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Head: Prof. Dr. Heinz-Eberhard Mahnke

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HMI-Structural Research

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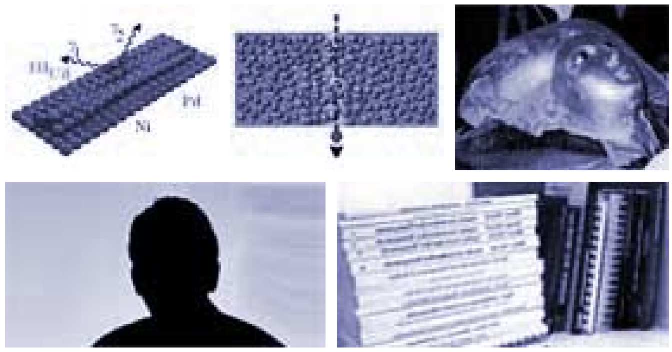

Diffusion, relaxation and phase transitions in condensed matter are due to the dynamics of individual atoms or their collective motion. The department "Structure & Dynamics" investigates these phenomena in the undisturbed solid state and as a consequence of the interaction with charged particles.

The temporary or stable local structures resulting from ion-impact are studied under scientific aspects and in addition are used for industrial applications. Furthermore the high-energy ions are applies for solid state analytics. Neutrons from BER II and photons from BESSY II are used as complementary probes. Untill dec. 2006 ions from the ion beam laboratory (ISL Berlin) were used also.

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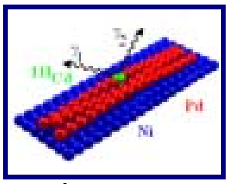

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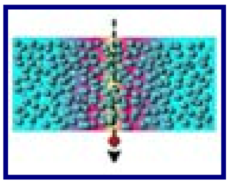

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- High-Energy Ion-Solid Interation
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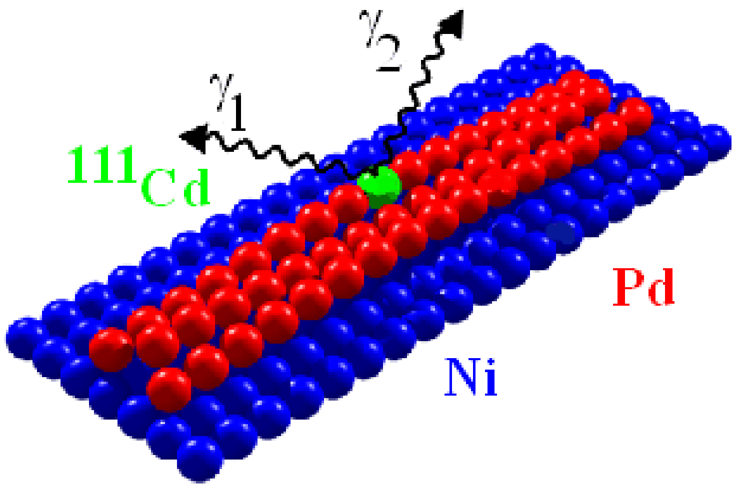
Structural Research Structure & Dynamics SF8

Interface Magnetism

In magnetic multilayer systems magnetic properties may vary from atomic layer to atomic layer. These variations are hardly accessible to most conventional techniques. Using radioactive probe atoms it is possible to trace the magnetic properties differentially through ferromagnetic layers and layers with induced magnetic properties by the measurement of hyperfine interactions at the probe nuclei. Such monolayer-resolved studies include the measurements of magnetic hyperfine fields at ferromagnetic surfaces, in magnetic-nonmagnetic dilayers, in trilayers etc.

The experiments are performed at the mass separator ISOLDE / CERN in Geneva, using the UHV-Chamber ASPIC (Apparatus for Surface Physics and Interfaces at CERN).



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Interface Magnetism - The physics in short

Our purpose

is the investigation of magnetic and electric properties (the magnetic hyperfine field and the electrical field gradient) of radioactive isotopes

(^{111m}Cd / ^{111}Cd, ^{111}In / ^{111}Cd, ^{77}Br / ^{77}Se, ^{100}Pd / ^{100}Rh ...)

located

- as adatom on the surface or
- in the topmost or deeper layer or
- at the interface of a binary layer system

transition-element systems

(Ni(001), Ni(111), Pd(001), Pd(111), Co(0001), Fe(001)...).

