin $a$-$SiO_2$ Films

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Recently, interest in hyperthermal oxidation of the Si-surface as an alternative to thermal oxidation has been rapidly increasing, especially for semiconductor applications and spacecraft investigations, especially since hyperthermal oxidation can be carried out at room temperature [1]. Although numerous studies have elucidated the overall oxidation behavior, various aspects are still poorly understood [e.g., 2, 3]. There are still open questions regarding the growth mechanism in hyperthermal oxidation. This contribution therefore focuses on the study of the oxidation of ultrathin amorphous silica ($a$-$SiO_2$) surfaces by both atomic and molecular oxygen with initial energies of 1 eV and 5 eV. These atomic-scale investigations were carried out using reactive molecular dynamics simulations employing the ReaxFF potential.

Hyperthermal oxygen adsorption on and penetration depth in an $a$-$SiO_2$ film with an initial oxide thickness of about 10 Å is analyzed and compared with impacts on a pure Si(100){2x1} ($c$-Si) surface at room temperature. Our results demonstrate that the oxygen mostly resides in the silica region rather than in the $a$-$SiO_2|c$-Si interface at low temperature. However, at higher temperatures, starting at about 700 K [4], oxygen atoms can diffuse through the oxide layer and react with the $c$-Si region. The new oxide layer formation by diffusing oxygen atoms at high temperature is discussed as well. The oxidation mechanism is similar to the oxide formation mechanism in the thermal oxidation case, which can be explained by well-known Deal-Grove mechanism [5].

This study is useful for the fabrication of silica-based devices in the micro and nanoelectronics industry, and more specifically for the fabrication of metal-oxide-semiconductor devices.

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# Characterisation of nanostructures induced by slow highly charged ion bombardment of HOPG

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Earlier studies, which have identified highly charged ion - induced defects on HOPG surfaces as regions of enhanced friction [1] have been extended by measuring the microscopic friction coefficient at the impact sites and the surrounding matrix by means of lateral force microsopy. Additional investigations have been performed on samples irradiated with ions in very high charge states ($Xe^{40+}$ and $Bi^{62+}$), and, for the first time, defects have also been found employing the intermittent contact AFM mode (Figure 1), where friction forces are basically eliminated from the measuring process (no pseudo-topographic contributions arising from friction). This is a strong indication that there is indeed a true topographic modification (as found for other target surfaces; see [2] and refs therein) if the impinging ions exceed a certain potential energy threshold. Furthermore, defects have been imaged in the conductive AFM mode, where strong local changes (imaging at atomic resolution) in the conductivity are apparent.

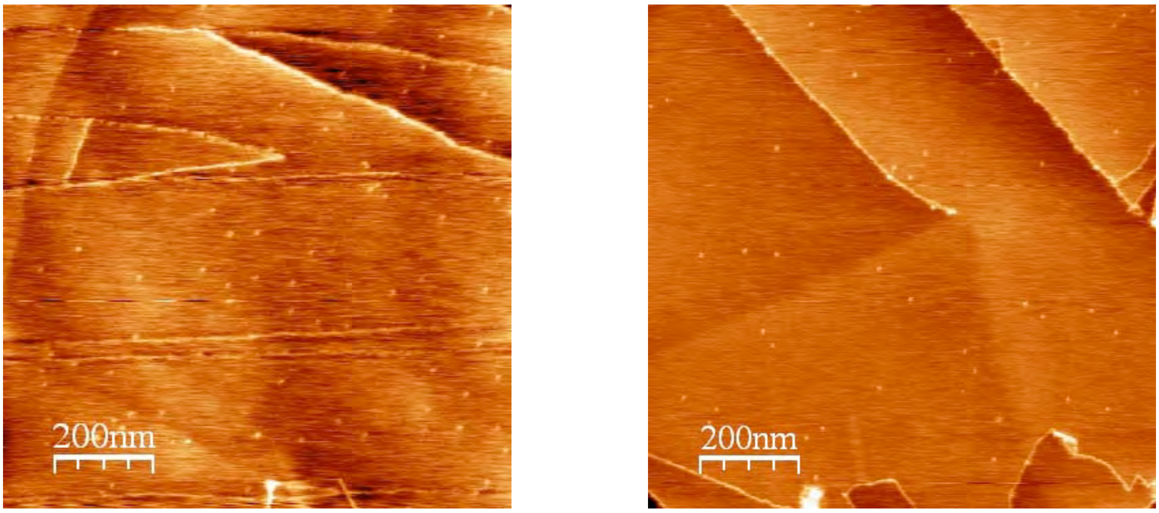

Figure 1: Intermittent contact mode AFM images showing defects induced by $Xe^{40+}$ ($E_{kin}$ = 40 keV) ions (left) and $Bi^{62+}$ ($E_{kin}$ = 37 keV) ions (right) on HOPG.

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# Energy Loss and Electron transfer processes in fluorine scattering on oxygen covered Ag (110) – crystal azimuthal dependence

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We present measurements of energy-losses and electron transfer processes in fluorine ions and atoms scattering on clean and oxygen covered Ag(110) surface. In this system chemisorption of oxygen results in an added row (nx1) reconstruction and in an increase of surface work function. Our oxygen covered Ag(110) measurements correspond to various added row reconstructions (e.g. 8x1, 4x1 and ultimately 2x1). Measurements were performed for 1 to 4 keV ion energies under surface channelling conditions for different surface azimuths. Energy losses for the clean and oxygen covered surface are measured for various azimuthal orientations and are observed to change strongly after oxygen adsorption. In general, adsorption of oxygen results in a fairly strong decrease in the negative ion fraction. Some variations on crystal azimuth were observed. The decrease in $F^-$ production can be associated with changes in electronic structure as a function of oxygen coverage and trajectory dependent changes. Energy loss results are discussed in the light of trajectory calculations of ions scattered under grazing incidence conditions on the surface. Using non-linear models for stopping power, *ab initio* crystal structure calculations of the electronic density and semi-classical simulations [1, 2], we obtain data that is in good agreement with experimental results. These simulations in particular allow us to properly take into account the variations of the surface electronic density and hence obtain an accurate description of the energy loss processes for ion scattering along various azimuthal orientations of the target. We are thus able to describe the multi peaked structures observed in the energy losses for certain azimuthal orientations and assign them to specific types of trajectories.

* The authors regret the untimely death of Ana Rita Canario-Bettencourt.

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# Surface Nanostructuring of $LiNbO_3$ by High-Density Electronic Excitations

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Lithium niobate ($LiNbO_3$) single crystals were irradiated with high energy gold ions (0.5-2.2 GeV) at the UNILAC (GSI) and with 150-keV highly charged Xenon ions from an EBIT (Electron Beam Ion Trap, HZDR). The surfaces of the irradiated crystals were analyzed by scanning force microscopy showing very similar topographic changes. Swift heavy ions and slow highly charged ions produce hillock-like surface nanostructures on this surface. In both cases, the energy deposition of the ions is characterized by dense localized electronic excitations and efficient transfer to the lattice. Furthermore, the irradiation results in a shift in the band gap as evidenced by UV-Vis absorption spectroscopy. Specific modifications (e.g. hillock size, energy loss threshold) induced by slow highly charged ions are discussed in comparison with effects due to the electronic energy loss by swift heavy ions.

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Tu-017

# Modeling Secondary Electron Emission from Nanostructured Materials in Helium Ion Microscope

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The scanning ion microscope (SIM) using a helium ion beam [1] has been a new tool that gives us for nanometer-scale resolution and effective contrast schemes for structural and compositional analysis. Although the image formation in SIM by detecting secondary electrons (SE) is similar to that in conventional scanning electron microscopes (SEM), there are some differences in the properties [2]. We present here a Monte Carlo study on imaging for nanostructures and charging for analyzing insulating $SiO_2$ layers.

Irrespective of whether a material is conducting or insulating, SE emission can be modeled by a three-stage process [3]. The first stage involves generation of internal SEs by ions penetrating the material and target atoms recoiled by them. The second stage is transport of these SEs to the surface. In the third stage, the SEs escape over the surface barrier. For $SiO_2$, the model is combined with charge accumulation, inducing electric field formation in the material and in the vacuum, and analysis of equation of motion for SEs emitted in the vacuum [4]. The sample nanostructures consist of $SiO_2$ layers with trapezoidal lines and trenches formed on a Si substrate, the surface of which are scanned by a zero-sized He ion beam for calculation of the SE profile. There appears large and sharp peak of the SE yield at the edge of the structures. The height of the peak is much more than that for an electron beam, whereas the width is less. This indicates that the structures are more clearly observed by SIM than by SEM.

The $SiO_2$ layer is charged positively due to ejection of SEs and injection of positive ions, which draw the ejected SEs back to the surface. The charging voltage progressively increases and the net SE yield decreases more strongly than for the electron beam, eventually vanishing.  However, it increases when the ion incidence occurs at the position near the edge of the structure in a similar way to that observed for the electron incidence. The increase in the yield is more localized than for electron incidence. Furthermore, when the trench is irradiated with the ion beam, the side wall of the trench becomes negatively charged from re-entrance of SEs emitted from the bottom of the trench. The negative charging increases the SE yield at the bottom, because it assists SEs, which may be reabsorbed by the side wall if they are not charged, to exit the narrow trench. This enhancement in the SE yield is stronger for the ion beam than for the electron beam.

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Tu-018

# THE EROSION COEFFICIENT OF A METAL SURFACE UNDER ION BEAM IRRADIATION

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The charged particle beams and plasma flows are successfully used for modifying material properties. The action result is determined by a great number of physical processes. One of them is the erosion of an irradiated surface due to sputtering, radiation heating up, and subsequent evaporation. The developing plasma-beam technologies demand to control the erosion properties and to choose the optimal processing mode and parameters. The numerical investigation results of evaporation kinetics for a metal target under high-power pulsed ion beams have been presented in [1]. But, contribution of collision sputtering has not been considered due to high ion energy (hundreds of keV) and high power density of a beam ($10^6 \ldots 10^9$ W/cm$^2$). However, for adequate calculation of erosion coefficient, in particular at low ion energy (less than 100 keV), the energy losses on collision sputtering should be taken into account.

The present work is devoted to the investigation of erosion processes on a metal surface under pulsed irradiation with 1 keV…1 MeV ions. The erosion coefficient is determined by the expression:

$$Y = \frac{\left(\frac{S}{e}\int_0^\tau j(t)dt + n\int_0^t V_f(t)dt\right)}{\frac{1}{e}\int_0^\tau j(t)dt}, \qquad (1)$$

where $S$ – sputtering coefficient, calculated according to the statistical model [2, 3], $\tau$ – impulse duration, $j(t)$ – current density varying during an impulse, $n$ – atomic density of a target material, $V_f$ – evaporation rate, calculated according to the heat erosion model [1], $e$– the electron's charge. The calculations have been implemented for copper and silver targets irradiated by argon ions with $10^{-7}$ s impulses. The obtained values of erosion coefficient vary in the range of $0.1 \ldots 10^4$ atoms per ion depending on the current density of a beam. The developed program code can be successfully used to predict the amount of removed substance and the velocities of atom emission in ion-beam technologies.

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Tu-019

# Structural changes of water ice analyzed by infrared spectroscopy

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$H_2O$ is the most abundant component of astrophysical ices. The aim of the present work is to contribute for the understanding of the structural changes that occur in the amorphous component when water ice is warmed up. For this, the dependence of infrared band absorption (FTIR) on ice temperature has been analyzed from 15 to 180 K. Results are compared to the chemical and physical effects induced by ion irradiation on frozen pure water ($H_2O$) over the same temperature range, obtained from the secondary ion yield measurements performed with 1.5 MeV $N^{2+}$ ion beam bombardment at Van de Graff Accelerator at PUC-Rio [1]. In both experiments, a thin ice film was prepared by vapor deposited into a substrate at about 10 K. The goal is to investigate if phase transitions in the ice could influence the desorption yield of $(H_2O)_nH_3O^+$cluster ions and also the FTIR water band areas. In Fig.1 the FTIR and the mass spectrometry (MS) results are compared. The left side axis represents the ratio between the $(H_2O)_1H_3O^+$and the hydronium $H_3O^+$ desorption yields. For water, three predominant IR bands are observed: 3250 $cm^{-1}$, 1651 $cm^{-1}$ and 760 $cm^{-1}$. The right side axis represents the area correspondent to the vibration mode of water, $\nu_1$ (3250 $cm^{-1}$) IR band. The agreement in the evolution of both curves during annealing (warming up in a very slow process) suggests that both techniques are sensitive to the high-density amorphous ice ($I_{ah}$) and the low-density amorphous ice ($I_{al}$) structures.

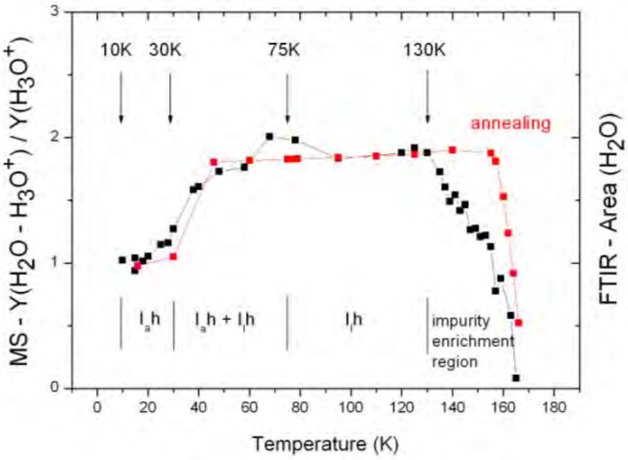

Figure 1. MS and FTIR analyses of phase change of water ice: during annealing, the high density $I_{ah}$ ice changes gradually into the low amorphous $I_{al}$ ice.

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Tu-020

# Channeling and Parametric X-ray Studies at the SAGA Light Source

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We present experimental results on channeling and parametric X-ray radiation (PXR) which have been obtained at the SAGA Light Source (SAGA-LS). The SAGA-LS is a synchrotron radiation facility newly constructed in Japan. The SAGA-LS accelerator complex consists of a 255-MeV injector linac and a 1.4-GeV storage ring, and an electron beam from the linac was used in the experiments.

Figure 1 shows the schematic of the experimental setup [1]. (i) We have observed both channeling phenomena and doughnut scattering through measurements of profiles of the electron beam transmitted through a 20-μm-thick Si crystal using a screen monitor [2]. (ii) We have measured PXR angular distributions from channeled electrons using an imaging plate as a two-dimensional X-ray detector [3]. These experimental results were compared with new [3] theory which takes into account combined effect of channeling and PXR, and good agreement is obtained.

Combining the experimental methods described above, we plan to search diffracted channeling radiation (DCR). Although the existence of DCR is predicted theoretically [4,5], the DCR has not yet been observed. The strategy for detecting DCR is also discussed.

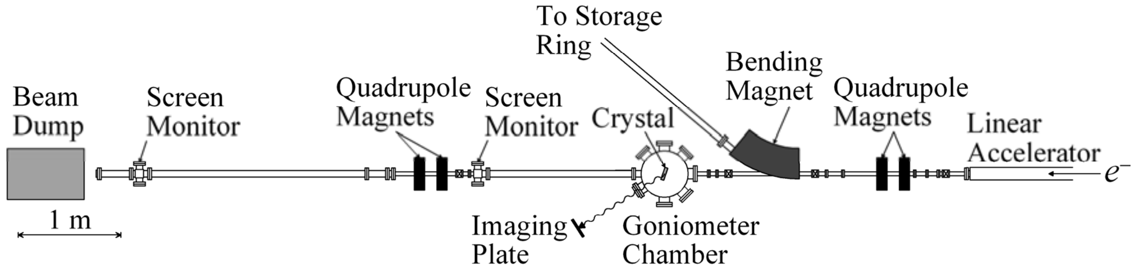

Figure 1. Schematic of the experimental setup.

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# Change of Diameters of Multi-walled Carbon Nanotubes by Multiply Charged Ar Ion Irradiation

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Nanostructured carbon materials such as carbon nanotubes (CNTs)[1] and graphenes[2] have been extensively studied toward realization of potential nanodevice applications. On the other hand, irradiating nanostructured carbon materials with energetic particles is thought to be capable of tailoring their structure and properties, and can be applied to process of nanodevice fabrication[3,4]. Multiply charged ions (MCIs) are recognized as having unique properties. The approach / collision of MCIs to solid surfaces results in multiple electron emission, since the MCIs have relatively high potential energy. This electron emission process strongly modifies the local electronic states of the materials. It was reported that the transformation from $sp^2$ to $sp^3$ hybridization by modification of the local electronic states of HOPG was demonstrated using the MCI irradiation[5]. However, the effect of MCI irradiation on the structural proeprties of nanostructured carbon materials has not been fully understood.

In this study, singly and multiply charged Ar ions ($Ar^+$, $Ar^{2+}$, $Ar^{4+}$) were irradiated to multi-walled CNT (MWCNT) films. The structural properties of irradiated MWCNT films were characterized by scanning electron microscopy (SEM), Raman spectroscopy, and transmission electron microscopy (TEM). In addition, soft X-ray photoelectron spectroscopy (XPS) and soft X-ray absorption spectroscopy (XAS) measurements were performed to characterize electronic states of the irradiated MWCNT films at BL17SU of SPring-8 and BL09 of NewSUBARU, respectively. It was found that the diameter of the MWCNTs was changed after the ion irradiation. Moreover, the change of the diameter was dependent on the charge state of multiply charged Ar ions. The increase of the diameter of the MWCNTs can be explained by bending and randomizing the orientation of broken graphene sheets, which is the origin for the large volume expansion of the irradiated graphite[6].

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Tu-022

# Analysis of the C 1s X-ray Photoelectron Spectrum and the C Kα X-ray Emission Spectrum of Multi-walled Carbon Nanotubes Irradiated by Multiply Charged Ar Ions

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Nanostructured carbon materials, such as carbon nanotubes (CNTs)[1] and graphenes[2], have been promising nanomaterials for various nanodevice applications because of their superior properties. Modification of the electronic states of nanostructure carbon materials has been essential to improve the nanodevice performance. For example, singly charged Ar ion irradiation enhanced the field emission properties of CNTs. Singly charged H ion irradiation improve the response time of the electrochemical sensors using CNTs. Thus, singly charged ion irradiation has been commonly used technique to modify the electronic states of nanostructured carbon materials. On the other hand, multiply charged ion (MCI) irradiation induced unique modification with solid surface, not observed with singly charged ions[3,4]. However, the effect of MCI irradiation on the electronic states of nanostructured carbon materials has not been fully understood.

In this study, singly and multiply charged Ar ions ($Ar^{+}$, $Ar^{2+}$, $Ar^{4+}$) were irradiated to multi-walled CNT (MWCNT) films. The electronic states of irradiated MWCNT films were characterized by soft X-ray photoelectron spectroscopy (XPS) and soft X-ray emission spectroscopy (XES) at BL17SU of SPring-8. The C 1s photoelectron spectra of the as-grown and irradiated MWCNT films were analyzed by means of a least-squares fitting procedure using Doniach-Šunjić functions convoluted with a Gaussian function[5]. The spectra were basically decomposed into five components (bulk $sp^2$ C, surface $sp^2$ C, surface $sp^3$ C, C-O bonds, and C=O bonds). It was found that intensity ratio of $sp^2$ C to $sp^3$ C was decreased after $Ar^{+}$ ion irradiation, and $\Gamma_G$ (FWHMs of the Gaussian function) was increased. Moreover, the spectra for $Ar^{4+}$ ion irradiation showed different shapes from $Ar^{+}$ ion irradiation. The C Kα X-ray emission spectra were also changed after the ion irradiation. These results were attributed to decrease of $sp^2$ C region, and increase of disordered region in the irradiated MWCNT films. Differences of XPS spectra between charge states of Ar ions will be discussed, and detailed results of analysis of XES spectra will be also presented.

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Tu-023

# Measurements of an Ion Beam Diameter Extracted into Air through the Various Capillaries

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A beam optics with a capillary has proposed a unique way to obtain PIXE spectra from any type of samples: solids, liquids and gases. The result of the PIXE measurement for the seabed sludge has demonstrated the ability of this method[1]. Since this technique is simple and effective to obtain micro beams in an atmospheric pressure, various laboratories have begun to use it. We have also performed in-Air-PIXE with glass capillary(GC) and a metal capillary(MC) and developed a 2D-mapping technique with a copper wire of 25 μm in diameter on an aluminum basement[2]. In order to estimate the position resolution, the diameter of the ion beam extracted through the capillaries into air should be estimated of this system. Here, we measured using a PIXE technique.

In this experiment, we have employed a conventional injection needle with a 200 μm inner diameter as the MC and a tapered GC with a 50 μm inner diameter. In order to extract the ion beam through the GC and MC, the capillary was fixed on a stage which are movable along three directions perpendicular to each other and the angle of which with respect to the incident beam axis was also adjustable. The wire was fixed another stage which is movable two dimensionally, that is, directions perpendicular and parallel to the ion beam axis. Induced characteristic X-rays by the beam irradiation were detected by a High-Purity Germanium photon detector. We measured the intensity of the characteristic X-rays as a function of the wire positions. The details of the beam diameter in air will be presented at the conference.

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# Ion beam irradiation effects on Ge nanocrystals synthesized by using RF sputtering followed by RTA

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Ge nanocrystals embedded in Silicon oxide matrix have been synthesized on Si substrate by using RF magnetron sputtering technique. The pristine samples were annealed at various temperatures using rapid thermal annealing (RTA). Eventually, these Ge nanocrystals are irradiated with heavy ions of various fluences at room temperature. Rutherford backscattering spectrometry (RBS) has been used to estimate the thickness and Ge composition of the composite films. The structural characterization was performed by using X-ray diffraction which confirms the formation of Ge nanocrystals. Raman scattering spectra showed a peak of Ge-Ge vibrational mode shifted with respect to its bulk value which is due to quantum confinement of phonons in the nanocrystals. Size and shape of irradiated Ge nanocrystals embedded in silicon oxide matrix are studied using transmission electron microscopy (TEM). Surface morphology of the samples is studied by Atomic Force Microscopy (AFM). Variation of the nanocrystal size and shape due to ion beam irradiation will be discussed in detail. The basic mechanism of interaction of ions with Ge nanocrystals at various ion fluences is being investigated and will be presented during the conference.

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# Structural characterization of CdSe/ZnS quantum dots using Medium Energy Ion Scattering

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Compound quantum dots QDs are promising materials that can be used in many fields of the technological development, but the accurate knowledge of compositional depth profiling inside of them is still a technological challenge. Medium energy ion scattering (MEIS) is an ion beam analysis technique, capable of elemental depth profiling with subnanometric depth resolution. Recently, the MEIS technique was optimized for nanostructured materials analysis [1] and became a promising tool for structural characterization inside of QDs [2,3]. In this work, we use the MEIS technique to characterize a core-shell nanostructure of CdSe/ZnS. The crystal size of 5.2 nm, determined by MEIS, is in good agreement with optical measurements and TEM images. The core-shell structure is resolved by the present configuration of MEIS in contrast to the present TEM measurements. The commercial CdSe/ZnS QDs has non-stoichiometric Cd and Se concentrations. The sample selected for this work have a Cd:Se ratio of 0.69:0.31. Our investigation shows that there is Cd present on the shell and the CdSe core tends to be a stoichiometric crystal. That indicates that, despite the unbalance of material, the CdSe crystal is preserved during the industrial process which allows the control of the QDs diameters.

This study shows that the MEIS technique, combined with other analytical techniques, is a powerful method to determine elemental distribution profiles, inside nanoparticles with diameter about 5 nanometers. This allows for studies of the formation and stability of the internal structure of the QDs when exposed to several kind of processes, like heating and ion irradiation. We also observed that for the present analysis the line-shape asymmetry of the energy-loss distribution is of minor importance. This is due to the use of a helium beam combined to a large number of isotopes of cadmium, selenium and zinc whose energy variation overshadows the asymmetrical effects from the backscattering collision.

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Tu-026

# A study on hydrogen performance in high-*k* stacks by high-resolution ERDA

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With continuously decreasing in the thickness of high-*k* stacks along the advances of semiconductor process technology, negative bias temperature instability (NBTI) has shown its increasing influences on the lifetime of electronic devices. NBTI occurs in *p*-channel MOS devices stressed with negative gate voltage at elevated temperature. It manifests as absolute drain current $I_{\mathrm{Dsat}}$ decrease and threshold voltage $V_{\mathrm{T}}$ increase. [1]

Currently, two major models have been proposed to explain NBTI. One explanation is referred as a "diffusion-limited" model in which $H^+$ diffuses to $SiO_2$/Si interface and reacts with Si-H traps to produce the silicon dangling bond and $H_2$. The other major explanation can be regarded as a "reaction-limited" model in which holes diffuse to $SiO_2$/Si interface and reacts with Si-H trap and neutral water-related species to produce $H^+$. In addition, some of the $H^+$ ions diffuse from the interface to the oxide layer. However, no explanation of NBTI is firmly accepted because there still lacks an observation of the diffusion of elements in the devices under the NBTI stress.

In this work, we have measured the hydrogen performance in high-*k* stacks by high-resolution elastic recoil detection analysis (ERDA) [2]. The influence of the different kind of metal layer on the hydrogen distribution in metal/$HfO_2$/$SiO_2$/Si was examined. Because 260 ºC is the typical stress temperature for NBTI, we also observed the H distribution at 260 ºC.

The results indicate that large amount of hydrogen has been introduced into the n-type Si substrate by the deposition of palladium layer. This result supports the "diffusion-limited" model which is consistent if $H^+$ can exist in the silicon. Hydrogen density in the high-k stacks has a small accumulation at the interface between high-k film and the $SiO_2$. Due to the 260 ºC vacuum annealing, the H density in the $HfO_2$ film and Si substrate can be significantly reduced.

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# Electronic energy loss of slow Ne ions in ultrathin Au-films deduced by TOF-MEIS

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The electronic stopping power $S_e$ for slow Ne ions in Au with energies between 80 and 180 keV was deduced experimentally. Time-of-Flight spectra for Ne ions backscattered from a 159 Å Au-film deposited on a Si substrate were recorded. The obtained energy-converted spectra were simulated by a TRIM based Monte-Carlo simulation [1] which employs a screened scattering potential applicable at these low energies. The electronic energy loss in the simulations can be tuned, until a best fit between experiment and simulation is obtained. Furthermore, the use of Monte-Carlo simulations permits to handle contributions from multiple scattering and the corresponding nuclear energy losses. Fig. 1 shows an energy-converted experimental spectrum obtained for 180 keV Ne primary ions and TRBS-simulations for three different magnitudes of $S_e$.

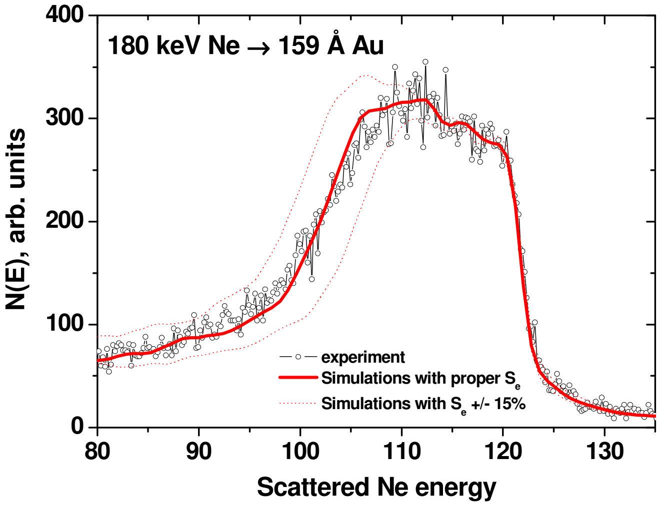

Fig.1: Energy converted Time-of-Flight spectrum for Ne ions backscattered from a thin Au film on Si. Also shown are Monte-Carlo simulations using different electronic stopping powers.

In this contribution the deduced stopping powers are also compared to earlier investigations, which were performed in transmission geometry (e.g. [2] and references therein).

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Tu-028

# Molecular Effect on Damage Accumulation in Si under $PF_4^+$ Ion Irradiation: Effect of Ion Energy

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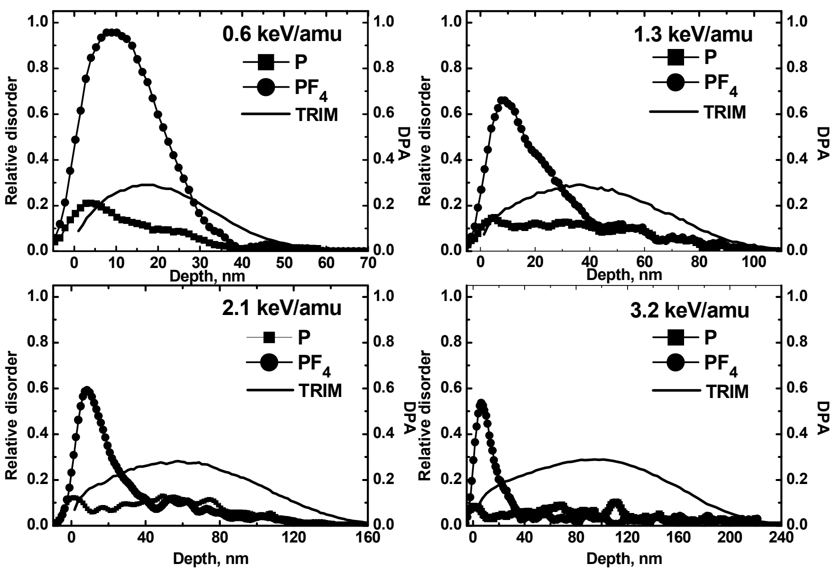
The efficiency of radiation damage accumulation differs for atomic and cluster (molecular) ion bombardment regimes under correct irradiation conditions. This is the so-called molecular effect (ME). The ME in damage accumulation has been attributed (i) to increased disordering in nonlinear energy spikes (such as thermal and displacement spikes) [1], which form due to spatial overlap of collision cascades produced by the atoms comprising a molecular ion or (ii) to nonlinear dynamic annealing processes (i.e. processes of annihilation and clustering of point defects during ion irradiation) [2].

In this contribution, we study the ME in (001) Si irradiated at room temperature in a wide ion energy range of (0.6 – 3.2 keV/amu) with cluster $PF_4$ ions comprising different atomic species. Implantation was carried out at 7° off the (001) direction in order to minimize channeling. Damage concentration was measured by RBS/C technique (0.7 MeV He ions) with low glancing angle of detecting (13°) to improve depth resolution. For correct estimation of the ME the following parameters were kept constant: ion energy normalized to amu, ion dose normalized to the number of displacements per atom (DPA) in maximum of elastic energy loss, and ion beam flux normalized to DPA $s^{-1}$ [3]. As an example, shown in the figure are depth distributions of relative disorder formed after implantation of $P^+$ and $PF_4^+$ ions to doses resulting in a DPA of 0.29 at the maximum of the nuclear energy loss profile. Also shown by lines are DPA depth distributions calculated by TRIM code. The molecular effect is clearly seen in this figure which results from both mechanisms mentioned above.



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Tu-029

# The Distribution of Induced Charge in Ion-Metal Surface Collisions

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In ion-metal collisions, an induced charge is produced inside the metal; this drastically affects formation of electronic states of the system under consideration. Spatial distribution of the induced charge within the metal was analyzed using the classical electrostatic model [1], and the following formula for electron density distribution ρ was obtained: $\rho(R) = 1/(2\pi)\, R_0 / \{R^3(R-R_0)\}$. Here $R$ is the distance between the incoming ion and electron, $R_0$ is the ion-surface distance.

Quantum-mechanically, electron cloud is expanded into vacuum via tunneling mechanisms. Therefore, dependence $\rho(R) = A\, exp\{-?(R-R_0)\}$ can be expected, while inside the metal the $\rho(R)$ dependence is almost classical. To satisfy both asymptotics, we choose the following form of $\rho(R)$: $\rho(R) = A/\{(R+d)^3\, [(R-R_0)^2 + b^2)]^{1/2}\, [1+exp(\gamma(R-R_0)]\}$.

Parameters can be found from the minimum of the energy functional that depends on electron density distribution [2, 3]:
$E[\rho] = \int U(\vec{R})\, \rho(\vec{R})d\vec{R} + \iint \rho(\vec{R})\rho(\vec{R}') / (?\vec{R} - \vec{R}'?) d\vec{R}\, d\vec{R}' + 2{,}87 \int \rho(\vec{R})^{5/3} d\vec{R}\ ) + \int E_{exc}[\rho]\ \rho(\vec{R}) d\vec{R} + 1/72 \int [\nabla\rho(\vec{R})]^2 / \rho(\vec{R}) d\vec{R}$ . Here $U(\vec{R})$ describes the interaction between the induced electron and incoming ion, the second is for the electron-electron interaction, the third is the electron kinetic energy, the fourth is the electron subsystem correlation-exchange energy, and the last is the gradient correction of the second order [4]. Calculations for the $C^{6+}$ - Cu case are shown in Fig.1. $R_0$ = 10 at.u. The arrow indicates the position of the first row of metal ions. Obtained density distribution is shifted towards vacuum (left side). The electron wall radius in Cu is 1.6 at.u. The incoming ions field shifts slightly the potential wall position towards vacuum.

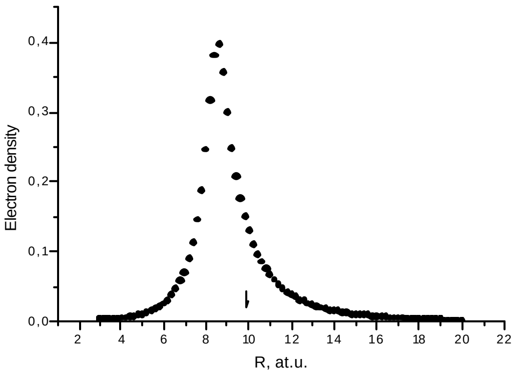

Fig.1. Obtained induced electron density distribution for $C^{6+}$ - Cu case, $R_0$ = 10 at.u.

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# Fragmentation of $^{56}$Fe on C, Al and $CH_2$ targets at 471 A MeV

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The total charge-changing cross sections, the partial cross sections of fragment productions, the emission angles and transverse momentum distributions of fragments of the fragmentation of $^{56}$Fe on Al, C, $CH_2$ and H targets at 471 A MeV are measured using CR-39 plastic nuclear track detector and compared with other experimental results and the predictions of the theoretical models. The total charge-changing cross sections agree will with other experimental results at different energies and the predictions of Bradt-Peters semi-empirical formula, which are approximately independent of the beam energy but increase with the increase of target mass. The partial cross sections are consistent with other ones at close energies and show a significant enhancement for the fragments with even-Z, especially for the fragments with charge $10 \leq Z_F \leq 20$. The improved quantum molecular model (ImQMD) combined with the GEMINI model can well represent the production of charged projectile fragments. The emission angles and transverse momentum distributions of fragments are compared with the predictions of ImQMD model, it is found that the model agree well with our results. The transverse momentum distributions of fragments can be explained by a single Gaussian distribution and the average transverse momentum decreases with the increase of the charge of fragment. Finally, the temperature parameter of emission source of fragment is discussed and it decreases with the increase of the size of fragment.

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# Microscopic Model of Material Excitation in Swift Heavy Ion Tracks

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Swift heavy ions (SHI, M>20 amu., E>1 MeV/nucl) lose the largest part of their energy for excitation of the electron subsystem of a target (up to 95%, 10-70 keV/nm). Subsequent transfer of even small parts of the deposited energy and momentum into the lattice can cause unusual nanometric structure transformations which kinetics crucially depends on the parameters of the initial excitation. This transfer occurs at femto-pico timescales after the projectile passage and can not be properly described in terms of the macroscopic models.

The molecular-dynamics model (MD) combined with the formalism of the dynamic structure factor (DSF) [1-3] is employed to calculate the cross sections of electron-lattice interaction at such short timescales. DSF takes into account the complete spectra of lattice excitations originated from spatial and temporal correlations in positions and dynamics of target atoms. It can be applied when (a) no thermal equilibrium of the lattice can be assumed [2], and (b) at times much shorter than the time of atomic vibrations when electron-to-lattice coupling differs from the electron-phonon mode appearing in the DSF as the low energy/long timescale limit [1,3]. The short timescale and high excitation results in the plasma-like electron-lattice energy exchange [3]. All the intermediate Warm Dense Matter states are also covered by the DSF formalism [4].

The obtained cross sections are introduced into the Monte-Carlo (MC) model of event-by-event simulations describing the kinetics of the electron subsystem in a SHI track. Based on the Complex Dielectric Function (CDF) formalism for inelastic scattering [5,6], this MC model takes also into account the dynamics of all collective modes appearing in the electronic subsystem.

Application of the combined MC-MD-DSF model supplies us with the spatial and temporal distributions of fast electrons, valence and core holes as well as the rates of the energy and momentum exchange between electrons and atoms in SHI tracks in different materials ($SiO_2$, $Y_2O_3$, LiF, Al, Si).

This approach can be used in *ab-initio* models and for obtaining the initial conditions for kinetic MC or MD models describing the structure transformations and defect formations in relaxing SHI tracks at longer timescales.

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# Dynamic Structure Factor Based Approach for Electron-Lattice Coupling in Swift Heavy Ion Tracks

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The spatial and dynamic couplings of atoms affect considerably the kinetics of energy and momentum transfer from the excited electronic subsystem to the lattice in nanometric tracks of swift heavy ions (SHI, E>1MeV/amu) decelerated in the electronic stopping regime. The Dynamic Structure Factor formalism (DSF) [1] is applied in the developed Molecular Dynamic (MD) model to describe the cross sections governing these transfers. DSF takes into account the complete spectra of the lattice excitations and can be applied when (a) no thermal equilibrium of the lattice can be assumed [2], and (b) at times much shorter than the time of atomic vibrations when the modes of electron-lattice coupling are similar to those in plasma and differ from the electron-phonon mode appearing in the DSF formalism as the low energy/long timescale limit [1,3]. All the intermediate Warm Dense Matter states are also covered by the DSF formalism [4].

LiF and Al are chosen as system for application of the developed MD model. Aluminum is chosen as a typical metal with a simple free-electron-like band structure. Alkali-halides find wide applications in investigation of the kinetics of damage formation in SHI tracks. The widest band gap supplies with the direct mechanism of point defects creation based on formation and decay of self-trapped excitons during relaxation of the excited electronic subsystem. To keep the electoneutrality, point defects catch electrons and holes forming the color center electron energy levels inside the gap. Transitions between these levels result in photon emissions providing with the quantitative information for the analysis of the electron and damage kinetics in SHI tracks.

Application of the MD-DSF model provides us with the frequency and wave vector dependencies of DSF, which are then used to construct realistic cross sections of electron-lattice interaction in SHI tracks in Al and LiF. This gives a possibility to investigate the effect of the different modes of dynamical coupling of lattice atoms, which can be realized in SHI tracks (e.g. the electron-phonon mode vs the “instantaneous” plasma-like approximation), as well as the effect of thermalization of the electronic subsystem on the kinetics of lattice excitation.

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Tu-033

# Fabrication of Planar Waveguide in KNSBN Crystal by Swift Heavy Ion Beam Irradiation

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We demonstrate the application of swift heavy ion implantation to generate optical waveguides in photorefractive materials. Potassium sodium strontium barium niobate (KNSBN) crystal is irradiated with 17 MeV $C^{5+}$ ions at a dose of $2\times10^{14}$ ions/cm$^2$. A nearly 10μm thick planar waveguide is fabricated after implantation. The properties of waveguide have been characterized using prism-coupling, microscope, and end-fire coupling. A refractive index increasing is formed in waveguide region based on the electronic energy deposition. The two-dimensional modal profiles of the planar waveguides, measured by using the end-coupling arrangement, are in good agreement to the simulated modal distributions.

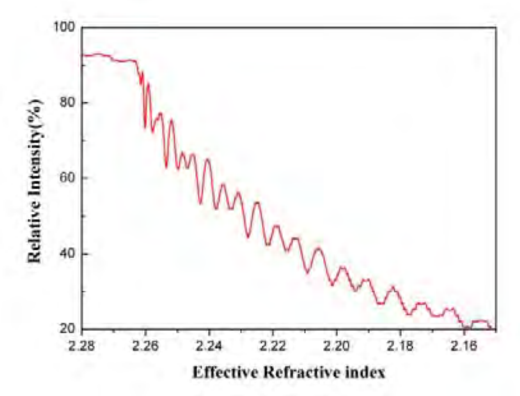

Figure 1. (Color online) Dark-mode spectra of TE modes of the KNSBN planar waveguides irradiated by 17 MeV $C^{5+}$ at a fluence of $2\times10^{14}$ ions/cm$^2$.

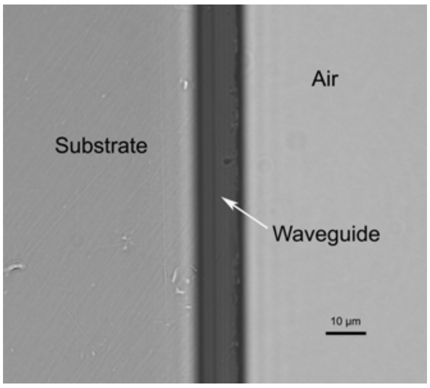

Figure 2. Optical microphotograph of cross section of the KNSBN waveguide sample irradiated by 17 MeV $C^{5+}$ at a fluence of $2\times10^{14}$ ions/cm$^2$.

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# Stopping Power in Magnetized Plasma

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In many-electron systems of the ionosphere around the earth, there appears the frequency of precession of electron in a magnetic field, $\omega_{0,}$ in addition with the plasma frequency, $\omega_{p.}$ Such a kind of magnetic effect is mainly expressed by $\omega^{-3}$ term of the dielectric function $\varepsilon(\omega)$ at the high-frequency approximation. The dielectric function $\varepsilon(\omega)$, in which up to $\omega^{-3}$ term is taken into account, is given as the following expression in a uniform magnetized plasma by Jackson[1].

$$\varepsilon(\omega) \cong 1 - \frac{\omega_p^2}{\omega^2} \pm \frac{\omega_0 \omega_p^2}{\omega^3} \boldsymbol{bn}. \tag{1}$$

In the above, ***b*** and ***n*** indicate unit vectors of the uniform magnetic field $\boldsymbol{B}_0$ and the wave number ***k*** of electro-magnetic field involved in interaction with an incident projectile. We note that the stopping power discussed here has the direction dependence toward to $\boldsymbol{B}_0$ through ***bn*** in Eq.(1). The stopping power $S$ is derived from the following general formula.

$$S = \frac{(Z_1 e)^2}{\pi^2 V} \int \frac{d^3k}{k^2} \int_0^\infty d\omega \omega Im \left[ \frac{-1}{\varepsilon(\boldsymbol{k}, \omega)} \right] \delta(\omega - \boldsymbol{kV}), \tag{2}$$

where $Z_1e$ and $\boldsymbol{V}$ are the charge and the velocity of the projectile, respectively. The integrand in Eq.(2) has $\varphi$-dependence in spherical coordinate ($r$, $\theta$, $\varphi$) generally, because of the direction dependence toward to $\boldsymbol{B}_0$ mentioned above. In this presentation, we mainly report theoretical results of the cases that the incident direction of projectile are parallel or anti-parallel to the uniform magnetic field.

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# Single-mode Waveguides Generated in $Nd^{3+}$-doped Silicate Glass by Nickel Ion Irradiation

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In this paper we describe the fabrication of single mode waveguides in $Nd^{3+}$-doped silicate glass substrates by ion implantation technique. $Nd^{3+}$-doped silicate glass is irradiated with 3MeV Ni ions at a dose of $5\times10^{14}$ ions/cm$^2$. The prism-coupling method is used to measure the effective refractive indices of the waveguide dark modes. Only one mode is found, its effective index($n_{\mathrm{eff}}$=1.5207) is higher than the substrate index ($n_{\mathrm{sub}}$=1.5202). The near-field intensity distribution and propagation loss of the light in the waveguides were measured by the end-fire coupling method. It is found that after annealing the propagation loss of waveguide is effectively reduced.

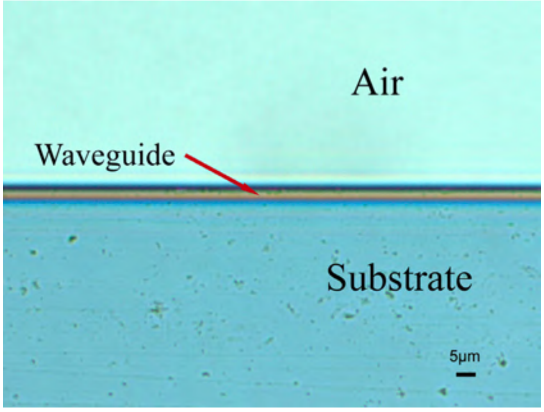

Figure 1. Optical microphotograph(500×) of cross section of the $Nd^{3+}$-doped silicate glass waveguide sample irradiated by 3MeV Ni ions at a fluence of $5\times10^{14}$ions/cm$^2$.

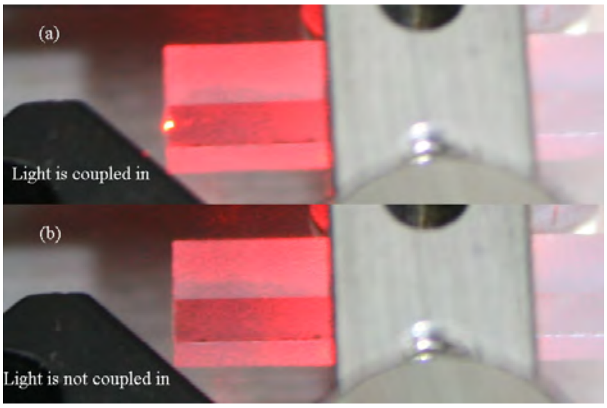

Figure2. (a)Light propagates out from the left ending of the waveguide, when light is coupled in by prism at the right angle for single-mode propagation. (b) Light is not coupled into the waveguide.

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# Bridge-Like Radiation Defects in Few-Layer Graphene

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Few-layer graphene structures as well as graphene itself become objects of great interest for the nearest future applications. It can be predicted, that in some cases few-layer graphene-based devices will be subjected to irradiation, which will result in changes of their properties. Therefore, study of possible radiation defects in these structures attracts attention of researchers and technologists. In the work presented few layer graphene fragments were produced by mechanical exfoliation and placed on a copper grid for TEM. Specimens were preliminary characterized by optical microscopy and Raman spectroscopy and after that exposed to electron beam irradiation (100 keV) with a mean exposure dose $3 \cdot 10^{19}$ el /cm$^2$. Raman spectra of the irradiated specimens showed the essential changes in intensities and positions of G and 2D peaks and apparent contribution of the D peak, indicating radiation damage of the structures. Computer simulation of the possible process of damaging in few layer graphene was performed by molecular dynamics and density functional theory. Results of modeling displayed that under the energetic conditions of irradiation the stable and strong-coupling bridge-like radiation defects [1,2], linking graphene sheets together can be produced as predominanting. Results of simulation allow making the interpretation of Raman spectroscopy data of the irradiated structures.