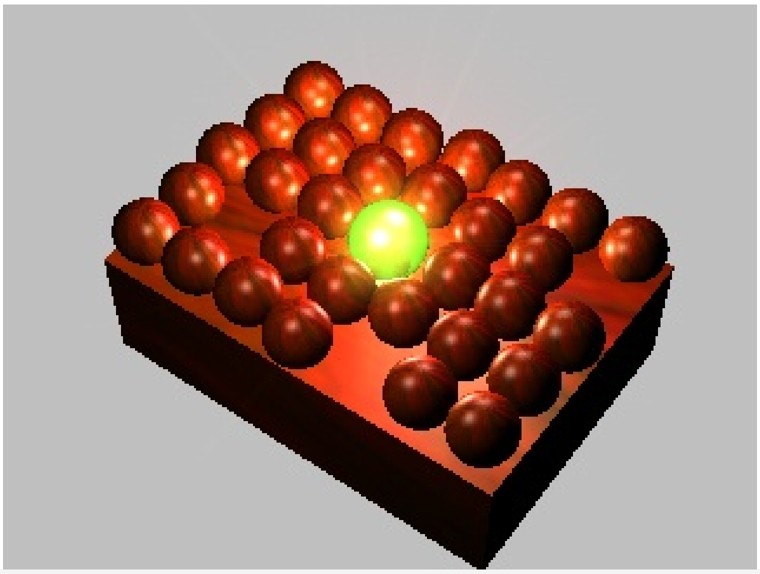

Fig. 1: The probe ^{111m}Cd atom (green) embedded in the topmost layer of Ni(001)

The Perturbed Angular Correlation Method: PAC

Applying the PAC method we observe the interaction between the electrical quadrupole moment of the radioactive probe nucleus and the electrical field gradient created in the very immediate vicinity of the nucleus by the surrounding electrons.

We also observe the interaction between the magnetic dipole moment of the radioactive probe nucleus and the magnetic hyperfine field created by polarized s-electrons at the nucleus.

These interactions perturbe the angular correlation between two successively emitted gamma rays of the probe nucleus. Only special nuclei posses a suitable gamma cascade with an intermediate isomeric state.

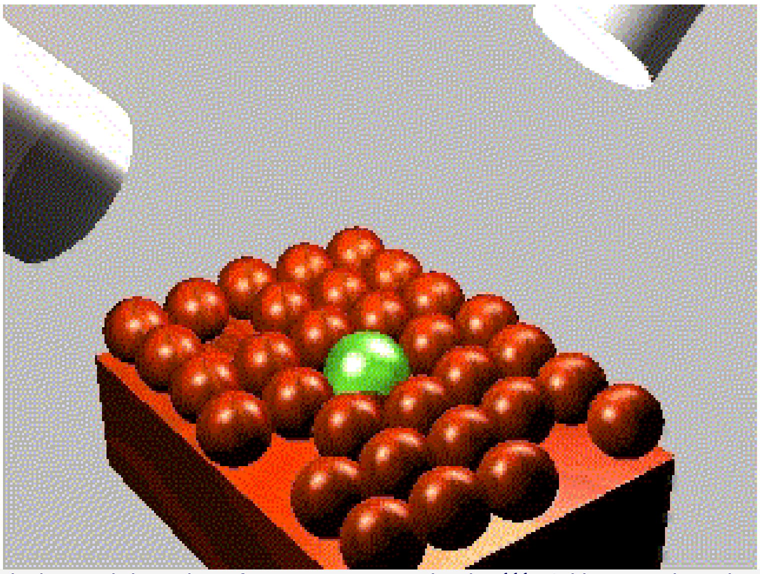

Fig. 2: Emission and detection of two gamma rays by the ^{111m}Cd isotope decaying to ^{111}Cd;
the perturbed angular correlation is measured by counting the number of gamma rays detected at two fixed angles of 90° and 180°

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Interface Magnetismn - Experimental Methods