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# SiC Surface Damage Originating from Synergy Effect of Ar Plasma Ion and Plasma-Induced Ultraviolet Light Irradiations

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SiC has been attracting much attention for applications to high power electronic devices [1], which originates from the fact that SiC has a high breakdown field and a high thermal conductivity. These characteristics result from a wide band gap energy and a high sound velocity. A large number of issues still exist in fabricating SiC-based devices because SiC is a binary compound [2]. In particular, plasma-induced damage to SiC in the etch process is a crucial issue; namely, surface roughening and/or spatial disordering lowers SiC-based device performances [3].

In the present paper, on the basis both of an experiment and of a simulation, we discuss Ar plasma etch damage to SiC at the different gas pressures from the viewpoint of synergy effect of Ar plasma ion and plasma-induced ultraviolet (UV) light irradiations: at the low gas pressure (10 mTorr), no UV light is emitted from the plasma, whereas at the high gas pressure (50~100 mTorr), the UV light corresponding to ArII is emitted from the plasma [4]. We focus on changes in the morphology, roughness, etch depth, and Si/C ratio at the SiC surface under the different gas pressures.

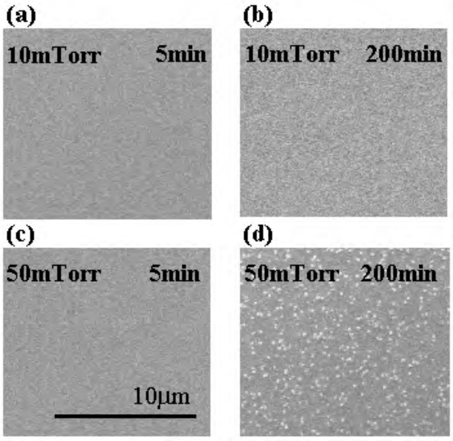

Fig. 1. SEM images of SiC surfaces etched by Ar plasmas at different gas pressures.

In the absence of UV light emission at the low gas pressure of 10 mTorr, the etched SiC surface morphology is quite similar to that of the as-grown sample, regardless of the etch time, as shown in Figs. 1(a) and 1(b). Si/C ratio at the etched surface, however, decreases with an increase in the etch time, which agrees with the simulation: Si is preferentially removed by $Ar^+$ plasma ions impinging on the surface. This agreement indicates that the physical etch effect, which originates from the impact of $Ar^+$ plasma ions, contributes to the surface damage. In the presence of the UV light emission resulting from ArII, the surface morphology at the high gas pressure (50~100 mTorr) depends on the etch time: the change in the surface morphology occurs in the case where the etch time increases to 200 min, as shown Figs. 1(c) and 1(d). The experimental etch depth at the etch time of 200 min does not agree with that of the simulation: the experimental etch depth is much higher. The difference connecting with the gas pressures can be related to the factor whether the UV light is emitted: the result at the high gas pressure suggests the contribution of the synergy effect caused by the following possible phenomenon: Si-C bonding is much weakened.

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Tu-038

# Evaluation of Electronic Stopping Cross Section for Well-Channeled Ions Using New Formula

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In previous work, we have determined the screening length with shell effect of an isolated atom adopting the average radius of the Thomas-Fermi electron distribution instead of that of Hartree-Fock electron distribution [1]. Based on the Firsov theory, we have also derived a formula of the electronic energy loss, which has a simple form $\Delta E_{\mathrm{e}}(b) \propto S_{\mathrm{e}}(E)\exp(\gamma b)/(1+\beta b)^6$, where $b = p/a$ ($\beta$ and $\gamma$ are the fitting parameters, $p$ and $a$ are the impact parameter and the screening length, respectively), and $S_{\mathrm{e}}(E)$ is the electronic stopping cross section.

In present study, we suggest a new formula of the electronic energy loss taking account of the interaction effect between the incident ion and the conductive electron in the Firsov model. For low ion velocity, the ion is moving slowly compared with the electrons at the Fermi surface. Electrons at the Fermi surface are viewed as being scattered by the screened potential of the ion [2]. The stopping power for a slow ion can be written by the phase shifts at the Fermi energy [3]. The energy spectra of channeled B ions impinging along the <110> axes of a silicon crystal were calculated by the ACOCT simulation code included the screening lengths with shell effect and the new formula for 400 keV B incident on a sample thickness of $0.55\,\mu$m [4]. It was manifested that the energy loss of well-channeled ions consists mostly of the electronic energy loss.

In addition, we calculated the electronic stopping cross sections for well-channeled ions by the present ACOCT code employing treatment on the maximum energy of transmitted ions as a function of energy of the incident ions for channeling along the <110> direction of silicon in the Eisen's experiments [4]. We obtained that the electronic stopping cross sections against the atomic number of incident ions at a constant velocity show an oscillatory dependence owing to the shell effect of electron.

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# Planar Waveguide Formed in $LiNbO_3$ by Proton Exchange Combined with Cu Ion Implantation

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We report on the fabrication of planar waveguide in lithium niobate by proton exchange combined with copper ion implantation. A z-cut $LiNbO_3$ crystal was immersed in a molten benzoic acid for 20 min and then was implanted with 1.5 MeV copper ions at a fluence of $3\times10^{14}$ions/cm$^2$. The guiding modes of the planar waveguides before and after copper ion implantation were measured by the prism-coupling method at 633nm. The modes in proton exchanged waveguide can be modulated by copper ion implantation. The reflectivity calculation method (RCM) was used for reconstructing refractive index profiles. The near-field intensity distribution and propagation loss of the light in the waveguides were measured by the end-face coupling method. We used the finite-difference beam propagation method (FD-BPM) to simulate the light propagation. Absorption spectra of the bulk $LiNbO_3$ before and after copper ion implantation were measured. Absorption bands of the bulk LiNbO3 crystal have been preserved after copper ion implantation. The Rutherford backscattering/channeling technique was used to investigate the damage of the waveguides.

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# Electronic Stopping for Swift Carbon Cluster Ions connected with Average Charge Reduction

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Interaction of cluster ion with solids has attracted intensive attention in that the so-called cluster effect will be expected in the electric excitation phenomena, e.g., the energy-loss[1-3] and secondary electron emission[4]. These processes induced inside a material are related to the charges of constituent ions in a bulk, whose average charges are known to be less than that of a single ion in a bulk with an equivalent speed. The reduction of the average charge is also characteristic in cluster-solid interaction[5], and its structure dependent feature was measured [6]. To our knowledge, however, basic data on the above phenomena were not ample till now. The aim of this study is to provide as an elemental quantity the electronic stopping cross section, S(n), for swift carbon cluster (Cn) ions in linear-chained structure, and C60 fullerene as a function of ion speed in connection with reduction of cluster average charge in a bulk. The average charges of constituent ions for a Cn incidence are estimated in self-consistent manner, where the average charge per ion Q(n) for a C60 reduces at most about sixty percent of that of a single carbon ion Q(1) with an equivalent speed, though Q(n) and Q(1) increases monotonically with increasing speed. By inclusion of the average charge reduction, the electronic stopping cross section is estimated in the dielectric function formalism as a function of speed and inter-ionic separation. At high speed, the positive cluster effect appears. In particular, the electronic stopping for a C60 represents the giant increase which is due to contribution of the collective resonance excitation.

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# Effects of energetic ions on the structural and vibrational properties of bonded hydrogen in silicon

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It is well known that hydrogen is an important impurity in semiconductors. Hydrogen plays a key role in crystal growth and can change electrical, optical and mechanical properties of many materials. Most importantly, the hydrogen passivation of defects in silicon has been an essential processing step in modern integrated circuit technology. Hence it is important to study the factors that can influence the stability, structural and vibrational properties of defect associated hydrogen in silicon. Here we present a study on the influence of swift heavy ion irradiation on the structural and vibrational properties of Si-H complexes associated to various defects in silicon. These defect associated Si-H complexes were obtained by low temperature (80 K) implantation of protons into silicon followed by room temperature annealing. Energetic protons (250 KeV, 190 KeV and 95 KeV at doses of $1\text{x}10^{13}$ to $1\text{x}10^{17}$ $H^+/cm^2$) were implanted into high resistivity, double side polished Si samples at 80 K using the low energy ion beam facility at IUAC, New Delhi. Presence of various defect associated Si-H complexes was confirmed by Fourier Transform Infrared spectroscopy (FTIR). It is shown that the concentrations of these Si-H complexes initially increase monotonically with increase in dose and saturate at higher doses. The influence of swift heavy ion irradiation on the stability of these Si-H complexes will be studied as a function of silicon resistivity, local structure, irradiation temperature and electronic energy loss of incident ions. These results will be discussed in detail during the conference.

Keywords: Hydrogen passivation, Si-H complexes, FTIR, SHI.

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Tu-042

# Effects of swift heavy ion irradiation on the structural and electrical properties of $HfO_2$ and $HfO_2/SiO_2$ films deposited on silicon

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Hafnium based high dielectric constant materials are critical for the *state-of-the-art* integrated circuit technology. As the size of the transistor decreases, the thickness of the gate dielectric ($SiO_2$) should be reduced to maintain device capacitance at a desired level. This thickness reduction results in high OFF-state leakage current due to quantum tunneling (~ 100 $A/cm^2$ for 1 nm $SiO_2$ on Si). Eventually high-k materials, like $HfO_2$, have recently been introduced as gate dielectrics. However deposition of these high-k materials on Si wafers results in high concentration of interface defects due to their thermodynamic instability on Si. Introduction of thin inter layer of Silicon oxide / nitrides between Si and $HfO_2$ is expected to improve interface quality. Hence it is important to study the composition, thickness and intermixing effects to optimize the fabrication of Hafnium based MOS devices. Here, we have performed High Resolution Rutherford Backscattering Spectrometry (HRBS) and X-Ray Reflectivity (XRR) studies of Atomic Layer Deposition (ALD) grown $HfO_2/SiO_2/Si$ samples obtained from SEMATECH, USA. HRBS measurements and Synchrotron based XRR measurements were performed at National University of Singapore (NUS). These results will be discussed in view of possible inter diffusion and straggling effects. In addition, the influence of swift heavy ion irradiation on the structural and electrical properties of $HfO_2$ films deposited by e-beam evaporation on Si and SiO2/Si will also be discussed in detail

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Tu-043

# Effect of Atomic and Cluster Ion Irradiation on Mechanical Properties of DLC Films

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The dependence of internal residual stress and film thickness of thin diamond-like carbon (DLC) films on ion irradiation conditions is described. These films (0.01 – 1μm) were grown on Si substrate by PECVD technique and had significant residual compressive stress about few GPa. Grown samples were irradiated to atomic $P^+$ and molecular $PF_4^+$ ions. Post-growth ion irradiation causes decrease of compressive stress followed by its inversion to tensile one. For all ion energy combinations used residual stress changes linearly with normalized fluence up to 0.2 DPA with slope (8.7 ± 1.3) GPa/DPA. In all cases anomalous swelling (up to 50% of initial film thickness) was observed after irradiation. The step on the film between irradiated and virgin regions depends on ion dose and cascade density similarly to internal stress. We propose a model which explains the swelling by appearance of the energy spikes in film during ion stopping. According to this model the superheated regions around a spike near the surface of the film are extruded above the surface, where they cool down. Thus, the density of the film decreases, and its thickness increases. This process is saturated when the loosened film can no longer squeeze the material to the surface due to the presence of internal pores and accumulated tensile stress in the film. Dose measurements of internal stress and XPS measurements confirm the conclusions of our theory. Also we observed some increasing of the roughness on irradiated regions of film.

The change of internal stresses as well as the film thickness is similar in nature and to a dose of ~ 2 DPA is linear and then saturates. Moreover, irradiation of molecular ions (with high cascade density) leads to a rapid change in properties when compared with the case of atomic radiation (at the same amount of totally generated knock-ons), i.e., the molecular effect takes place.

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# Molecular dynamics simulations of subsurface Ar bubble rupture in copper after the impact of Ar atoms

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Noble gas bubbles in solids can be created by a high-dose ion implantation of noble gases into solids and it is of practical interest for the local modification of material properties. Franzreb & Williams [1] observed the formation of noble-gas cluster ions ejected from bursting subsurface bubbles during noble-gas ion sputtering. We present a molecular dynamics simulation of the rupture of a subsurface Ar bubble in Cu(100) and the ejection of small Ar clusters initiated by the impact of sub-keV Ar atoms. In addition we calculated local temperature and pressure maps inside the Ar bubble as a function of time elapsed from the impact and discussed mechanisms of the bubble burst.

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# Radiation damage and annealing effects in diamond implanted with high-dose, high-energy carbon ions

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Diamond is one of candidate materials for fabrication of high power, high frequency devices, because of its excellent characteristics such as a wide band gap (~5.5 eV), extremely high thermal conductivity, high breakdown voltage, high radiation hardness, etc. However, to realize such semiconducting diamond devices, we need high-quality and large-size single crystal (SC) diamond wafers, similar to conventional semiconductor materials. To date, we have developed a chemical vapor deposition (CVD) SC diamond growth method, which will allow one to produce large SC diamond wafers in the future, and attempted to fabricate freestanding thick SC films (plate). Among them, separation of a thick diamond film from the seed substrate is one of central issues because of high hardness and chemical inertness of diamond. To remove the substrate at ease, we have developed a “lift-off method”[1]. The procedure of this process is as follows: prior to the film growth, a highly defective layer is formed in the subsurface of the substrate using high-dose, high-energy ion implantation. After the implantation, a thick SC diamond film is grown on the substrate. After the film growth, the above highly defective layer is etched away, finally resulting in the fabrication of a freestanding thick diamond film (CVD SC wafer). In this paper, we will present investigations of crystallinity of the diamond substrate damaged by high-dose, high-energy ion implantation, mainly by means of measurements of optical properties. It is important to estimate crystallinity of the substrate, because CVD films are grown on such ion-implanted substrate surfaces.

As samples, high-temperature, high-pressure synthetic type-Ib SC diamond plates were used. The diamond plate was implanted with 3 MeV carbon ions to a fluence of $2 \times 10^{16}$ $\mathrm{cm}^{-2}$ (post-implantation annealing was 1200 °C/5min). The TRIM simulation showed that the depth profile of radiation damage has a sharp peak of $2.5 \times 10^{23}$ $\mathrm{cm}^{-3}$ with 0.1 μm (FWHM) at a depth of 1.6 μm. On the other hand, the radiation damage is not much in the depth region from the surface to 1.6 μm ($3 \times 10^{21}$ $\mathrm{cm}^{-3}$ at the surface).

The optical transmission spectrum less than ~700 nm of as-implanted sample is almost zero, while more than ~700 nm it steeply increases with the wavelength and finally reaches 60 % at 3.2 μm. In that of the post-implantation annealed sample, the optical transmission less than ~1 μm is zero, and it gradually increases with the wavelength above ~1 μm, but remains at most ~4 % at 3.2 μm, unlike the as-implanted sample. On the ion implanted diamond, accumulation of radiation damage over $\sim 1 \times 10^{22}$ $\mathrm{cm}^{-3}$ followed by annealing over ~1000 °C results in the structural transition to a graphitic phase. Thus, the lowering of the optical transmission observed after annealing reflects graphitization of the depth region over $\sim 1 \times 10^{22}$ $\mathrm{cm}^{-3}$ as indicated in TRIM. On the other hand, in the depth region from the surface to the depth below radiation damage of $\sim 1 \times 10^{22}$ $\mathrm{cm}^{-3}$, the diamond structure should be preserved. In fact, an interference pattern is seen in the optical transmission spectrum of the post-implantation sample. From this interference pattern, it is calculated that a thickness of the above preserved thin diamond layer is ~1.7 μm, consistent with the result of TRIM simulation. In addition, an optical luminescence from this layer was observed, also indicating that the diamond layer was preserved, while the observed luminescence spectrum was a broad band, most likely related to radiation damage, which stretches in the wavelength 600–900 nm and consists of several peaks, unlike the pristine substrate.

Acknowledgment: They are also grateful to members of DRL at AIST for various technical support.

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Tu-046

# An Electrostatic Quadrupole Lens for Focusing Swift Heavy Ions in MeV-SIMS

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The importance of imaging mass spectrometry (MS) for visualizing the spatial distribution of molecular species in biological tissues and cells is growing. SIMS imaging has been used to visualize elemental distribution at the cellular level because of its low molecular ion yield. In conventional SIMS with keV-energy ion beams, elastic collisions occur between projectiles and atoms in constituent molecules. The collisions break the molecules and produce fragments, which makes acquisition of molecular information difficult. In contrast, MeV-energy ion beams excite electrons and enhance the ionization of high-mass molecules, and a SIMS spectrum of ionized molecules can be obtained. In a previous study, we have developed a new system for imaging mass spectrometry using MeV-energy heavy ion beams, termed MeV-secondary ion mass spectrometry (MeV-SIMS), and demonstrated more than 1000-fold increase in molecular ion yield from a peptide sample (1154 Da), compared to keV ion irradiation. In addition, we successfully obtained mass spectrometric imaging of the deprotonated peptides (m/z 1153) without any matrix enhancement [1]. However, obtaining molecular imaging data at present, takes a long time, because the current density of the primary beam is not high enough. We have developed an electrostatic quadrupole lens to focus the swift heavy ion beam and reduce measurement time. MeV-SIMS imaging using the Q lens was performed with the instrument depicted schematically in Fig.1. The primary beam of 6 MeV $Cu^{4+}$ was focused with the Q lens and introduced onto the sample surface through an aperture with a hole of 100 μm diameter. Secondary ions were analyzed with an orthogonal acceleration (oa) time of flight (TOF) mass spectrometer [2]. Using the quadrupole lens, the current density increased by a factor of ~60 and we obtained an MeV-SIMS image of 100 × 100 pixels of protonated distearoyl phosphatidylcholine (DSPC) (m/z = 790.6) over a 4 mm × 4 mm field of view with a pixel size of 40 μm within 5 min, showing that the Q lens reduces measurement time of current imaging by a factor of ~30.

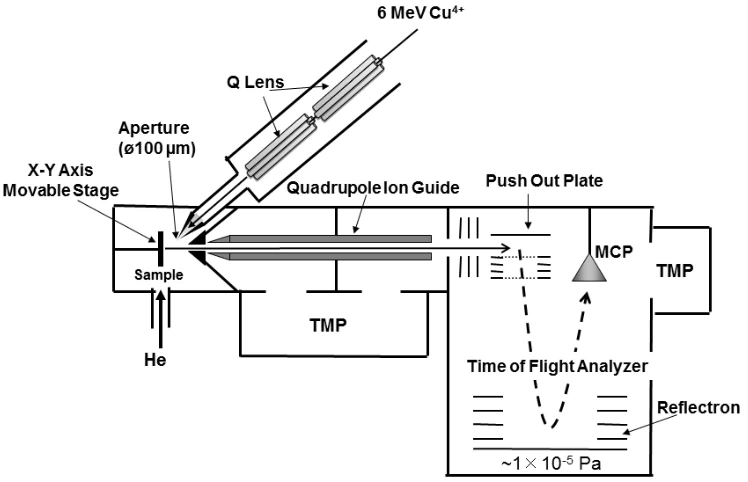

Figure 1. Schematic diagram of the MeV-SIMS instrument with Q lens.

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# The near-infrared waveguide properties of LGS crystal formed by swift $Kr^{8+}$ ion irradiation

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In this work, we report on the optical properties in the near-infrared region of $La_3Ga_5SiO_{14}$ (LGS) planar waveguide formed by swift-heavy-ion (SHI) irradiation. The planar optical waveguide in LGS crystal was fabricated by 330-MeV $Kr^{8+}$-ion implantation at a fluence of $1 \times 10^{12}$ ions/cm$^2$. The SHI irradiation was carried out at the Heavy Ion Research Facility in Lanzhou (HIRFL). The initial beam had an energy of 2.1-GeV and was slowed down by passing through a 259-um-thick Al foil which is determined by the Stopping and Range of Ions in Matter (SRIM) simulation [1]. The guided mode was measured by using a model 2010 prism coupler at the wavelength of 1539 nm. The refractive index profile was reconstructed using the reflectivity calculation method (RCM). The near-field intensity distribution of the mode was recorded by a CCD camera using the end-face coupling method. The finite-difference beam propagation method (FD-BPM) was used to simulate the guided mode profile. There is a good agreement between the recorded and the simulated mode profiles. The lattice damage induced by SHI irradiation in LGS crystal was studied by the micro-Raman spectroscopy. The Raman spectra are consistent with the energy loss distributions of Ar ions simulated by SRIM and the micro-photograph of the waveguide taken by a microscope using a polarized light.

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Tu-048

# Coulomb explosion in swift-heavy-ion-irradiated tracks: a hybrid PIC/MD simulation

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We study the coupled electron and ion dynamics in swift-heavy-ion-irradiated dielectric materials. As a prototypical case we investigate a LiF crystal irradiated in perpendicular direction at a deposited energy of around 400 eV/nm.

Our hybrid code is based on a molecular-dynamics study of the ionic Li+/F- system. The electron dynamics in the track is described by a microscopic particle-in-cell (PIC) scheme. As an empirical fit parameter we use the lifetime of excited electrons, before they recombine with ions.

We evaluate the sputter yield as well as the energy and angular distributions of the ejected ions. We find:

- the sputter yield decreases with the lifetime of excited electrons,
- the angular distribution is peaked along the surface normal (jet-like emission),
- the energy distribution of emitted ions has a bimodal structure, in which a low-energy component (~ 1 eV) is accompanied by a high-energy (> 5 eV) contribution characteristic of a Coulomb explosion.

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Tu-049

# Experimental investigations of synchrotron radiation at the onset of the quantum regime

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The classical description of synchrotron radiation fails at large Lorentz factors for relativistic electrons crossing strong transverse magnetic fields. In the rest frame of the electron this field is comparable to the so-called critical field of $4.414 \cdot 10^9$ T. When the Lorentz factor times the magnetic field is comparable to the critical field, quantum corrections are essential for the description of synchrotron radiation to conserve energy. With electrons of energies 10-150 GeV penetrating a germanium single crystal along the <110> axis, we have experimentally investigated the transition from the regime where classical synchrotron radiation is an adequate description, to the regime where the emission drastically changes character; not only in magnitude, but also in spectral shape. The spectrum can only be described by quantum synchrotron radiation formulas. Apart from being a test of strong-field quantum electrodynamics, the experimental results are also relevant for the design of future linear colliders where beamstrahlung - a closely related process - may limit the achievable luminosity.

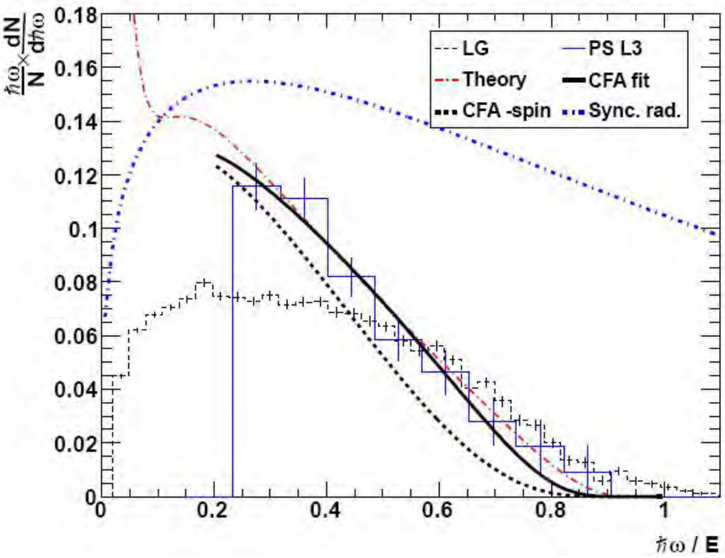

Figure 1. The radiation spectrum from a 100 GeV electron traversing a Ge crystal along the <110> axis.

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Tu-050

# Formation of Noble Metal Nanoparticles on Damaged and Undamaged Graphite Studied by Photoelectron and Auger Electron Spectroscopies

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A metal nanoparticle (MNP) depoisited on a substrate exhibits unusual physical properties, such as optical, electrical, and magnetic properties. The properties greatly depend on the size and shape of MNPs.It is, therefore, necessary to establish the method to control morphology of MNPs. The particle-substrate interaction is a key factor to effect the morphology. Ion-irradiation damage produced on a substrate can modify the interaction between MNP and a substrate through defects, e.g., vacancies and dangling bonds.

Highly oriented pyrolytic graphite (HOPG) was used as a substrate. The HOPG was irradiated with 1 keV-Ar ions at several irradiation times ranging from 0.1 to 30 s. Au, Pt or Ag NPs were deposited by sputtering of respective bulk sheets by using 0.8 keV-Ar ions. The areal densities of the noble metal atoms deposited on the substrate were determined by Rutherford backscattering spectrometry. X-ray photoelectron spectroscopy (XPS) and x-ray induced Auger electron spectroscopy (XAES) have been applied to examine the effect of ion irradiation to a substrate on size of the noble MNPs. The $4f_{7/2}$ binding energy (BE) can be used to size estimation for the Au and Pt NPs. In the case of Ag NPs, on the other hand, the kinetic energy of $M_{4,5}VV$ Auger electrons is a measure for sizing.

Fig.1 shows Ag $M_{4,5}VV$ Auger electron kinetic energy (KE) shifts from a bulk value at various areal densities of deposited Ag atoms. For deposited Ag NPs at areal density of $7.0\times10^{14}$ atoms/cm$^2$, for example, the KE shift is −0.80 eV for the Ar$^+$-irradiated HOPG, much larger than that for the pristine HOPG (−0.40 eV), indicating that the smaller NPs form on the damaged HOPG. A material dependence as well as defect density dependence of particle size will be discussed.

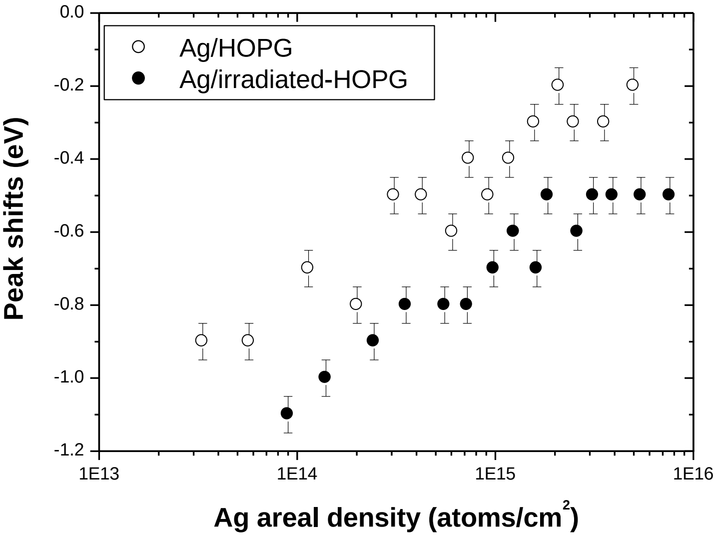

Fig. 1 :XAES Ag $M_{4,5}VV$ kinetic energy shifts as a function of coverage (number of deposited Ag atoms) for Ag/HOPG (○) and Ag/irradiated-HOPG (●).

# Kinetic electron emission from monocrystalline Ru and Cu induced by impact of slow $Cs^+$ ions

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We have studied the energy distributions of electrons emitted from the surfaces of Ru(0001) and Cu(100) bombarded by slow $Cs^+$ ions below the classical threshold. The electron yields at $Cs^+$ impact energies between 100 eV and 5000 eV are presented as a function of the inverse $Cs^+$ impact velocities 1/v. We have analyzed the data in terms of Sroubek's phenomenological model for a sub-threshold ion-induced kinetic electron emission [1].

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# Characterization of Epitaxial Transformation Phenomena Induced by the Interaction of Implanted N-Ions with Ti Thin Films

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Non-stoichiometric titanium nitrides, $TiN_y$, have covalent properties as well as metallic and ionic properties, which make them fascinating for both fundamental research and technological applications. Recently, it has been revealed that the interesting physical properties are related to the crystallographic (preferred oriented) and electronic structures [1]. In the present study, the formation mechanisms of preferred orientation of epitaxial $TiN_y$ films, especially epitaxial formation phenomena induced by the interaction of implanted N-ions with Ti thin films, will be clarified.

The as-deposited Ti films on thermally cleaned NaCl substrates consisted of both $TiH_x$ and hcp-Ti with some preferred orientations at RT. Nitrogen ions ($N_2^+$) with 62keV were implanted into the deposited Ti films held at RT in the 400kV analytical TEM connected to an ion accelerator at JAEA-Takasaki [2]. The hydrogen component measurement by ERDA was performed to elucidate the H depth profile change, by heating and nitriding Ti films. Furthermore, EELS measurement and DV-Xα MO calculations were used to clarify the electronic structure changes in as-deposited Ti films during N-implantation.

By careful analysis of these results, the following has been clarified. Nitriding of $TiH_x$ in the deposited Ti with N-occupations of octahedral sites of H-released fcc-Ti sublattice leads to the formation of $TiN_y$ without transformation of the Ti sublattice. However, the shift of the atoms on the closed-packed (00・1) plane of hcp-Ti induced by the bonding interaction of Ti sublattices with implanted N atoms plays an important role in the epitaxial transformation of hcp-Ti sublattices to fcc-Ti sublattices due to the occupation by N atoms, partially inheriting the specific atomic arrangements of hcp-Ti. Moreover, it has been found from the analyses of EELS measurements that the hcp-fcc transformation would occur preferentially above a critical concentration ratio $N/Ti \approx 0.25$ during N-implantation. This means that above the $N/Ti \approx 0.25$, the invasion of implanted N atom to the N-unoccupied octahedral site in the neighboring unit cell next to the N-occupied one occurs preferentially and induces the growth of nucleus of the hcp-fcc transformation.

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# Effects of low energy electrons and thermal annealing on the formation of color centers in nitrogen implanted diamond

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Color centers in diamond, e. g. the nitrogen-vacancy center (NV) are promising quantum bit candidates and they enable advanced magnetometry schemes [1]. Implantation of nitrogen ions into single crystal diamonds followed by thermal annealing is a straightforward approach that leads to the formation of some NV-centers. But the reliable formation of NV-centers with long spin coherence times and high spatial resolution is challenging. The established mechanism for NV-formation following nitrogen ion implantation is a two step process that takes place at annealing temperatures above ~600° C. Nitrogen is first incorporated onto a lattice site, followed by the capture of a vacancy by the substitutional nitrogen. We report an unexpected effect of exposure to low energy electrons on the formation of NV-centers in nitrogen implanted diamonds. Exposure to electrons (2–30 keV) in a scanning electron microscope induces formation of NV-centers without any thermal annealing [2]. We find that non-thermal, electron-beam-induced NV-formation is about four times less efficient than thermal annealing. But NV-center formation in a consecutive thermal annealing step (800º C) following exposure to low-energy electrons increases by a factor of up to 1.8 compared to thermal annealing alone. These observations point to the reconstruction of a precursor defect complex (which possibly includes interstitial nitrogen and two vacancies) that is induced by electronic excitations from low-energy electrons as an NV-center formation mechanism. The finding of enhanced NV-formation when exposure to low energy electrons is followed by thermal annealing indicates the importance of microscopic charging effects on the formation of NV-centers. In our presentation we will discuss strategies for the enhancement of NV-formation efficiencies.

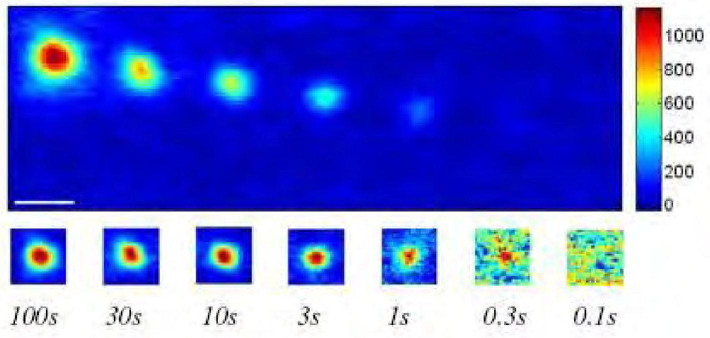

**Figure 1.** Confocal photoluminescence image of NV− centers (integrated spectral intensity 635–642 nm). The image was recorded following exposure of 1μm squares with a 2 keV, 9 pA electron beam. Insets show locally auto-scaled spot details. The scale bar is 3μm.

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# Acetone Cluster Ion Beam Irradiation on Solid Surfaces

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The efficiency of polyatomic cluster ion beam irradiation in the surface processing and modification of solid materials has been demonstrated [1]. The characteristic features of the polyatomic cluster ion irradiation may be attributable to the chemical properties of polyatomic molecules as well as the common characteristic properties of the cluster ion beam irradiation such as high sputtering yields and surface smoothing effect. According to molecular dynamics calculations, the local temperature of the area bombarded by a cluster increase within approximately 1 ps [2], which may result in the enhancement of the chemical reactions between the surface and molecules that comprise the cluster. In this study, the irradiation effects of acetone cluster ion beam on solid surfaces were investigated to enlarge the applicability of the polyatomic cluster ion beam technique. Acetone is a common material in the industry, and has different chemical properties from ethanol or water molecules that have been used as the source material of clusters [1].

Acetone clusters were produced by the adiabatic cooling effect during the adiabatic expansion of a supersonic nozzle flow. The production of acetone clusters were performed without helium support gas. The acetone clusters were ionized by electron impact ionization. The acetone monomer and small cluster ions were removed by the retarding voltage method. The typical acceleration voltage was from 3 to 9 kV. The cluster size distributions were measured by the time-of-flight (TOF) method, where singly charged clusters were assumed.

Figure 1 shows the cluster size distributions of the acetone cluster ion beam measured by the TOF method. The mode of the cluster size distribution was approximately at 2000, and gradually increased with source pressure. The typical source pressure used for the production of acetone clusters for the irradiation on the solid surfaces was 0.3 MPa.

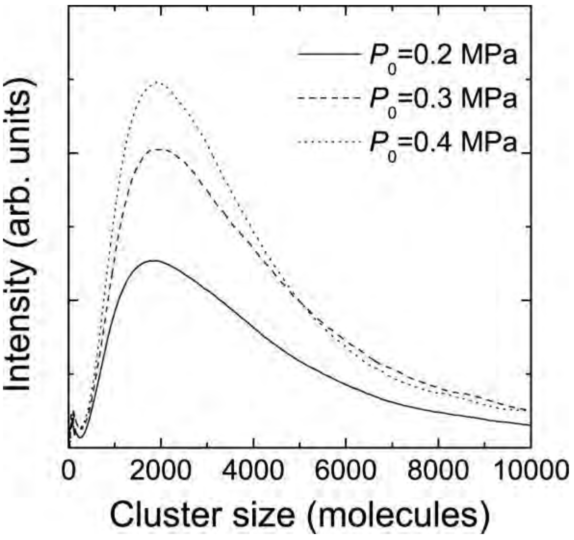

Figure 1. Cluster size distributions of acetone cluster ion beam.

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Tu-055

# Development of TOF-MEIS and the limitation of existing ion-interaction models

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We have developed, for the first time, a time-of-flight (TOF)-MEIS system with a collection efficiency 4 orders of magnitude higher than that of conventional MEIS to minimize the ion beam damage while maintaining a similar energy resolution. Furthermore, it can detect neutrals and ions which removes the ion neutralization problems in absolute quantitative analysis. A TOF-MEIS system was designed and constructed to minimize the ion beam damage effect by utilizing a pulsed ion beam with a pulse width < 1 ns and a TOF delay-line-detector with an 8 inch diameter and a time resolution of 300 ps. TOF-MEIS spectra were obtained using 70 keV $He^+$ ions that can rastered over 500 x 500 μm$^2$ and with an ion beam diameter of 10 μm. The TOF-MEIS system was applied for ~ μm small spot analysis of gate oxides and ultrashallow junctions and profiling of nanoparticles that are susceptible to ion beam damage. We report the quantitative compositional profiling with single atomic layer resolution for 0.5~3 nm CdSe/ZnS QDs with a conjugated layer. A large non-stoichiometry in sub nm CdSe cores with the Cd/Se ratio of 2.3 and its diameter dependence in the initial growth stage were clearly observed.

In spite of practical and exciting applications of TOF-MEIS for nanostructured materials analysis, a few questions regarding to physics on ion-surface interactions remain not clearly answered such as the effect of multiple scattering, electronic stopping power, the electronic straggling, and ion beam damage in the abnormal MEIS ion energy range. Discussions how to overcome these physics issues and extend applications to various nanotechnology and biotechnology shall be be invited.

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Tu-056

# Study of the Stopping Power of $H^+$ and $H_2^+$ in Silicon in E<90keV Energy Region

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The experimental measurement of ions' stopping power in low energy region is always a challenge work. The uncertainty of existed experimental stopping power data is rather large in keV energy region and can only be used for modifying the extrapolated curve based on higher energy data. In this work, the stopping power of $H^+$ (proton) and $H_2^+$ (hydrogen molecular ion) have been obtained from the depth profile of $H^+$ and $H_2^+$ in silicon. The $H^+$ and $H_2^+$ ions with energies of 10, 25, 35, 80 and 90 keV/amu were implanted into silicon with a fluence of $1\times10^{17}$ p/cm$^2$, the hydrogen depth profiles in implanted samples were then measured by $H(^{15}N,\alpha)^{12}C$ resonance Nuclear Reaction Analysis (NRA). The projected ranges of implanted ions are therefore obtained from the depth profiles. Then, a code based on the Projected Range Algorithm given by Biersack, Andersen and Ziegler has been developed to extract the stopping power data. In this code, the nuclear stopping power is the same as that from SRIM, but $^2He^+$ is used to instead $H_2^+$. The best coefficients have been obtained by fitting the experimental range data. As a result, the stopping power of proton in silicon is larger than the data used in SRIM, a maximum difference reaches to 15% at 30 keV/amu. The stopping power of $H^+$ and $H_2^+$ molecular ion is also different. The difference of the stopping power of $H^+$ and $H_2^+$ are velocity dependent. A critical velocity is found at the energy of 40 keV/amu. Below the velocity, the difference is positive, and it is changed to negative above the velocity. An interpretation related to the vicinage effect of $H_2^+$ is given.

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# The Restoration Spikes of Local Phonon During the Post Annealing in Diamond

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A long time is required for the thermal annealing after ion implantation to restore the once damaged crystal, e.g., it requires a few millisecond at shortest. For the target crystal, the whole process from ion-implantation to the end of post-annealing is the phase change of "crystal-amorphous transition (order → disorder)" and "amorphous-crystal transition (disorder → order)" in the atomic distribution in the same crystal. We have evaluated this order in terms of the long-range-order (LRO) parameter rather than the short-range one [1] based on the analysis of crystalline defects called the Pixel mapping method [1]. The degree of the order is simply indicated by the LRO parameter, that spans from $LRO = 1$ (order) to $LRO = 0$ (disorder). The atomic distribution is obtained by an atomistic simulation of molecular dynamics (MD) simulation. Therefore, we have used the MD and the PM to study the effect of post-annealing. Here, the projectile is the $N_2$ molecule with energy ($E_0$) of sub-keV per atom, which is implanted into a pure diamond at room temperature. After a period of thermal stabilization, until the bulk temperature became equilibrated by interacting with heat-bath, we started the post-annealing. Before the start of heating, the CA transition has already identified through the change in the *LRO*. The temperature of the heat-bath was raised up to the annealing temperature ($T_A$), which should enhance the lattice vibrations in a crystal simulated in MD. Just after the start of heating up to the order of tens ps, no appreciable change appeared in the *LRO* parameter. Then, we observed temporal *restoration spikes* [2] in the *LRO* parameter, where each spike changes "0 → 1 → 0" quickly. The time-interval between restoration-spikes was almost same for each case defined by a set of ($E_0$ and $T_A$). For example, in the case of 200 eV/atom and $T_A = 1000$ K, 9 regular spikes were identified between 60 ps and 670 ps, i.e., spikes appeared every 70 - 80 ps. We suppose such a regular profile of the restoration spikes signifies the trigger toward a final state of nearly ordered. The critical conditions for achieving the post-annealing will be presented at the conference.

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# Quantitative evaluation of charge-reduction effect in cluster constituent ions passing through a foil

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It is known that an average charge of the constituent ions resulting from the foil-induced dissociation of cluster ions is smaller than that of monatomic ions at the same atomic number and speed. Such a charge-reduction effect would decrease with increasing of the internuclear distance of the constituent ions moving in the solid. The internuclear distance is thus one of the most important parameters for understanding the mechanism of the charge-reduction effect. However, it is difficult to measure accurately and directly the internuclear distance increasing gradually by the screened Coulomb force between constituent ions, because of an interference correlation between the internuclear distance and the charge state. Therefore, we developed a method for estimating the internuclear distance distribution through the divergence angle distributions in each combination of charge states of the constituent ions after foil penetration [1], and then succeeded in quantitatively evaluating the empirical relationship between the internuclear distance and the charge state. As shown in Fig. 1, it was demonstrated regarding 6-MeV $C_2^+$ ions that the charge-reduction effect can be described as a function of the internuclear distance. Furthermore, a theoretical value indicated in a solid curve in this figure, calculated by the model considering the cluster effect on average charge [2], was well consistent with our experimental value.

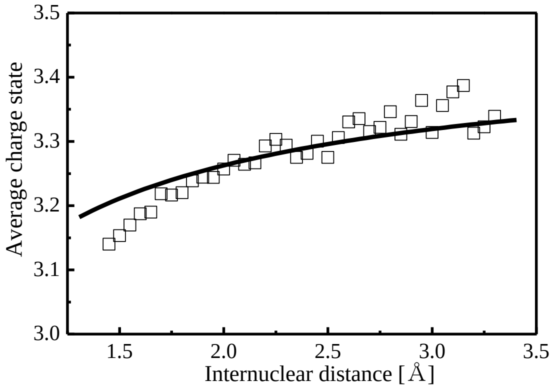

Figure 1. Average charge state of the constituent ions dissociated from 3-MeV/atom $C_2^+$ ions moving in a carbon foil, as a function of internuclear distance. The solid curve indicates a calculated result using the cluster average charge theory reviewed in Ref. [2].

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# A Positron Beam Analysis on Defect Formation in Iron by MeV Ion Beam

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Defect formation by energetic particles such as neutron and ion in metals has been studied for many years, and recent computational simulation in atomic scale has contributed to further understanding of cascade damage processes. However, experimental validation of these computational works is not sufficient mainly because of experimental difficulties in investigating such a fast (~ps) and fine scaled (~nm or less) process. This study is an experimental challenge to investigate defect production involving cascade damage processes produced by MeV ion irradiation.

Defect configuration after cascade damage is expected to be preserved at low temperature below stage I where interstitial atoms begin to migrate. MeV ion beam irradiation to pure-iron was carried out at 12 K, and then positron beam is implanted at the same temperature to the irradiated surface as a vacancy probe to evaluate vacancy concentration remained in the irradiated specimens. By this method, defect production efficiency which is defined as a ratio of residual defects to defect formation predicted by NRT model [1] was evaluated for iron irradiated with proton and carbon ions. Most of generated vacancy-type defects were likely to monovacancies, independent of PKA energy spectrum. Defect production efficiency values qualitatively represent the difference in PKA energy spectrum of $H^+$ and $C^+$, but the values were lower than simulation-based ones, possibly due to inhomogeneous distribution of vacancies caused by cascades and enhanced mutual annihilation of Frenkel pairs. Post irradiation annealing results and electric resistivity experiment results will be also discussed.

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Tu-060

# "The mechanism of emerging catalytic activity of Gold nano-clusters studied by ion scattering coupled with photoelectron spectroscopy"

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This paper reveals the fact that the O adatoms ($O_{ad}$) adsorbed on the 5-fold Ti rows of rutile $TiO_2$(110) react with CO to form $CO_2$ at room temperature and the oxidation reaction is pronouncedly enhanced by Au nano-clusters deposited on the above O-rich $TiO_2$(110) surfaces. The optimum activity is obtained for 2D clusters with a lateral size of ~1.5 nm and two-atomic layer height corresponding to ~50 Au atoms/cluster. This strong activity emerging is attributed to an electronic charge transfer from Au clusters to O-rich $TiO_2$(110) supports observed clearly by work function measurement, which results in an interface dipole. The interface dipoles lower the potential barrier for dissociative $O_2$ adsorption on the surface and also enhance the reaction of CO with the $O_{ad}$ atoms to form $CO_2$ owing to the electric field of the interface dipoles which generate an attractive force upon polar CO molecules and thus prolong the duration time on the Au nano-clusters. This electric field is screened by the valence electrons of Au clusters except near the perimeter interfaces, thereby the activity is diminished for three-dimensional clusters with a larger size.

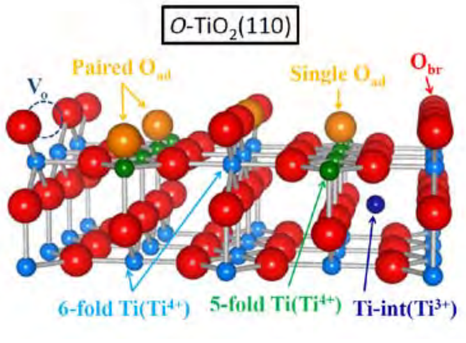

Fig. 1 Ball and stick model of *O*-$TiO_2$(110)

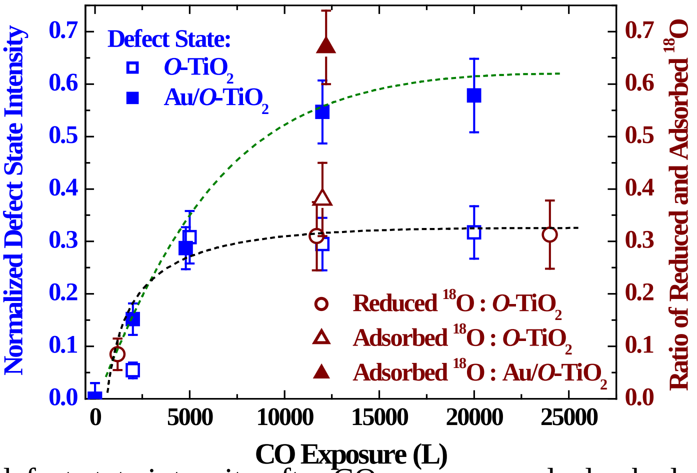

Fig. 2. Normalized defect state intensity after CO exposure and adsorbed $^{18}O$ after CO exposure followed by $^{18}O_2$ dose for *O*-$TiO_2$ and Au/*O*-$TiO_2$.

# Irradiation Effects on Hexagonal Boron Nitride Coated Titanium Diboride Reinforced Boron Carbide-Silicon Carbide Composites

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Boron carbide has wide application areas including nuclear technology [1]. Boron carbide has high hardness, wear resistance, chemical stability and thermal neutron cross section value [1]. However it has some disadvantages such as high sintering temperature, low mechanical strength and fracture toughness. So some additives such as silicon carbide and titanium diboride are used to reach high densities of boron carbide [2]. In this study hexagonal boron nitride (h-BN) coated titanium diboride reinforced boron carbide- silicon carbide composites were studied. In the sintering process of the materials hexagonal boron nitride was used for coating. Average thickness is 1 μm for hexagonal boron nitride. The materials were sintered by hot pressing method which has 2250 °C temperature, 130 MPa pressure and 2 hours sintering time properties. The titanium diboride ratio in the composites varies up to 4% by volume [2,3]. The wide using area of boron compounds in nuclear technology has generated interest to irradiation damage mechanism in boron compounds [4,5]. The composite materials were irradiated by 4 MeV electrons to fluence ranging from $10^{15}$ to $10^{17}$cm$^{-2}$ at room temperature.For the initial and irradiated samples XRD, SEM and EDX analyses were performed. The parameters of crystalline lattices and stresses were investigated for bulk (substrate) materials (boron carbide, silicon carbide and titanium diboride) and coated material (h-BN) at each dose value and titanium diboride ratio. The structure features of boron carbide, silicon carbide, titanium diboride and hexagonal boron nitride were carried out. The effects of dose and titanium diboride ratio on the crystalline lattice parameters and stresses (micro and macro) were discussed. We also discussed possible mechanism of accumulation and evaluation radiation defects by high energy electron irradiation.

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Tu-062

# Ion Scattering on Polarity-controlled ZnO Surfaces by MeV ions

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An almost complete reflection of a 2.5-MeV proton beam on an evaporated Au layer was found at a grazing-incidence angle [1]. Focusing of 2-MeV $He^+$ ions by means of tapered glass capillary optics was achieved by Nebiki et al. [2]. It has generally been considered that small-angle scattering on the surfaces play important roles in the reflections. However, the details of the mechanism have not been clarified yet. On the other side, the polarity-controlled ZnO crystals have been available, recently. They have two different surfaces, or “faces”, terminated with Zn and O atoms. We studied the mechanism of collisions between MeV ions and polarity-controlled ZnO surfaces aligned to the *c*-axis in order to investigate the efficient reflection of swift ions on solid surfaces.

The experiment was performed at the the JAEA Takasaki laboratory. $C^+$ (1–2 MeV) ions of a continuous beam (~50 pA) was modulated to a 10-kHz pulsed beam after attenuating the fluence rate to 1/300 or 1/30. Free-standing ZnO single crystals with two opposite surfaces, so-called “Zn and O faces,” were set on a manipulator in the chamber. The two crystals were of the same dimensions 10 mm × 10 mm × 0.5 mm. The energy of the ions scattered at 3° with respect to the beam axis was measured by a conventional Si surface barrier detector. The energy distribution was recorded by a multichannel analyzer. Figure 1 shows the energy distribution of the scattered ions in collisions of 2-MeV $C^+$ ions on the ZnO surfaces at an incidence angle of 2°. The distributions on the two opposite surfaces are significantly different. A larger energy loss and a higher yield of scattered ions on the Zn face compared to the O face suggest that elastic collisions with surface atoms play key roles.

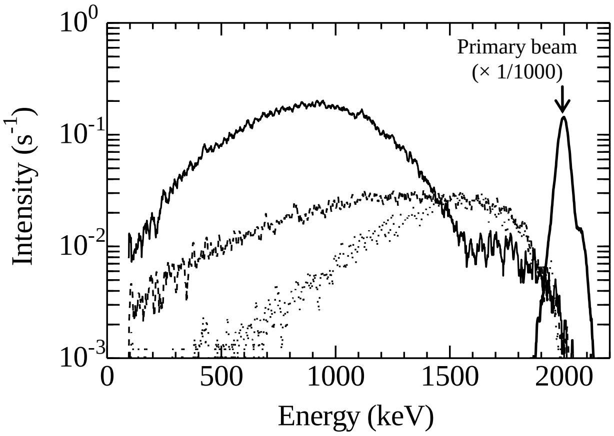

Figure 1. Energy distributions of scattered ions on Zn face (———) and O face (− · − · −) of ZnO crystals, and Au (- - - - -) surfaces in grazing-incidence collisions of $C^+$ (2 MeV) ions.

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Tu-063

# Stopping power for 5.2 – 6.8 MeV C ions into Si [110] direction

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Stopping powers for channeled H and He ions in single crystal silicon have been investigated for long time. There are also needed for surface, interface or impurity structure analysis by ion scattering. In contrast to H and He ions, there are few experimental studies of stopping powers for channeled heavy ions. Jiang et al [1] measured the energies of various heavy ions though the silicon foil in [100] axis and {110} plane channeling incidence.

We investigated stopping powers for C ions along the [110] direction in silicon single crystals with the energy regime from 5.2 to 6.8 MeV. Backscattering spectra for [110] direction incident C ions were measured from SIMOX (Si(100)/$SiO_2$/Si(100)) as target sample. Ion trajectories and energy loss were calculated by Monte Carlo simulation.

We assumed that the impact parameter dependent stopping powers were expressed by simple exponential formula. Stopping power $S$ ($E$,$r$) is expressed by next equation.

$$S(E,r) = a \cdot \exp(-b \cdot r)$$

Hence, $r$ is the closest approach, $b$ is fitting parameter and $a$ is appropriate normalizing coefficient.

Figure 1 shows the observed and simulated RBS spectra for 6.0 MeV. We determine parameter $b$ to reproduce the RBS spectra for the channeling incidence. The best fitted parameter $b$ values are 1.8, 1.8, and 1.95 for the incident energies of 5.2-MeV, 6.0-MeV, and 6.8MeV respectively. Figure 2 shows averaged stopping powers for axial channeling and random (SRIM2008). The ratio of [110] channeling to random stopping powers for 5.2, 6.0, 6.8 MeV are 0.67, 0.68, and 0.64, respectively.

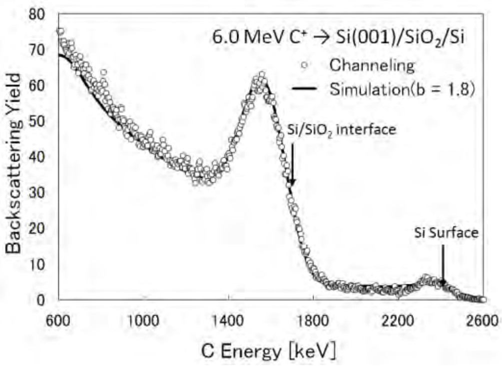

Figure 1. Observed and simulated RBS spectra for 6.0 MeV.

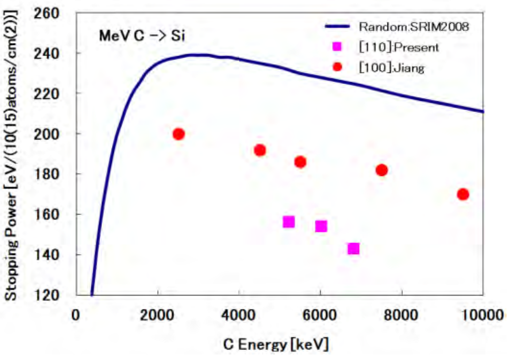

Figure 2. Averaged stopping powers for axial channeling and random (SRIM2008).

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Tu-064

# Trajectory dependent energy loss in grazing collisions of keV He atoms from a LiF(001)-surface

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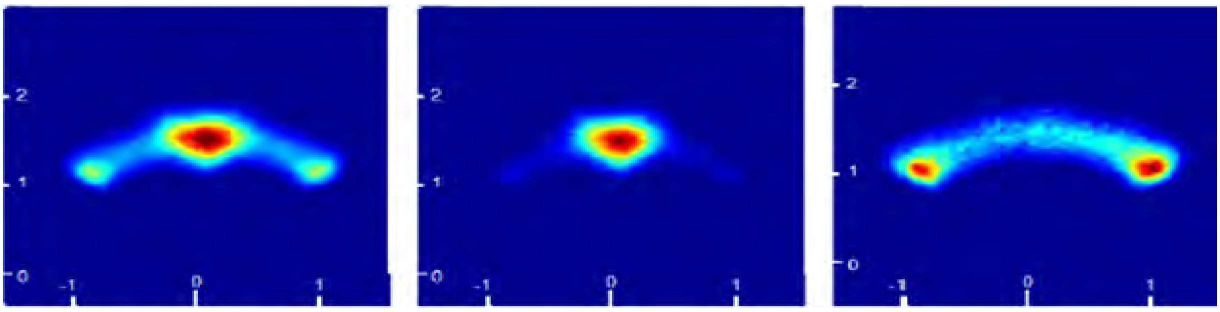
Scattering of fast atoms from insulator surfaces under grazing angles of incidence is accompanied by electronic excitation and emission processes based on the formation of transient negative ions. This implies that the capture process of well localized valence band electrons from so-called “active” sites dominates charge transfer and projectile energy loss giving rise to discrete peaks in the energy loss spectra for scattered ions [1]. In experiments on the coincident detection of energy loss and number of emitted electrons the basic mechanisms of the interaction scenario could be cleared up in some detail [2].

In the work presented here, we have extended these studies by recording the angular distribution of scattered projectiles in coincidence with the projectile energy loss in the regime of axial surface channeling. For scattering along strings of atoms in the surface plane the projectiles are deflected out of the incident scattering plane and at the extreme of the azimuthal angle an intensity enhancement is observed (“collisional rainbow”) [3]. In our experiments, the scattered atoms were recorded by means of a position sensitive micro-channelplate-detector and the projectile energy loss is obtained making use of a time-of-flight setup. As an example, we show in Figure 1 the angular distributions for 12 keV He atoms scattered from a LiF(001) surface under an angle of incidence of 1.4°. For scattering along <110>, i.e. along channels formed by alternate strings of $Li^+$ and $F^-$ ions, the coincident distributions reveal that rainbow scattering is accompanied with a discrete energy loss and proceeds primarily from $F^-$ strings, whereas scattering from $Li^+$ ions is fully elastic. This finding fully agrees with the concepts of charge transfer between atoms and insulator surfaces.



intensity of all scattered atoms intensity of elastically scattered atoms intensity of atoms with 15 eV energy loss

Figure 1. Angular distributions as recorded by means of position sensitive micro-channelplate-detector for scattering of 12 keV He atoms from LiF(001) along <110> direction with incidence angle of 1.4°.

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# Gas Cluster Ion Beam Accelerator: First Results

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Gas cluster ion beams and their interaction with solid surface is a rapidly developing area during the last years. In this work gas cluster ion beam accelerator is described. Clusters are formed by supersonic expansion of gas through Laval nozzle. The gas passes through a valve operating in pulsed regime to reduce gas load on the pumping system and to support pressure below $10^{-2}$ Torr in the expansion chamber. Neutral clusters are ionized by an originally designed ionizer; electrostatic field accelerating cluster ions can be set up to 20 kV. Magnetic field is used to remove monomers, and then focused beam is directed onto a sample.

In the experiments, argon was employed as the working gas. Using variable homogeneous magnetic field it was shown that $Ar_N^+$ clusters with N>500 are there in the beam when the stagnation pressure is above 2,5 bar. Time of flight technique was applied to measure argon cluster size distribution; the spectra obtained are in good agreement with literature [1]. Cluster sizes are in a range from 200 to a few thousands of atoms in a cluster.

Surface relief and structure of different materials after cluster irradiation was investigated.

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Tu-066

# Sputter Induced Cesium Luminescence: In Situ Optical Information During ToF-SIMS Depth Profiling With Cesium

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Low energy (<500 eV) $Cs^+$ sputtering allows molecular depth-profiling of organic materials, from amino acids to polymers [1,2]. Depending on the sample, molecular ions or characteristic molecular fragments can be monitored. Like in inorganic materials, anionic signals are much improved upon Cs irradiation, mostly due to reduction reactions with implanted cesium atoms. Those atoms also react with free radicals, therefore inhibiting cross-linking reactions.

We have used Optical Emission Spectroscopy (OES) in order to observe light emission induced during the sputtering mechanism [3]. The $6P_{1/2}$ and $6P_{3/2}$ to $6S_{1/2}$ neutral cesium transitions are intense. Peak intensities can be easily monitored during a depth profile simultaneously to ToF-SIMS measurements and can be attributed to neutral cesium atoms, excited by atomic collisions.

In this communication we will discuss typical differences between light emission from organic/inorganic depth profiles with cesium. We also have the ability to simultaneously use cesium and xenon as primary ions for sputtering (Cs/Xe co-sputtering). We will show that, on polystyrene, collisional excitation with cesium or xenon can be discriminated thanks to a Stark effect on those transitions. Sputtering yield differences have also an implication on the IR yields at the interface by OES. Through this communication we will show that Sputter Induced Optical Emission Spectroscopy can give access to fundamental processes occurring during depth profiling.

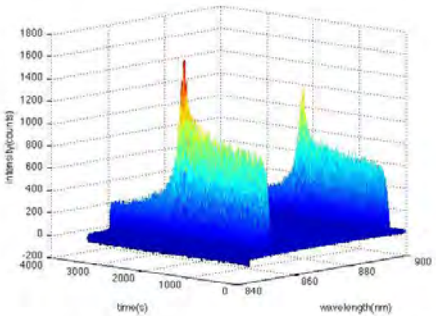

Figure 1. $6P_{3/2}$ and $6P_{1/2}$ to $6S_{1/2}$ transition monitored during a cesium depth profile of polystyrene on silicon

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# Highly charged Xe ions inducing nanostructure on $CaF_2$ surface at low energy and characterized by SFM in tapping mode

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Nature and intensity of ion-surface interactions are intimately connected to projectile energy deposition in the target and therefore depend both on the kinetic and the potential energies [1]. A coherent synergy of nuclear and electronic energy losses is suggested in ion-irradiation processes from the nuclear to the electronic energy regime [2]. In comparison with swift heavy ions (SHI), highly charged ions (HCI) carry several tens of keV of potential energy which is delivered into only a few atomic layers of the surface, resulting in many different phenomena that are significantly dependent on the potential energy deposition. Defects on dielectric surfaces irradiated by the energetic ions are usually tested by scanning force microscope (SFM). SFM has three modes: tapping, contact and non-contact. It is noted that a contact-SFM observation is often not very reliable in discussing topological structures while the tapping mode SFM was successfully applied to observe protrusions [3].

Experiments on nanostructure formation on $CaF_2$ single crystals irradiated by highly charged $Xe^{30+}$ ions with kinetic energies of 0.54 and 3 MeV have been carried out on the 320 kV ECR highly charged ions experimental platform at the Institute of Modern Physics (IMP), Lanzhou. In the tapping mode SFM image, the nano-sized hillocks protruding from the surfaces are probed. Results show that the height is equal to 3.1 ±1.1 nm and radius is equal to 13 ± 7 nm by irradiation of 0.54MeV $Xe^{30+}$. Such results are compared to hillocks created also by $Xe^{30+}$ at an energy of 0.3 MeV studied by El-Said et al. [4]. Using SFM in contact mode, the measured height is equal to 0.4 ± 0.1 nm and radius to 20 ± 4 nm. The height is lower and the radius is larger in contact mode than in tapping mode as already observed for hillocks on $CaF_2$ surface irradiated by swift heavy ions and measured by contact mode [5] or tapping mode [6].

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Tu-068

# High resolution depth profile analysis of ultra-thin STO/TiN layers on Si by LEIS

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(4) IMEC, (5)Linz University

Low-energy ion scattering (LEIS) can selectively analyze the atomic composition of the outermost atoms of a surface. Just like in higher energy RBS techniques (High and Medium Energy Ion Scattering) the incident projectiles may also scatter back from atoms in deeper layers. The effective neutralization of ions like $He^+$ strongly reduces the LEIS signal from subsurface layers and is thus responsible for its extreme surface sensitivity. However, above a particular threshold energy, a small fraction $P^+$ of the $He^o$ projectiles is reionized again upon leaving the surface. Details of this LEIS process and values of the energy threshold are given in [1]. From the analysis of ions, including reionized projectiles, information can thus be obtained on both outer surface and sub-surface layers. By use of the sensitive Qtac LEIS analyzer, which combines a very large acceptance angle with parallel energy detection, this is done with high-resolution and high efficiency. Since at low energy E the energy loss along the ion trajectory scales with $\sqrt{E}$, the depth resolution improves when using lower primary energies. Thus with1.2 keV $He^+$ scattering one can detect, for instance, the increase of a layer thickness by 1 carbon atom [2].

For a quantitative analysis of the depth profile it is crucial to know the (energy dependent) ion fraction $P^+$ or perform a calibration using well-known reference samples. A fast Monte Carlo simulation program (TRBS) developed for ion backscattering [3] has been used to determine the energy distribution of all (ions + neutrals) backscattered particles. The code accounts for multiple scattering, straggling and electronic stopping. Since it is essential to use the correct electronic stopping power, and no reliable data are available in the energy range of interest, a 3 nm TiN/Si sample was used to obtain this information on the TOF-LEIS setup ACOLISSA at Linz University.

It will be shown how the energy dependence of $P^+$ can be determined by combining LEIS (only backscattered ions) with the TRBS code. Using TRBS corrected for the ion fraction (TRBS-I) the in-depth profiles of ultra-thin layers of TiN and $SrTiO_3$ deposited on silicon were determined with 3 and with 7 keV $He^+$ scattering. These layers were grown by ALD and PVD. TRBS-I and complementary analysis using techniques such as MEIS have yielded results that serve as a guide for choosing optimum scattering conditions for in-depth analysis by LEIS in future.

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Tu-069

# Multiple scattering effects in the MEIS analysis of buried nanoparticles systems

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The synthesis of 2-dimensional nanostructured systems buried into a solid matrix has attracted interest in connection e.g. with plasmonic or magnetic applications. For both, the properties of the nanoparticle (NP) system are strongly dependent on the size, shape, areal number density and spatial order of the NP set. Medium energy ion scattering (MEIS) is an ion beam characterization technique, which have a great potentiality to investigate such kind of systems through the use of PowerMeis software [1], that considers any geometry, size distribution, composition and density of the nanostructures, and also the asymmetry of the energy loss-distribution. However, multiple scattering effects have not been taken into account. These effects can be important for the analysis of systems of buried NPs [2] and also for new MEIS setups using ions heavier than He [3] at lower energies. In this work, the energy loss due to multiple scattering effects was included in the PowerMeis program. Our results show a large contribution of multiple scattering effects in case of the analysis of a 2D buried array of Pb and Au NPs distant from the surface by about 60nm using 100 keV He ions. [2]. The inclusion of such effects improves the precision of the MEIS analysis of buried NPs and affects the determination of the shape and mean volume of the NPs. Other examples of the importance of multiple scattering effects, in particular their dependence with the shape, volume and density of buried NPs will be discussed.

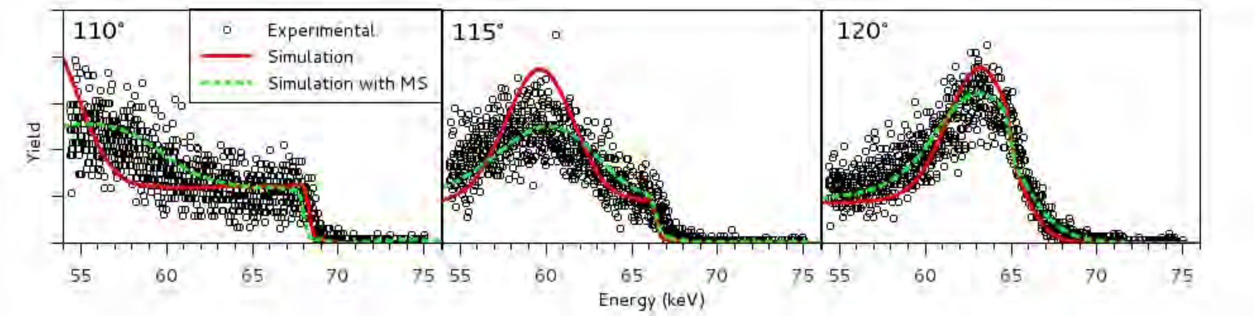

Figure 1. MEIS energy spectra of a 2D set of Pb NPs covered by 61nm SiO2 layer [2] using 100keV He$^+$ ions compared to PowerMEIS simulations, with and without multiple scattering effects for different scattering angles.

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# Effect of Low Energy Deuterium Ion Irradiation on Iron Oxide ($Fe_2O_3$)

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Iron oxide ($Fe_2O_3$) is one of rich materials in the nature world. However, there is little knowledge about the irradiation effects on the iron oxide by low-energy ions of hydrogen-isotopes. In this study, we have measured the depth distribution of deuterium (D) and the change in the X-ray diffraction (XRD) pattern of $Fe_2O_3$ films by low-energy D ion irradiation and investigated the D-incorporation effect and irradiation (energy deposition) effect on $Fe_2O_3$. Here, D is chosen because D can be easily detected by nuclear reaction analysis (NRA), $D(^3He,\alpha)H$.

Samples were prepared by deposition of Fe layers on $SiO_2$-substrates (RF-magnetron-sputter method) and followed by thermal oxidation [1]. The crystal structure of the oxide was confirmed to be $\alpha$-$Fe_2O_3$ (hexagonal, corundum structure), and the film thickness was evaluated by Rutherford backscattering spectroscopy (RBS) of 1.8 MeV $He^+$. Samples were irradiated by D ions generated using D-plasma of grow discharge in $D_2$ gas with 60 Hz AC-applied voltage of 1.5 kV [1].

Depth distribution of D was measured by using 1 MeV $^3He$ and by detecting $\alpha$-particles at the angle of 90 ° measured from the incident beam direction. It appears that D's in $\alpha$-$Fe_2O_3$ (100 nm thickness) are distributed deeper than the range distribution (< 30nm) calculated by using TRIM code, but, not uniformely distibuted in the film and more than 90 % of D's are located in the film, indicating small D diffusivity near room temperature. By integrating the D-density and consodering $^3He$ beam induced desorption, the amount of D-retention in $\alpha$-$Fe_2O_3$ is evaluated to be $50 \times 10^{15}$ $cm^{-3}$, in reasonable agreement with the reported value [1] and the value appears to be saturated at the D-ion irradiation time of 15 min. It appears that the XRD intensity vs the diffraction angle of $\alpha$-$Fe_2O_3$ (60 nm thickness) becomes broader and the XRD intensity decreases to 1/3 of that of unirradiated film at D-ion irradiation time of 30 min and the patterns reveal two components. Thus, it is more likely that both D-incorporation effect and D-ion irradiation effect (limited within 30 nm) contribute to the XRD modifications.

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# Damage Processes, Structure and Magnetic Moments Distribution in $Fe_3O_4$ Magnetic Films Irradiated by Swift Heavy Ions: Theoretical Modelisation and Experimental Results

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Swift heavy ions (SHI) irradiation is a unique and effectual tool, which is recognized to produce controlled defects (point/cluster and columnar), structural disorder, stress, and phase transformations in the thin films and to modify the physical properties of materials [1,2]. In addition, it is well known that the distribution of the magnetic moments in the films depends on the competition among magnetocrystalline anisotropy energy ($E_k$), demagnetization energy ($E_d$) and magnetoelastic energy ($E_\lambda$), and the effective magnetic anisotropy ($E_{eff}$) is by the above components interaction results. So, can we modify $E_{eff}$ by SHI irradiation and model its damage processes?

The experimental were performed on the materials research terminal of the HIRFL-SSC (IMP, Lanzhou) and a micro-model of the damage were reasonably assumed to fitting experimental results. In experiment, $Fe_3O_4$ films were irradiated at RT with 2.03 GeV $Kr^{26+}$ ions for fluence range from $5\times10^{11}$ to $1\times10^{13}$ ions/cm$^2$.

By means of contrast of the CEMS spectra of pristine and irradiated $Fe_3O_4$ films, it is found that occupancy distribution of the metallic cations in the films has changed significantly and the electronic-excitation effects result in a change of magnetic anisotropy after SHI irradiation. And the corresponding value of $E_d$ is calculated according to the CEMS results. In consideration of the approximate infinite plane of films and a large number of columnar defects (latent tracks) in the films induced by SHI irradiation, we assumed that the modification of $E_d$ is dominated by SHI irradiation process. In order to understand the magnetic moment distributions in the films, a micro-model of the damage in the films were reasonably assumed and the $E_d$ of the pristine and irradiated $Fe_3O_4$ films were calculated. The value of $E_d$ from CEMS is very close to the calculated results from the micro-model of the damage, which indicated that our micro-model of the damage is right and SHI irradiation can modify $E_d$ ($E_{eff}$) effectually.

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Tu-072

# "The structure of $SrTiO_3$(001) surface analyzed by high-resolution medium energy ion scattering spectrometry"

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Strontium titanate ($SrTiO_3$) takes a perovskite structure with a large dielectric constant and recently attracts much attention due to formation of two-dimensional electron gas at a $LaAlO_3$(001)/$SrTiO_3$(001) interface and an H-terminated surface. The single crystal (001) surface consists of alternating $TiO_2$ and SrO planes. It was reported that the surface is terminated completely with a $TiO_2$ layer by chemical etching in a buffered $NH_4$F-HF (BHF: pH ~4) solution[1]. However, annealing in ultrahigh vacuum (UHV) leads to a clean surface with SrO face partly[2]. Recently, the surface X-ray diffraction analysis by Herger et al.[3] demonstrated that the single layer $TiO_2$ (S-$TiO_2$) on top is thermally unstable and the surface is terminated with a double layer $TiO_2$ (D-$TiO_2$) by annealing the chemically etched surface in UHV. We analyzed the $SrTiO_3$(001) surfaces by high-resolution medium energy ion scattering (MEIS) before and after annealing in UHV. As the results, it was shown that the surface chemically etched in the BHF is perfectly terminated with the S-$TiO_2$ layer and the surface annealed in UHV consists of the D- $TiO_2$ and SrO faces. Interestingly, re-etching the annealed sample in hot water at 50°C and then annealing again at 600°C in UHV led to almost D-$TiO_2$ termination although a small fraction of SrO face still existed. The present high-resolution MEIS checked the validity of the surface structure proposed by Herger et al. and found a significantly different structure.

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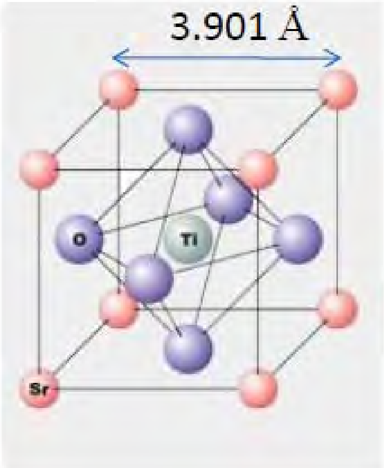

Tu-073

# Surface Modification of Teflon by Nitrogen Ion Beam Irradiation

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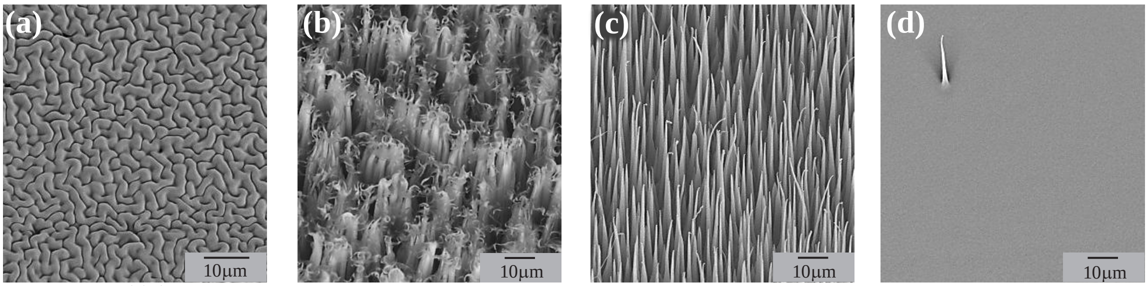
Polytetrafluoroethylene (PTFE) and fluorinated ethylene propylene (FEP) are typical fluoropolymers and well known as Teflon®. FEP has the excellent optical transparency unlike PTFE, and the melting temperature is lower than that of PTFE. When these surfaces are irradiated with ion beam, both are covered with a large number of small protrusions and show the superhydrophobicity due to lotus effect. Previously, we reported the morphological change of these surfaces by 80keV $N_2^+$ ion beam irradiation and sample heating [1]. At a low fluence, the melted layer and micropores were formed on the surface. When the fluence increased, the melted layer gradually diminished and the micropores enlarged. After the melted layer vanished, the surface was finally covered with small protrusions. In this study, we investigated the difference in densities and the sizes of the protrusions caused by the changes of the ion energy, the current density and the sample thickness.

PTFE and FEP films (50-500 μm in thickness) were irradiated with $N_2^+$ ions using an ion accelerator. The ion energy was controlled in the range from 80 to 380 keV. The current density was also controlled in the range from 0.3 to 1.0 $\mu A/cm^2$. The surface morphology and chemical bonding were observed with a scanning electron microscopy (SEM), an optical microscope, and an attenuated total reflectance/Fourier transform infrared (ATR/FT-IR).

When 500-μm-thick PTFE sheet was irradiated with 380keV $N_2^+$ ion beam at the current of 1.0 $\mu A/cm^2$, the flat surface became wrinkly at the fluence of $5\times10^{15}$ ions/$cm^2$ (Fig. 1(a)). Up to $1\times10^{16}$ ions/$cm^2$, many protrusions with a shaggy top were formed (Fig. 1(b)). When 100-μm-thick PTFE was irradiated with $N_2^+$ ion beam with the same condition, the protrusions were spiny as shown in Fig. 1(c). In the case of 100-μm-thick FEP, only at $1\times10^{15}$ ions/$cm^2$, the surface was nearly flat with very few protrusions (Fig. 1(d)). From the results, the surface morphology was controlled by the beam condition and the sample thickness. We will also discuss the chemical bonding of these surfaces.



500-μm-thick PTFE $5\times10^{15}$ ions/$cm^2$

100-μm-thick PTFE $1\times10^{16}$ ions/$cm^2$

500-μm-thick PTFE $1\times10^{16}$ ions/$cm^2$

100-μm-thick FEP $1\times10^{15}$ ions/$cm^2$

Fig. 1 SEM images of the surfaces irradiated with 380 keV $N_2^+$ ion beam. The uppers were sample and the lower were the fluence.

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Tu-074

# Guiding effect of tapered glass capillary optics for MeV ion beam

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Rutherford backscattering spectroscopy is known to be useful for the depth profiling and compositional analysis of materials. However, the lateral resolution is limited by the diameter of ion beam. For this limitation, Nebiki *et.al.*[1] proposed the tapered glass capillary as a compact optics of beam transport. Indeed, they demonstrated that this optics can focus the MeV ion beam to sub-μm size with a significantly enhanced current density (focusing effect).

We performed similar experiments to ref.[1], by using 1.5 MeV He$^+$ ion beam. Then, in addition to the focusing effect, we found a new effect. It is the *guiding effect*, by which the MeV ion beam can be tilted from the initial beam direction. For the glass capillary, the ion beam could be guided by ±3.5° with respect to the initial beam direction (solid circles in Fig.1), and the ion beam was transported without degrading the quality of beam over this angular range. For better understandings of the effects, the same experiment was performed by using the electrically conductive capillary, instead of the non-conductive glass capillary. The size and shape of the conductive capillary was practically the same as the non-conductive glass capillary, since it was prepared by silver-plating on the inner and outer surfaces of the tapered glass capillary used. Both focusing and guiding effects could not be observed for the conductive capillary (open circles in Fig.1), which was electrically held on the ground level. Therefore, the electric charging-up of the insulating capillary surface would be primarily responsible for both effects, even for the MeV ion beam.

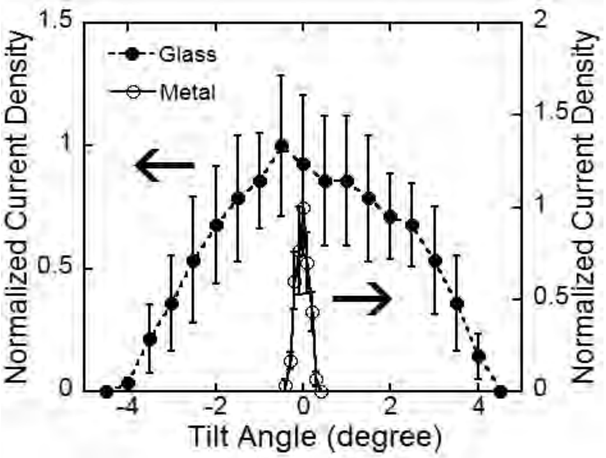

Figure 1. the guiding effect by glass capillary(solid circles) and silver plated capillary(open circles).

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Tu-075

# Spectroscopic Characterization of Ion-irradiated Multi-layer Graphenes

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Graphenes have been attracting attention as new semiconductor materials with intriguing properties, basic and applied researches have been intensively carried out in the world[1]. Interesting properties of graphenes can be employed in numerous potential applications such as transparent conductors and quantum devices. On the other hand, control of electrical and optical properties is essential to realize the graphene devices. It was reported that the band gap of the graphenes was controlled by introduction of defects into the graphenes. Soft X-ray absorption spectroscopy (XAS) has been one of powerful tools since it provides not only information on the local electronic structure surrounding excited carbon atom, but also orientation of the π bonds of carbon. However, there were a limited number of soft X-ray spectroscopic studies on multi-layer graphenes into which defects are introduced by ions.

In this study, multi-layer graphenes grown by catalytic CVD were irradiated with low energy Ar ions with different ion doses, and characterized by XAS, X-ray photoelectron spectroscopy (XPS), and Raman spectroscopy. Number of layers of graphenes used in this study was estimated to be 3 to 5 from 2D peak position and shape of Raman spectra of as-prepared graphenes. In order to investigate local bonding configurations and electronic states of the irradiated graphenes, XAS and XPS were used. The results revealed that &pi;* peak intensity was decreased with increasing dose of the ion in the XAS spectra (Fig. 1). This suggests that $sp^2$ component in the graphenes is decreased by the ion irradiation.

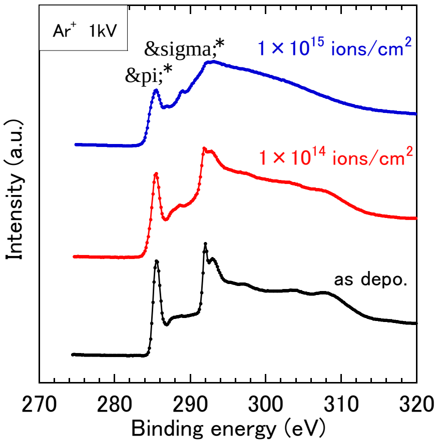

Figure 1. Soft X-ray absorption spectra of Ar ion irradiated multi-layer graphenes

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Tu-076

# Ion-induced luminescence and damage process of $LiTaO_3$

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Lithium-based oxide ceramics are promising candidates for tritium breedimg materials in a fusion reactor utilizing the D-T reaction. The tritium recovery strongly depends on the release behavior of tritium affeted by the defects that MeV energetic particles from the Li-n nuclear reactions bring about. Therefore the damage accumulation and its interaction with hydrogen isotopes are needed to be clarified. Among the conventional ion beam analysis techniques, the ion-induced luminescence is a potentially powerful tool capable of examining modifications and their evolution under irradiation conditions[1]. In the present study, the ion induced luminescence measurements were carried out to examine its basic characteristics of the light emission and the damage accumulation in Li oxide materials.

Samples used in the present work were commercially available $LiTaO_3$ single crystals having <0001> axis normal to the surface, with a size of $10\times10\times0.5$ $mm^3$. The sample was placed in a scattering chamber connected with a 1.7 MV tandem accelerator. The light emitted from the sample in the scattering chamber was collected through a synthesized silica window and a lens focused on a silica fiber connected to an optical spectrometer, which consists of a monochromator equipped with a CCD camera. The evolution of the ion-beam-induced luminescence spectrum was monitored for wavelengths from 300 to 900 nm during the irradiation of H, He and O ions for the various incident energies between 0.3 and 4 MeV. The photo-stimulated luminescence (PL) was also obtained in the same chamber using 266 nm (4.7 eV) photons from the fourth harmonic wave of an Nd:YAG laser.

A broad peak centered at about 500 nm was observed in a $LiTaO_3$ crystal under the ion bombardment and was essentially the same as the UV photon irradiation. The intensity of the luminescence drastically enhanced with a decrease of the temperature, with an activation energy of 0.15 eV estimated for the non-radiative transition process. The analysis of decay curves of the luminescence showed two components of lifetime, 5 and 50 ns. During the ion bombardment at room temperature the peak intensity from the $LiTaO_3$ crystal monotonically decreased with a relatively slower reduction rate in comparison to that of $Li_2ZrO_3$[2]. Assuming first-order kinetics of the annihilation process of the luminescence centers, the annihilation rate constants of the luminescence centers is proportional to the nuclear energy deposition of the incident ions, while the recovery of the damaged ones is effectively occured by the electronic energy deposition.

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Tu-077

# Surface Composition Analysis of Binary Mixtures of Ionic Liquids

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Ionic liquids (ILs) are composed entirely of cations and anions, and in a liquid state near room temperature (below 100°C in a broad sense). There are more than $10^6$ different ILs with various combinations of cations and anions. ILs commonly have some unique properties such as high ionic conductivity, negligible vapor pressure, incombustibility, and good thermal stability of wide temperature range. However, their properties can be turned in a wide range by varying the combination of cations and anions. This diversity of the properties allows them to be promising for applications in many fields, for example, as safer electrolyte of lithium secondary battery, lubricating oil under severe conditions where usual lubricating oil does not work, and so on. Furthermore, mixing two or more kinds of ILs is also considered to be effective to tailor the properties precisely for a specific application. For some applications, it is of great importance to understand the relation between the surface structure of ILs and their properties to select or design an IL with desirable properties. In the last decade the surface structure of ILs were intensively investigated with various techniques of surface analysis. However, there are only a few studies on surface structure of IL mixtures [1-3], and even the surface composition is not fully elucidated.

In this study, we analyzed surface composition of several binary mixtures of imidazolium-based ILs by two different techniques, time-of-flight secondary ion mass spectrometry (TOF-SIMS) with grazing incidence of MeV ions and high-resolution Rutherford backscattering spectroscopy (HRBS). Surface sensitivity in SIMS and high quantitativity in HRBS revealed the molecular composition and orientation at the surface of IL mixtures.

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Tu-078

# Surface structural analysis of MgO(111) using low energy atom scattering spectroscopy

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Fundamental concepts for surface science are well-established and their applications are straightforward for metals and semiconductors, but not for insulators and materials in the electric/magnetic fields. Bombardment of insulator surfaces by charged ions can be induced a charge on their surfaces. One can see the charging/discharging dynamics of the insulating material during this ion-beam bombardment. Sometimes, an electron shower using a tungsten filament placed nearby a sample is used to reduce the sample charging. However, electron-shower failure can cause sample damage. Therefore, we developed a low-energy atom scattering spectroscopy system for the analysis of these insulator surfaces [1]. Low-energy atom beams were produced using ion beams. Atom beams were converted from ion beams by charge exchange while the ion beams passed through a small gas chamber.

MgO is an exceptionally important material, which used in catalyst, toxic-waste remediation agent, or as an additive in refractory, paint as well as for fundamental and application studies. The 111 surface gives a hexagonal arrangement of atoms. We have been wondered which atoms, that is to say, Magnesium or Oxygen atoms are more dominant on topmost surfaces ? Here, low energy atom scattering spectroscopy will give answer and show experimental results on MgO(111) surfaces. Figure 1 shows the image of Mg atoms obtained from clean MgO(111) surfaces. In details will be shown in the conference.

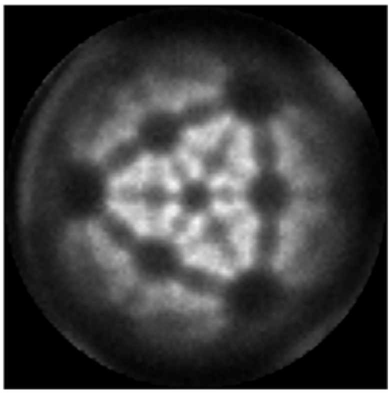

Figure 1. the Mg image of clean MgO(111) surfaces

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Tu-079

# Intensity Distributions of Reflected Surface-channeling Protons Scattered on Surfaces of Electron-bombarded Alkali Halide Crystals

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Surface-channeling at grazing incidence of 550keV protons on electron-bombarded surfaces of alkali halide crystals is investigated. Electron-stimulated desorption (ESD) resulting from the irradiation of electrons changes the morphology of the surface. As the result of the ESD, the surface is covered by rectangular holes of monolayer depth with edges oriented along the crystallographic directions of <100> and <010> on the (001) plane [1]. In order to investigate the change of the surface morphology by the electron irradiation, the luminous intensity distributions (scattering patterns) of reflected protons on a fluorescent screen under the surface-channeling conditions is observed. The samples are KCl(001) and KBr(001). Figure 1 shows an example of the measured scattering patterns. The intensity profiles containing the incident and the scattered beams along the direction normal to the crystal surface are inserted on the top of the figure. The peak-angle of the scattered beam profile depends slightly on the irradiation dose. It shifts to lower angle and comes to a standstill. The peak-angles are compared with calculated results of a computer simulation. The modeled ESD surface is obtained by a section of the computer simulation. An example of the obtained surface morphologies is shown in Figure 2(a). Figure 2(b) shows calculated scattering pattern on the surface shown in Figure 2(a). The calculated scattering pattern reflects the changes of the morphologies of the ESD surfaces. This tendency is similar to the experimental results.

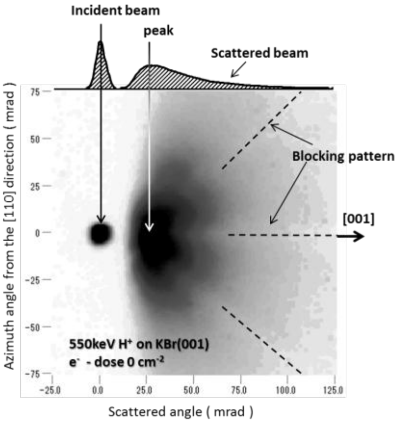

Figure 1 An example of measured scattering patterns.

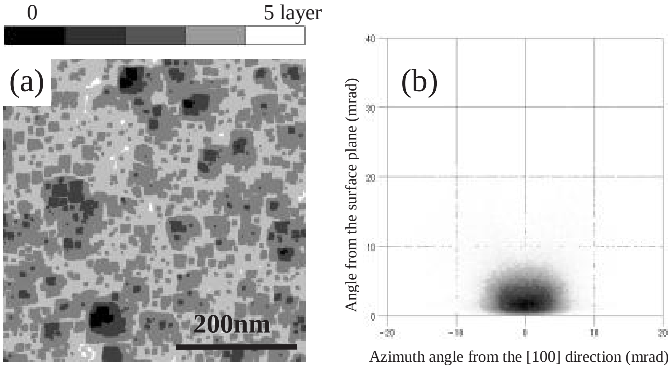

Figure 2 (a) Calculated surface for the irradiation dose of $1.5 \times 10^{15}$ cm$^{-2}$.
(b) Calculated scattering pattern on the surface.

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# Direct Observation of Fine Structure in Ion Tracks in Amorpous Thin Films by TEM

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There are a lot of studies on the ion tracks produced in crystalline substrates because they can be easily observed using transmission electron microscopy (TEM). On the other hand, ion tracks produced in amorphous materials have not been observed by TEM. It has been thought that direct observation is difficult due to a lack of sufficient contrast. In this study, thin films of amorphous $Si_3N_4$ were irradiated with 120 – 720 keV $C_{60}^{+,\,2+}$ ions and observed using TEM. The ion tracks produced in the amorphous material was directly observed by TEM for the first time. Figure 1 shows the observed TEM image. For quantitative analysis, the ion tracks were also observed using high-angle annular dark field scanning transmission electron microscopy (HAADF-STEM). The observed ion tracks consist of a low density core (radius ~ 2.5 nm) and a high density shell (width ~ 2.5 nm), which is very similar to the ion tracks in amorphous $SiO_2$ irradiated with high energy heavy ions observed by small angle x-ray scattering (SAXS) [1]. This suggests that the core-shell structure is a universal feature of the ion tracks produced in amorphous materials irrespective of the material and the ion. The observed track radius is almost independent of the incident energy in the observed energy region, where the electronic stopping power increases rapidly with energy while the nuclear stopping power decreases. This indicates that the nuclear stopping power is also responsible for the track formation and is more effective than the electronic stopping power.

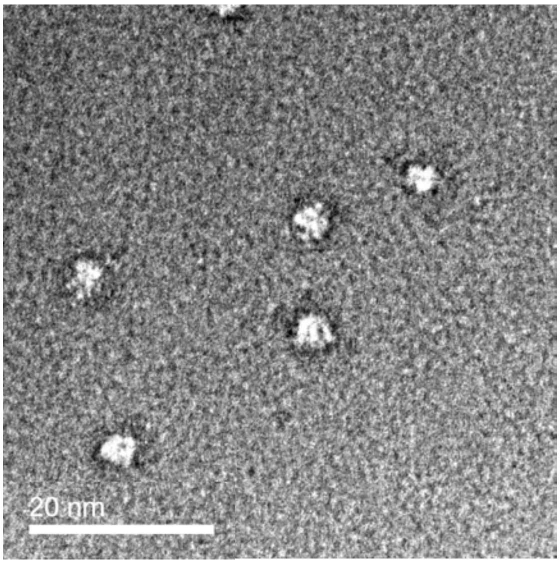

Figure 1. Observed TEM image of the amorphous $Si_3N_4$ irradiated with 720 keV $C_{60}^{2+}$ . Sample thickness is 20nm.

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# Measurements of Electron Attachment to Oxygen in Proportional Counter

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We have developed a proportional counter for measurements of low-energy β-rays and faced a problem on electron attachments which shows a clear energy-shift of the same event on spectra. This phenomenon is well-known as the negative-ion formation by electronegative molecule such as $O_2$ and $H_2O$ contaminated in the counter gas, which causes some deterioration of time resolution and detection efficiency. Recently these influences in a long drift counter and in gaseous plasma have been investigated to optimize the performance of the detection system. In the long proportional counter, the electron attachments were studied by the pulse height as a function of drift time for different values of the oxygen contamination in counter gases.

However, as shown in Fig.1, we clearly observed a similar phenomenon of electron attachments by measurements of 5-keV Auger electrons from thin Fe-55 source by varying the concentration of oxygen gases, actually by that of dry air. It is thought that our data indicate sensitive response to the electron attachment, because the primary electrons drafting through oxygen gases are finally multiplied just around anode wire by a factor of about $10^4$, i.e., a huge amplification known as a Townsend avalanche. We now systematically perform some meaurements to evaluate the electron attachment rate at different oxygen concentrations and also try to extract new information from these peak profiles on energy spectra. At this conference, we present our experimental method and newly obtained results.

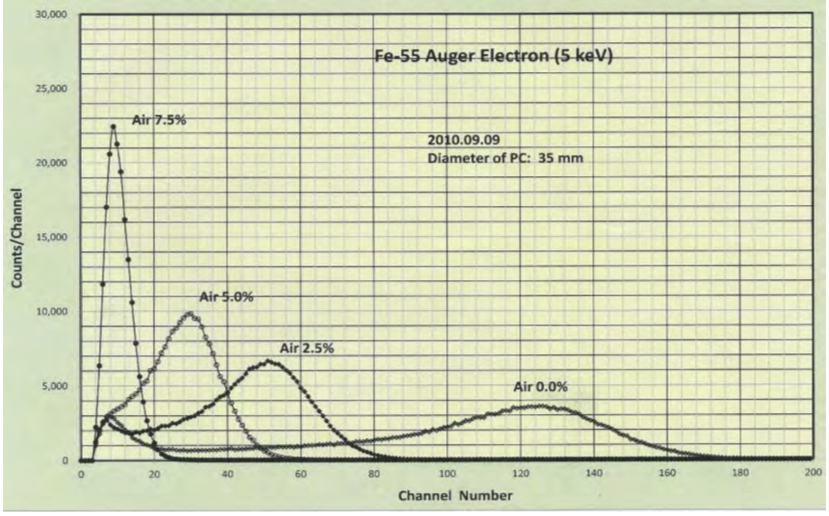

Figure 1. Energy spectra of 5-keV Auger electrons for differnt values of the oxyzen concentration controlled by that of dry air using the proprtional counter filled with $CH_4$. Fe-55 source was set on inner wall of the counter(50-cm-long and 3.5-cm-diam of cylindrical with 20-μm-diam tungsten wire).

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Tu-082

# Positron energy loss and the interaction between positrons and soliton-like electron density in Graphite-Alkali Metal Intercalation Compounds

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Alkali-metal graphite intercalation compounds(AGICs) are interesting and important materials, which have quasi-two dimensional electron structure. Cartier et al.[1] have reported very interesting results of the angular correlation of positron annihilation radiation (ACAR) for AGICs. That is, it is seen that a strong anisotropic and narrow component appears in the center of the ACAR of C8K and C24K. Then hydrogen chemisorption effect in AGICs have been studied by means of positron annihilation [2,3]. So far the origin of the narrow compound in the positron annihilation spectra has not been confirmed. Recently the present authors [4] have analyzed the narrow components of the positron annihilation spectra with the theoretical formula, which is extended from "topological quasi-positronium model" [5]. In this study, we will discuss positron energy loss and the interaction between positrons and Skyrmion-like electron density in Graphite-Alkali metal intercalation compounds.

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Tu-083

WITHDRAWN

Tu-084

# On the role of d-electrons in electronic stopping of slow light ions

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When ions traverse matter, they lose energy according to the stopping power S = dE/dx. These energy losses can be attributed to either collisions with target nuclei (nuclear stopping, $S_n$) or excitations of electrons (electronic stopping, $S_e$). For a free electron gas and projectile velocities below the Fermi velocity, $S_e$ is expected to scale linearly with projectile velocity: $S_e = Q \cdot v$, with the friction coefficient Q as proportionality factor [1]. In recent years, many experiments have revealed, that for light ions and low projectile velocities the specific band structure of a target may lead to pronounced deviations from velocity proportional stopping [2,3].

This investigation focuses on the particular role of the d-electrons in the interplay between band-structure and electronic stopping. It has been shown for Au and Cu that the onset of the excitation of d-electrons may cause a significant increase in Q. This behavior leads to a pronounced kink in $S_e$ at a certain projectile velocity. To gain a complete picture of the correlation between d-electrons and stopping power, materials with a different d-band configuration have been investigated, namely Ag and Pt. Ag is very similar to Au and Cu, except that the onset of the d-electrons is ~ 4 eV below $E_F$ compared to ~ 2 eV for Au and Cu. Pt, on the contrary, features d-electrons with energies ranging from 8 eV below $E_F$ up to $E_F$.

Experiments have been performed in backscattering geometry employing thin film targets. Electronic stopping has been deduced in two ways. First, at sufficiently high energy, electronic stopping was deduced from the width of the peak due to backscattering from the thin film, taking the influence of nuclear stopping and multiple scattering into account. The film thickness was determined quantitatively by RBS. Second, relative measurements were performed, relating the height of the backscattering spectrum to that of Au. In this case, no information on the film thickness was needed, but the absolute value of gold stopping was required instead.

Results are presented on electronic stopping of H and He ions in Ag and in Pt. To elucidate the role of the d-electrons, the present results are compared to the corresponding stopping values in gold. It is analyzed, to which extent surface impurities or the correction for nuclear stopping may introduce an uncertainty to the presented data.

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# XMCD-PEEM observation of focused ion beam induced magnetic patterns on FeRh surfaces

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Equiatomic ordered FeRh alloy with the B2 (CsCl type) structure is of much interest due to the first order anti-ferromagnetic (AF) – ferromagnetic (FM) phase transition near the room temperature. In our previous studies, we reported that deposited energy through elastic collision by ion irradiation induced the FM state in FeRh films below room temperature where they were originally in the AFM state. [1] Such ferromagnetic ordering was found to be ascribed to the lattice defects introduced in the B2 structure due to the keV-MeV ion irradiation. And we have successfully produced micrometer-size lateral magnetic modulation by 10 MeV I ion microbeam rradiation.[2][3]

In the present study, we have demonstrated the fabrication of micron scale magnetic patterns by 30keV Ga ion irradiation using a focused ion beam system (FIB). We also discuss the magnetic domain structure of the irradiation induced ferromagnetic regions by using the X-ray magnetic circular dichroism-photoemission electron microscopy (XMCD-PEEM).Thin FeRh films were deposited on MgO(001) substrates by using an ion beam sputtering from Fe-50at.%Rh target. In order to make magnetic modulations, we irradiated huge numbers of 5-30 $\mu$ m square regions at the surface of the FeRh thin films. The fluences were $1\times10^{12}/cm^2$, $5\times10^{12}/cm^2$, $1\times10^{13}/cm^2$ and $3\times10^{13}/cm^2$.

We successfully confirmed the formation of the designated ferromagnetic dot patterns by a magnetic force microscope. As for the magnetic domain structures of ferromagnetic patterns, we observed the corresponding bright square regions in the XMCD-PEEM images. We also confirmed that the contrast become absolutely clear with increasing in the ion fluence. This result suggests that ion-irradiated microm-scaled areas definitely show the ferromagnetic state, magnetization of which increases with increasing ion fluence. We will discuss these magnetic domain structures in conjunction with the ion irradiation fluence.

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Tu-086

# A new facility for *in-situ* analyses of slow highly charged ion modifications of various materials

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The interaction of highly charged ions (HCI) with materials has been investigated intensively in recent years. On different materials local topographic modifications at the ion's impact site could be identified by means of atomic force microscopy (AFM). The type of the produced nano-structures varies from pit-like (KBr, PMMA) to craters ($TiO_2$) and hillock-like structures on $CaF_2$ and others ([1, 2]). Most of the studies so far were performed under ex-situ conditions, meaning the target material was transported under ambient conditions from the place of irradiation to an AFM or scanning tunneling microscope. We present a new experimental set-up for in-situ investigations on HCI induced nano-structures. The set-up is based on an assembly of a Dresden-EBIT (Electron Beam Ion Trap) ion source and an Omicron ultra-high-vacuum-AFM. Samples can be mounted in the AFM and analyzed by means of AFM and STM before, during and after the irradiation with HCI. Samples can be heated in-vacuum to prepare clean surfaces before irradiation. The EBIT delivers highly charged ions with Xe charge states up to q=40+, which can be decelerated to kinetic energies of only 10 eVq.

Figure 1 shows a drawing of the set-up. The dimensions of the set-up are small compared to other HCI experimental set-ups. The EBIT is mounted in a high voltage cave and so a negative potential can be applied, while the AFM chamber is kept on ground potential. The final kinetic energy of the ions is defined by the difference of the extraction potential (respective to ground) and the target potential (ground) by $E^{final}_{kin} = (U_{ext} * U_{beamline}) * q$. A lens system focusses the beam onto the target with a beam diameter of less than 1 mm.

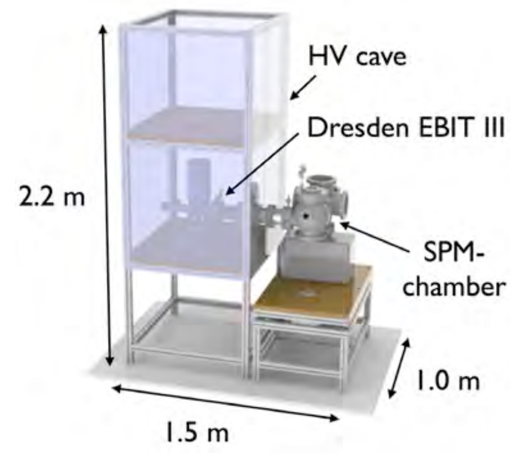

Figure 1. Schematic view of the set-up. The dimensions are indicated as well as the high voltage cave holding the ion source.

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# Characterization of the monoclinic-tetragonal phase transition of zirconia by using proton implantation

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The tetragonal (t)–monoclinic (m) transformation of zirconia has a great technological importance for mechanical application since it is the basis for the transformation toughening of ceramic components[1, 2]. As a result of the typically potential room temperature of high temperature polymorphs (tetragonal and cubic) of $ZrO_2$, their stabilization at low temperatures and understanding the associated phase stabilization mechanisms has been of intense interests[3]. Here, oxygen ion vacancies or strain energy is also one of factors associated t-phase stabilization. Therefore, the implantation parameters (energy, ion dose, substrate temperature, and ex-situ annealed temperature) could play a vital role to study the resultant phase transition of zirconia. In this study, zirconia of monoclinic (m) phase was first prepared by Sol-Gel sythesis and the internal oxidation of Ag-$AgZr_2$ alloys, respectively, to study the phase transition of zirconia under irradiation with free surface and nano-confinement situations. Here, the particles size or grains size of pure monoclinic zirconia are ranging from 20 to 60 nm. The two kinds of specimens, i.e., pure monoclinic zirconia particles with and without Ag cladding, were followed by using protons implantation of 1.5 MeV and 50 keV energy. The fluences are from $1\times10^{14}$ to $1\times10^{16}$ ions/cm$^2$. The effect of implanted doses, were studied and characterized by using transmission electron microscopy (TEM) and x-ray diffraction (XRD). Consequentially, tetragonal (t) zirconia characteristic peak appeared on the free particles of zirconia after proton implantation of 1.5 MeV energy at the proton doses above $1\times10^{15}$ ions/cm$^2$, while tetragonal zirconia characteristic peak all appeared on the Ag-cladding zirconia at the proton doses range from $1\times10^{14}$ to $1\times10^{16}$ ions/cm$^2$. Apparently, the m→t phase transition for zirconia free particle can be accomplished with the above threshold of requiring dose ($1\times10^{15}$ ions/cm$^2$), while the Ag-cladding zirconia could show the m→t phase transition at lower proton dose ($1\times10^{14}$ ions/cm$^2$) due to constraint effect. Moreover, there is no tetragonal zirconia characteristic peak appeared on the free particles and Ag-cladding zirconia at the same proton doses of 50 keV energy. It suggests that the implantation-induced lattice defects were not conducive to m→t phase transition. The further results and study on the m→t phase transition to the two kinds of zirconia will be discussed.

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Tu-088

# Damage and recovery process of PEN films irradiated by MeV ions

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Polymers consisting of benzene rings are known to effectively absorb UV light and some of them are accompanied by photo emission in visible wavelengths, which can be utilized for monitoring the intensity and special distribution of the ionizing radiation. Polyethylene naphthalate (PEN) film, exhibiting superior and desirable properties such as Young's modulus and permeability to water, also shows irradiation induced blue luminescence. On the other hand, the ion bombardment of the polymer materials causes drastic changes in the optical properties of the PEN films, depending on the energy deposition process[1]. Moreover, particle irradiation causes irreversible degradation of the films accompanying significant release of O and H atoms, especially in vacuum condition[2]. In the present study, we measured evolution of MeV ion and UV photo induced luminescence of PEN films to examine the relationship between energy deposition and damage/recovery of luminescence characteristics of the films.

The samples were commercially available PEN (Teonex@, Teijin DuPont Japan) films with a thickness of about 9 μm. Irradiation of 0.3–2.0 MeV $H^+$ and 2.8 MeV $He^{++}$ ions, which can penetrate the entire thickness of the sample film, was performed at room temperature in a scattering chamber connected with a 1.7 MV tandem accelerator. An area of about 100 $mm^2$ of the sample was irradiated with a current density less than 1 $nA/mm^2$ to prevent heating effects during the irradiation. The photo-stimulated luminescence (PL) was also obtained in the same chamber using 355 nm (3.5 eV) photons of a light emitted diode (LED) and of the third harmonic wave of an Nd:YAG laser. The evolution of the ion-beam-induced luminescence spectrum was monitored for wavelengths from 300 to 900 nm during the irradiation. Immediately after the irradiation, the PL measuements were continuosly carried out to observe recovery phanomena in the sacattering chamber filled with the air at a temperature range between 290 and 400 K

The PEN film exhibited characteristic luminescence bands mainly in the 400-500 nm wavelengths under the both ion and photon irradiation. At the beginning of the ion irradiation to a fluence of $10^{13}$ ions/$cm^2$, the peak intensity immediately diminished, followed by a smaller decrease rate at higher fluence. Similar two step reduction behavior of the PL intensity was found during the LED exposition where the energy fluence of photons was comparable to the total energy deposition of the incident ions. This indicates that the damage process of the luminescence centers is essentially the same for ions and photons. After stopping irradiation, the PL intensity recovered as a function of time with a rate depending on the deposited energy fluence. The elevating temperature, however, prevented the damaged luminescence centers from being annealed, probably owing to the formation of a non-irradiative structure.

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Tu-089

# Deposition of Ionic Liquid Ion Beams on Solid Substrate

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The ionic liquid(ILs) known as room-temperature molten solt show moderate electrical conductivity (1-100 S/m), high thermal stability (up to ~300 °C) and extremely low vapor pressure (< $1\text{x}10^{-9}$ Pa). Due to the typical ILs includes halogens in safety, reactive etching, surface modification and ILs deposition could be expected for silicon, silicon oxides and glasses. We developed an ionic liquid ion source(ILIS) with porous medium [1] known as a high current and stable method in the field of liquid metal ion sources. In this study, deposition of thin IL layer and surface modification of glass and silicon substrate by irradiation of IL ion beam was characterized.

1-butyl-3-methylimidazolium hexafluorophosphate(BMI-$PF_6$) was used for the source liquid. Positive and negative ion beams generated from an ILIS with porous emitter[1] were irradiated to a borosilicate glass substrate (Matsunami #7059) and a single crystalline Si (100) substrate. The positive ion beam was accelerated to 4, 6, 8 kV, and the negative ion beam was accelerated to -4, -6, -8 kV. The irradiations ware carried out under dose of $1\text{x}10^{13}$ - $1\text{x}10^{15}$ ions/$cm^2$ assumed as a single charge. Contact angle of pure water on the substrates were measured by sessile drop method before and after remove of deposited IL layer.

Surface liquid layer on the glass and Si substrate irradiated with positive and negative ion beam was observed. This is probably caused by mass of BMI-$PF_6$ ion which consists of at least 17 cation-anion pairs. Figure 1 shows dose dependences of contact angle of glass substrates irradiated with positive ion beam at acceleration voltage of 6 kV. Increase of the angle was observed for IL-removed, but not for as-irradiated. This means formation of thin IL layer on the surface-modificated glass substrate.

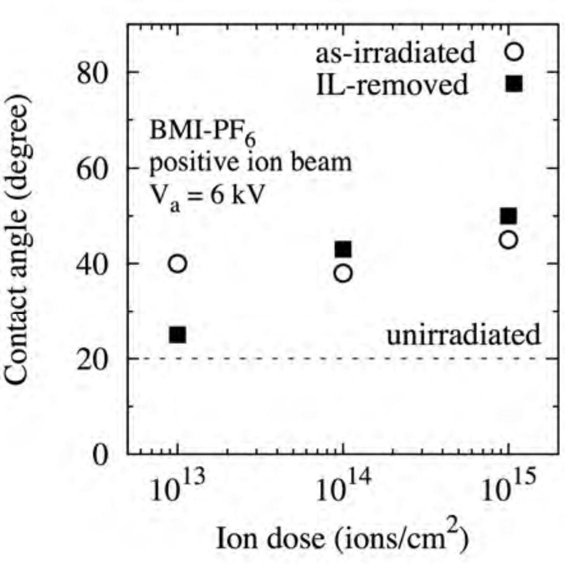

Figure 1. Dose dependences of contact angle of glass substrates irradiated with BMI-$PF_6$ positive ion beam.

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# Ion Induced Patterns on Crystalline Ge Surfaces

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Low energy ion irradiations of surfaces can induce the formation of patterns with periodicities in the range of tens to hundreds of nanometers. These patterns have been used as templates for growing thin films with interesting anisotropic properties resulting from the modulation of their interface and surface [1].

At off-normal angle of incidence between around 55° and 70° and at room temperature ripple patterns oriented perpendicular to the ion beam direction are observed. At normal incidence or for incidence angles smaller than 55° smoothing dominates on elemental materials, like Si and Ge. However, additional surface instabilities can exist due to the presence of a second atomic species on the surface. Furthermore, on crystalline surfaces anisotropic diffusion or kinetic restrictions can also lead to additional instabilities.

We studied ion induced pattern formation on Ge surfaces with 1 keV $Ar^+$ at elevated temperature. In contrast to irradiations at room temperature we found pattern formation even at normal ion incidence. Similar to the case of ion irradiated crystalline metal surfaces a new instability appears at higher temperature due to the Ehrlich-Schwoebel barrier [2]. Depending on the surface orientation checkerboard or isotropic hole patterns with the symmetry of the patterns reflecting the crystal structure of the irradiated surface are observed (see Fig. 1a, b).

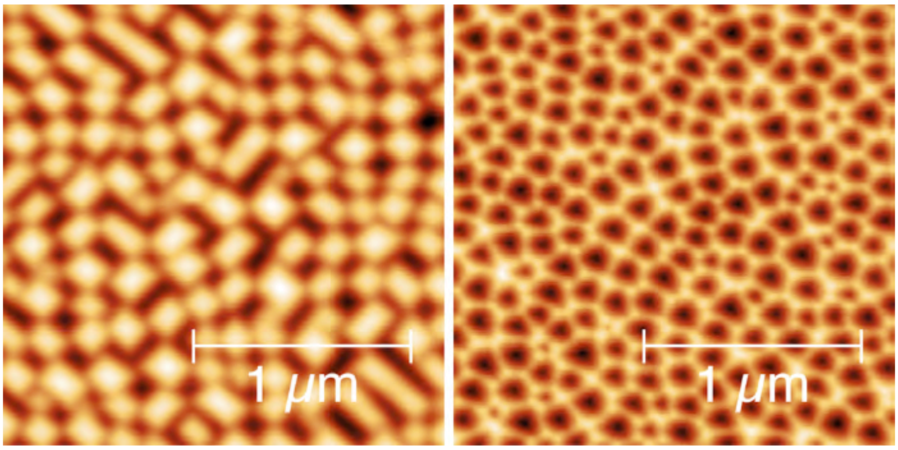

Figure 1. Atomic force microscopy images of ion induced patterns on crystalline (a) Ge (001) and (b) Ge(111) surface.

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Tu-091

# Development of Ionic Liquid Ion Source with Porous Emitter for Surface Modification

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Ionic liquid ion source (ILIS) has attracted attention for a space propulsion, a focused ion beam and a primary ion of secondary ion mass spectroscopy. The ionic liquid(ILs) known as room-temperature molten solt show moderate electrical conductivity (1-100 S/m), high thermal stability (up to ~300 °C) and extremely low vapor pressure (< 1x10-9 Pa). Due to the typical ILs includes halogens in safety, reactive etching and surface modification of semiconductor materials could be expected. Several types of ILIS, such as an externally wetted needle made of tungsten and a capillary, have been reported. We developed an ILIS with emitter of porous medium[1] known as a high current and stable method in the field of liquid metal ion sources. In this study, ion beam properties and mass spectra of positive and negative ionic liquid ion beams extracted from the porous emitter were evaluated.

1-butyl-3-methylimidazolium hexafluorophosphate(BMI-PF$_6$) and 1-ethyl-3-methylimidazo- lium tetrafluoroborate(EMI-BF$_4$) were used for the source liquid. The ion beams were extracted by field-emission from a carbon needle with the porous carbon felt connected to a IL reservoir. Mass spectra of positive and negative ion beam of BMI-PF$_6$ and EMI-BF$_4$ with 4-8 kV of acceleration voltages were evaluated by means of time of flight method. Extraction current of the ILIS with porous carbon felt were measured with respect to beam stubility.

Figure 1 shows a mass spectrum of positive or negative ion beam of BMI-PF$_6$. The modes of the mass spectra were about 5-10x10$^3$ mass/charge. With regard to molecular masses of 139 for cation and 145 for anion, the mass/charge of the modes corresponds to cluster ion with 17-34 cation-anion pairs.

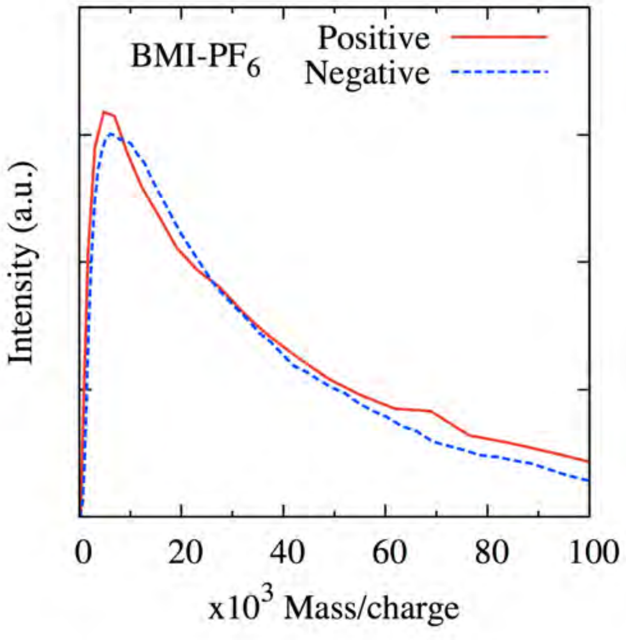

Figure 1. Mass spectra for positive or negative ion beam of BMI-PF6.

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# Measurements of $^4$He Elastic Scattering Cross Sections from Nitrogen for TOF-ERDA Using He beam

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A Time-of-flight Elastic Recoil Detection Analysis (TOF-ERDA) is one of the promising methods for the simultaneous measurements of multi light elements with good depth resolution [1,2]. We are developing a TOF-ERDA measurement system using He beams for the elemental analysis and depth profiling of light elements [3]. For quantitative measurements of elemental concentrations by the TOF-ERDA, reliable data of recoil cross sections are needed. For the TOF-ERDA using He beams of above about 2 MeV, the recoil cross sections are known to be non-Rutherford. In such case, experimental data for the recoil cross sections are necessary. Therefore, we plan to measure recoil cross sections for light elements such as Li, B, C, N, O bombarded by $^4$He ions. This paper presents measurements of recoil cross sections for nitrogen bombarded by $^4$He ions.

The experiments were performed using the 2MV tandem Pelletron accelerator at the Quantum Science and Engineering Center, Kyoto University. $^4$He ions with an energy range between 2 MeV and 5.5 MeV were utilized for the incident beam, and a silicon-nitride membrane of 50 nm thickness with a coated thin Au layer was used as a target. Scattered $^4$He ions were detected with silicon detectors at scattering angles of 83.6° and 165°. The scattering angle of 83.6° corresponds to the recoil angle of 40°, and recoil cross sections at 40° were evaluated from scattering cross sections at 83.6° using the kinematical calculation. We also measured the scattering cross sections at 165° for the backscattering experiments of nitrogen. This paper will present results of cross section measurements as well as details of the experimental setup. Comparison between the present data and calculations will also be indicated.

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Tu-093

# Structural characterization of planar set of buried Au nanoparticles

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In order to build nonvolatile memory devices with smaller size, faster operating speed, and larger storage capacity, the investigation of a floating gate transistor with discrete charge traps (nanocrystals (NCs)) has attracted great interest. In this case, the charge is trapped at discrete sites, and it is more stable than in a conventional conductive floating gate as the latter can lose trapped charge through a single leakage path in the gate oxide. Thus, NCs floating gate memory is expected to have a longer retention time than the conventional devices. One way to synthesize a sandwich structure with a 2-dimensional set of NCs between two dielectrics is by physical deposition of an ultrathin metal (such as less than 1 nm of Au, Ag, Ni, Pt and Co) [1]. The device efficiency depends, among other factors, on electric isolation of the NCs for the charge retention. Therefore, the understanding of the relationship between the amount of metal, which nucleates as NCs, and amount of metal retained in the dielectric around the particles, which can decrease the charge retention of the NCs, is of major importance. In this work we investigate a planar set of Au NCs buried ~30 nm into a $SiO_2$ matrix, synthesized by sputtering deposition of $1.8\times10^{15}$, $3.1\times10^{15}$ and $7.4\times10^{15}$ Au/cm$^2$, over a silica thin film over a Si (001) substrate and followed by a deposition of another $SiO_2$ thin film. The size distribution and areal number density of the NCs for each case were well characterized through transmission electron microscopy (TEM) and grazing incidence small angle X-ray scattering (GISAXS). The amount of Au not nucleated as NCs and the corresponding depth profile distribution around the NCs was measured by medium energy ion scattering (MEIS). The typical mean size, FHWM of the size distribution and areal number density obtained were 3 nm, 20% and $13\times10^{11}$ NCs/cm$^2$, respectively. The amount of non-nucleated Au is about 60-70% for some cases, and the highest concentration of atomic Au around the NCs is about 5 atomic percent. The MEIS data were analyzed through the PowerMeis software [2], where the structural information obtained from TEM and GISAXS was taken into account.

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# Study of optical, structural, chemical and dielectric properties of 145 MeV $Ne^{6+}$ ions irradiated PTFE polymer

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## Abstract

The bombardment of the polymeric materials with Swift Heavy Ions (SHI) results in the change of their significant optical, structural, chemical and electrical properties in the form of rearrangement of bonding, cross-linking, chain scission, formation of carbon rich clusters and changes in dielectric properties etc. Modification depends on the ion beam parameters (ion, energy and fluence) and the polymeric material itself. In the present work characterization of the optical, chemical, structural electrical modifications in PTFE induced by 145 MeV $Ne^{6+}$ ions were carried out through UV-Visible spectroscopy, Fourier Transform Infra Red spectroscopy (FTIR), X-Ray Diffraction (XRD) and LCR meter. 100 μm thick PTFE polymer procured from Good fellow, Cambridge Ltd. England (UK), were irradiated by 145 MeV $Ne^{6+}$ ions to various fluences at Variable Energy Cyclotron Centre (VECC), Kolkata, India.

From UV-Vis spectra the optical band gap ($E_g$), calculated from the absorption edge of the UV spectra of the films in 200-800 nm region varied from 2.23 eV to 1.63 eV for pristine and irradiated samples. At the highest fluence of $10^{13}$ ions/cm$^2$ the maximum change in optical band gap ~26% has been observed. The cluster size changes from 236 to 443 carbon atoms per cluster. Carbon enriched domains created in the polymer during irradiation may be responsible for the decrease in the band gap. In FTIR spectra, appreciable changes have been observed after irradiation, indicating molecular fragmentation, cross-linking, formation of unsaturated group and free radicals. X-Ray Diffraction (XRD) analyses show significant change in crystallinity with fluence. Dielectric constant (ε') decreases with frequency whereas it increases with the ion fluence. Variation of loss factor (tanδ) with frequency reveals that tan δ increases as the frequency increases. Tanδ also increases with fluence. Tan δ has positive values indicating the dominance of inductive behavior. A sharp increase in A. C. conductivity in pristine as well as in irradiated samples is observed with frequency. Due to irradiation the increase in conductivity with fluence at a given frequency may be attributed to scissoring of polymer chains, resulting in an increase of free radicals, unsaturation, etc.

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# Ion-induced Modification of Glassy Carbon Structure and Morphology

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The ion-induced modification of high-temperature glassy-carbon SU-2500 under 5-30 keV $Ar^+$ ion irradiation at high fluences ($10^{18}$-$10^{19}$ ion/cm$^2$) has been studied from room temperature (RT) to ~ 400 °C. The structure changes of glassy carbon surface layer has been carried out using *in situ* analysis of the temperature dependences of ion-induced electron emission yield $\gamma(T)$ and reflection high energy electron diffraction (RHEED) [1]. The morphology changes have been studied by scanning electron microscopy (SEM). The temperature dependences $\gamma(T)$ show a transition from a step-like behaviour with a jump at damage annealing temperature $T_a$ ~ 130°C for 30 keV ion energy to the temperature independent curves as ion energy decreases. The reason of such transformation is the decrease of disordering of a fullerene-related structure of high-temperature glassy carbons with decreasing of ion energy as a consequence of decreasing level of radiation damage $\nu$ (*dpa*). The calculations of the dependence of the amorphous fraction on $\nu$ using an error function have made it possible to find the threshold values $\nu_{am}$ when the structure of glassy carbon is virtually not disordered under ion irradiation at RT. The threshold of $\nu_{am} \approx 60$ *dpa*. At elevated temperatures ($T > T_a$) and ion energy > 15 keV the graphitization of SU-2500 surface layer takes place as the RHEED shows. SEM analysis shows that the structure changes lead to difference of ion-induced morphology. After irradiation at RT the SEM micrographs show the etch pits with pentagon and hexagon forms, Fig.1a. The elementary ordering of carbon lattice at $T > T_a$ results to the shallow-cellular pattern, Fig. 1b. At more higher temperatures SU-2500 graphitization leads to the morphology similar to irradiated polycrystalline graphite [2], Fig.1c.

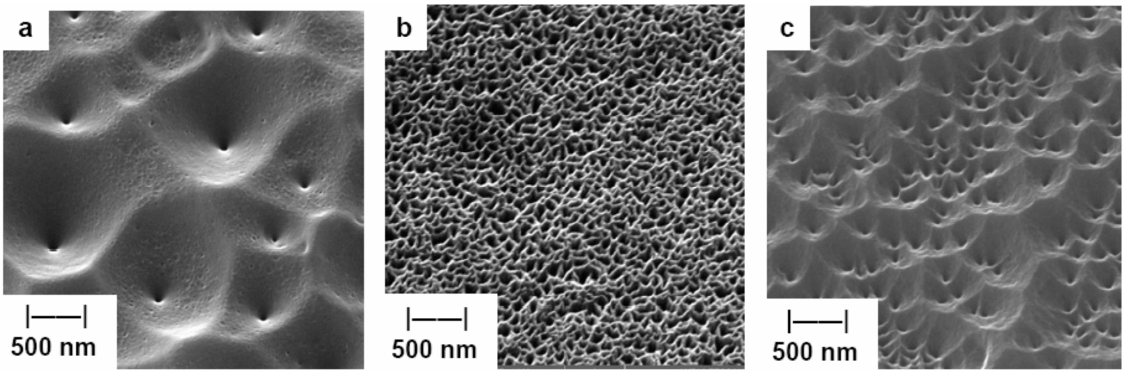

Fig.1. SEM micrographs (tilt 30°) of glassy carbon SU-2500 surface after 30 keV $Ar^+$ ion irradiation (normal incidence) at room temperature (a), 250 (b) and 400 °C (c).

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Tu-096

# Development of novel compact spin-polarized electron gun

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We have already developed a novel high brightness and high spin-polarized low energy electron microscope (SPLEEM) and applied it to clarify the magnetic property of [CoNix]y/W(110) and Au/CoNi2/W(110) during growth of ultra thin films[1-3]. Such thin film multi-layers are important for current driven domain wall motion devices [4]. Our developed SPLEEM can make us the dynamic observation of the magnetic domain images possible. However the size of the spin-polarized electron gun is large and we have started to develop a new compact spin-polarized electron gun with new idea. It is necessary two devices to operate 3 dimensional spin direction. One is a spin manipulator which changes the out of plain spin direction and another one is a spin rotator which can change the in plain spin direction. We have proposed a multi-pole Wien filter which can make 3 dimensional spin operation with one device possible. Fig.1 shows a drawing of the developing 3D multi-pole spin manipulator which has 8 poles.

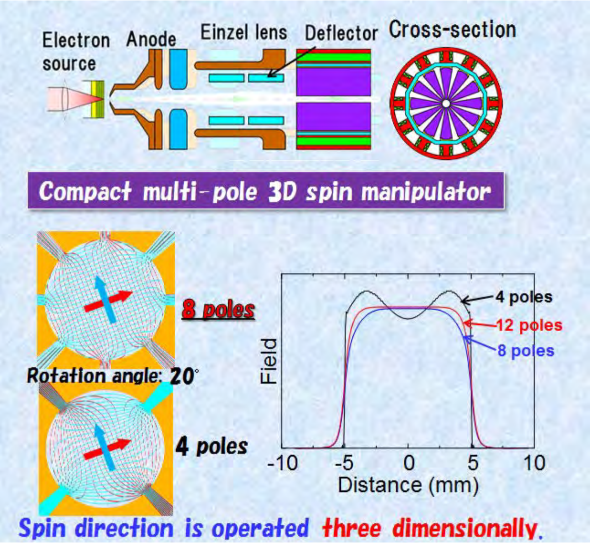

Fig. 1:  3D eight-pole spin manipulator and uniformity of magnetic and electric field

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# Harvesting and Storing Laser Irradiation Energy with Graphene-Cu Compound Structure

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Graphene-metal compound structure has been reported as a novel and outstanding component used in electrical and optical devices. We report on a first-principles study of graphene-cu compound structure, showing its capacity of converting laser energy into electrical power and storing the harvested energy for a long time. A real-time and real-space time-dependent density functional method (TDDFT) is applied for the simulation of electrons dynamics and energy absorption. The laser-induced charge transfer from copper layer to graphene layer is observed and represented by plane-averaged electron difference and dipoles. The effects of laser frequency on the excitation energy and charge transfer are studied as well. The enhancement of C-C σ-bond and decreasing of electron density corresponding to π-bond within graphene layer indicate the way in which the transferred-charges are stored. In addition, the shift and oscillations of dipole along z-direction after the application of laser pulse offer a concept that the compound structure has the ability of storing the harvested energy for a long time.

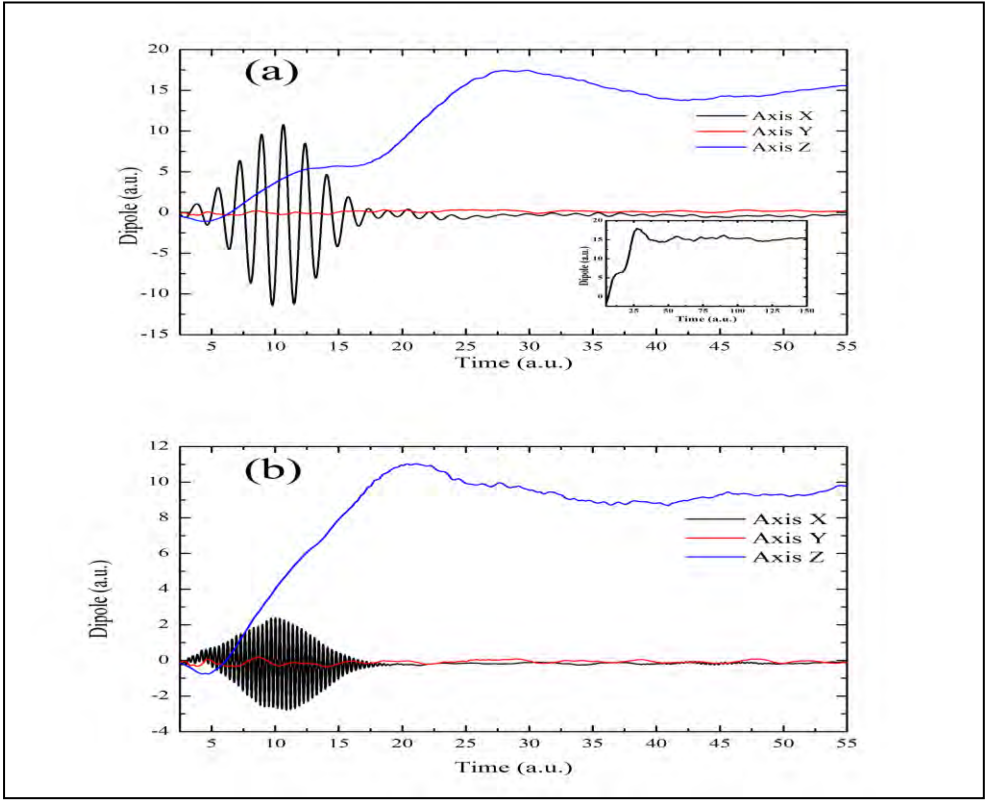

Figure 1. Dipoles along the 3 axes as a function of time under the irradiation of laser pulse with energy of (a) 100 eV and (b) 500 eV. The insert in (a) shows the changes of dipole along z axis for a relatively long time up to 150 a.u. (about 3.7 fs).

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# Magnetic Effects Following Proton Irradiation in Diamond

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Following recent experiments involving proton induced magnetization in graphite [1,2], we demonstrate related experiments in diamond. A proton micro-beam of 2.2 MeV energy generated using a nuclear microprobe is used to create microscale magnetic domains in ultra pure single crystal synthetic diamond. Characterization of the magnetized domains is achieved using Atomic/Magnetic Force microscopy analysis (AFM/MFM) and Raman Spectroscopy. Preliminary measurements using the Superconducting Quantum Interference Device (SQUID) are also presented. Sources of possible AFM/MFM induced artifacts are considered and discussed in detail.

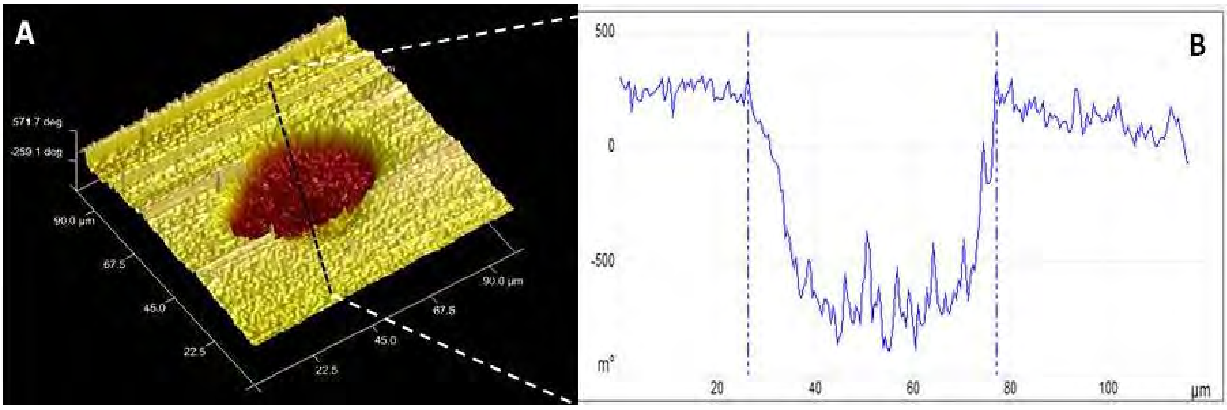

Figure 1. Example of a MFM phase image (A) showing a proton induced magnetic microscale domain together with a line profile across the microscale domain (B) in Diamond.

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# Photoluminescence and Thermoluminescence study of $K_2Ca_2(SO_4)_3$: Cu nanophosphor for gamma ray dosimetry

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Nanocrytstalline $K_2Ca_2(SO_4)_3$:Cu was synthesized by chemical co-precipitation method and annealed at 700 °C. XRD spectra shows the orthorhombic structure and the crystallite size ~ 20 nm. The same was also confirmed with TEM and shows nanorods of $K_2Ca_2(SO_4)_3$:Cu having diameter 20nm and length 200nm. These nanocrytstalline samples were irradiated with gamma radiation for the dose varying from 1Gy to 20kGy and their thermoluminescence (TL) and photoluminescence (PL) characteristics have been studied. In PL spectra, the emission bands are observed at 403 and 419 nm respectively and their respective intensity increases linearly with the increase in the gamma dose. The glow curve of the nanocrystalline material shows a major peak at around $163^0$C and one small peak at 290 $^0$C. Moreover, one peak at higher temperature around $365^0$C has been observed after the gamma dose of 100Gy. The TL response shows a linear behavior up to 1kGy and further saturates with increase in the gamma dose .This saturation occurs may be due to the generation of new peak. Moreover, a significant shift in the peak towards lower temperature has been observed. This indicates the disorganization of the initial energy bands in the $K_2Ca_2(SO_4)_3$:Cu nanophosphor.Computerized Glow Curve Deconvolution (CGCD) program was used for the analysis of TL glow curves. Trapping parameters for all the TL glow curves of $K_2Ca_2(SO_4)_3$:Cu nanophosphor from 0.1Gy to 20kGy have been calculated and correlated with the gamma dose. The property of linearity, simple glow curve and negligible fading makes the nanocrystalline phosphor useful for the estimation of high doses of gamma rays.

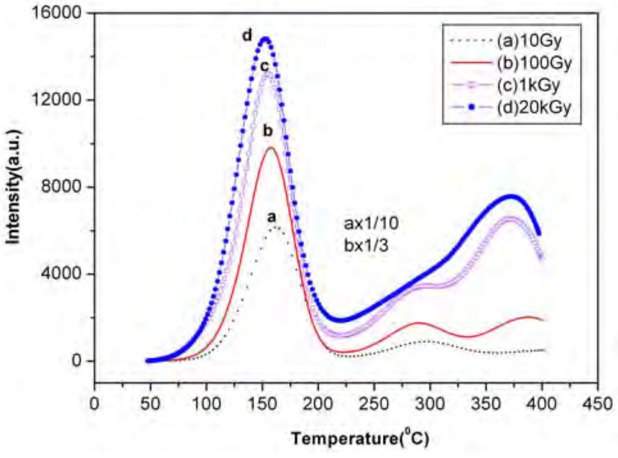

Figure 1. TL Glow curves of nanocrytstalline $K_2Ca_2(SO_4)_3$:Cu irradiated with different gamma doses.

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# Effects of Electron Beam Irradiation on Micro-porous Materials

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Zeolite is an aluminosilicate micro-porous material with periodically arranged nano-space in the structure. The general chemical formula of zeolite is $M_xSi_{n-x}Al_xO_{2n}\cdot mH_2O$, where the framework is composed of covalently bonded Si, Al and O atoms, M may be monovalent cations, usually alkali metals, and water molecules exist in the space as zeolitic water. It is well-known that zeolite has been widely used as industrial applications such as catalysts, ion-exchangers, and separation membranes. There have been more than 200 framework types registered in the Database of Zeolite Structures [1], and also many efforts devoted to synthesize new type of zeolite frameworks, especially with larger and three-dimensionally connected micro-pores. Thus, it is of particular importance to characterize their structures, and transmission electron microscopy (TEM) is one of the essential methods to clarify their framework structures (Figure 1). There is, however, always difficulty in their structural characterization since electron beam irradiation easily vitrifies their structures, which is caused by electron beam damage [2]. There are two kinds of damage processes have been reported, that is, radiolytic and knock-on [3]. Here, I have investigated effects of electron beam irradiation on micro-porous materials, and their damage processes under the electron beam accelerated by 300 kV. Dependence of (i) Si/Al ratio of their frameworks and (ii) electron beam irradiance level will be discussed, and other micro-porous materials such as aluminophosphate will also be investigated.

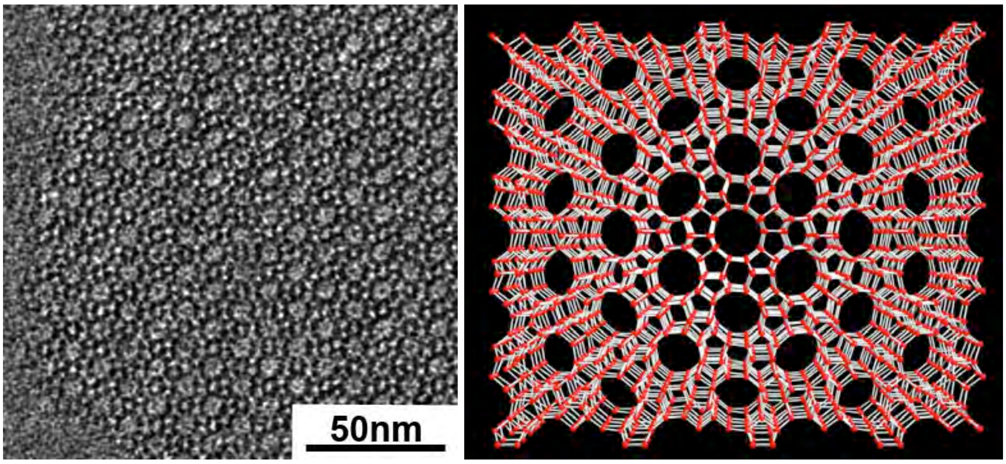

Figure 1. High resolution TEM image of zeolite MFI (left) and the framework structure (right).

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# γ-radiations effect on the electrical and structural properties of low dimensional Resonant tunneling diodes

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The total dose effect of γ-radiation effect on the electrical and structural properties of single barrier low dimensional resonant tunneling diodes (RTDs) have been studied. The morphology of the diodes was characterized by scanning electron microscope (SEM). The I-V characteristics of RTDs have been measured at room temperature by leaving the hetrostructures embedded in the insulating template membrane. The γ-radiation causes significant change in the electrical properties of the RTDs. The peak to valley ratio dropes by a factor 3.8 as compared to pre-irradiated samples. The magnitude of this effect is proportional to gamma dose. The X-ray diffraction study also shows the pronounced changes in the structural properties of the post –irradiation low dimensional RTDs.

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