Sample Preparation

our chamber

cleaning the samples

ultrathin metal films

Radioactive Probes

mass-separator ISOLDE
(Ion Separator Online Danish Engineering)

collection and probe transfer

PAC Spectroscopy

experimental setup

electronics

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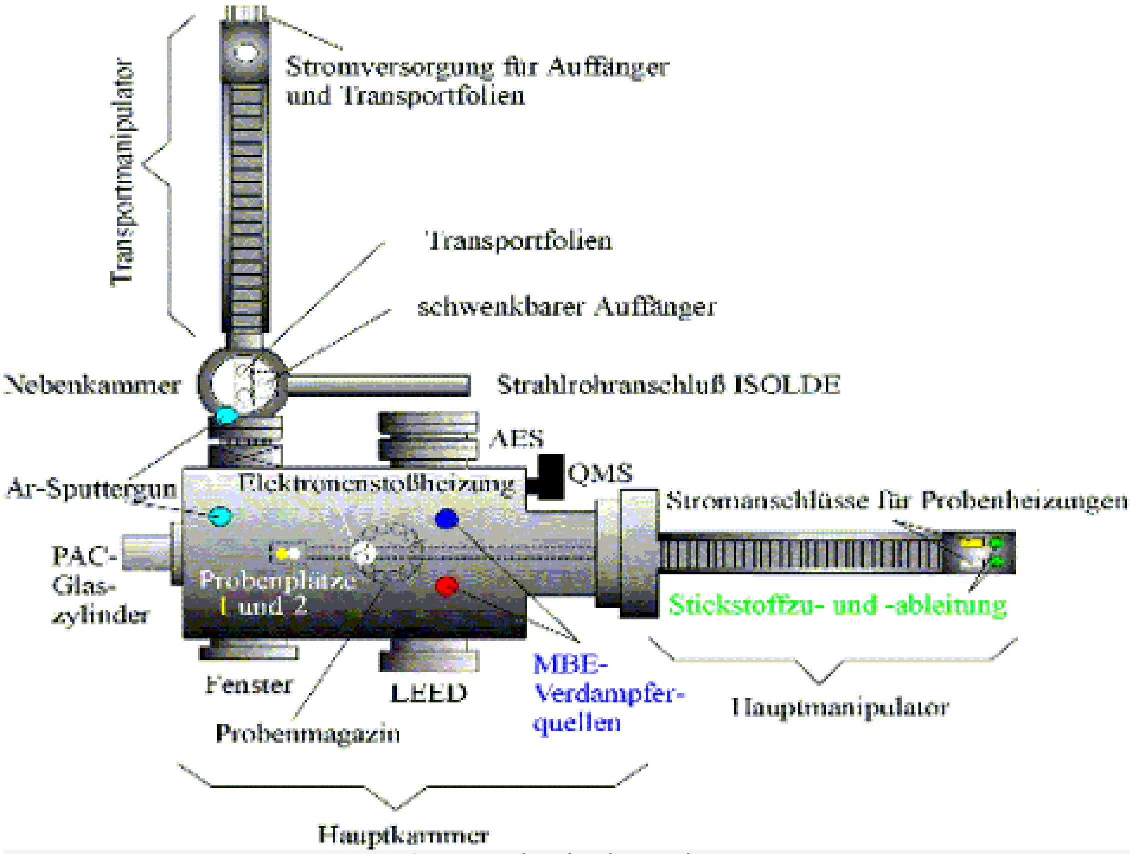
Interface Magnetismn - Experimental Methods

Our chamber



Our UHV-chamber in top-view;
the vacuum we reach is about 10^{-10} mbar

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Ion Impact

The impact of swift and slow ions can result in local structures, either short-lived or with long-term stability. The research focuses on the understanding of the ion-solid interaction. For swift ions, the deposition of the high electronic energy density and the follow-up processes leads to materials modification on a micro- and nanometer scale. For slow ions, the energy transfer from the high potential energy of highly-charged ions to near-surface electrons and atoms induces the modifications.

High-Energy Ion-Solid Interaction

Ion-Surface Interactions

Team

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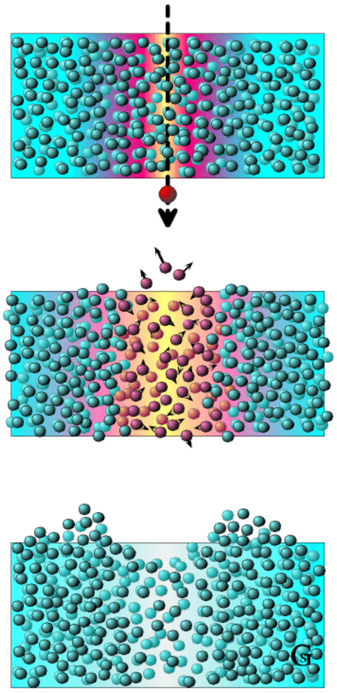
High-Energy Ion-Solid Interaction - Fast Ion-Matter Interactions

Studies at the ISL Cyclotron (the ISL operation ended Dec. 2006)



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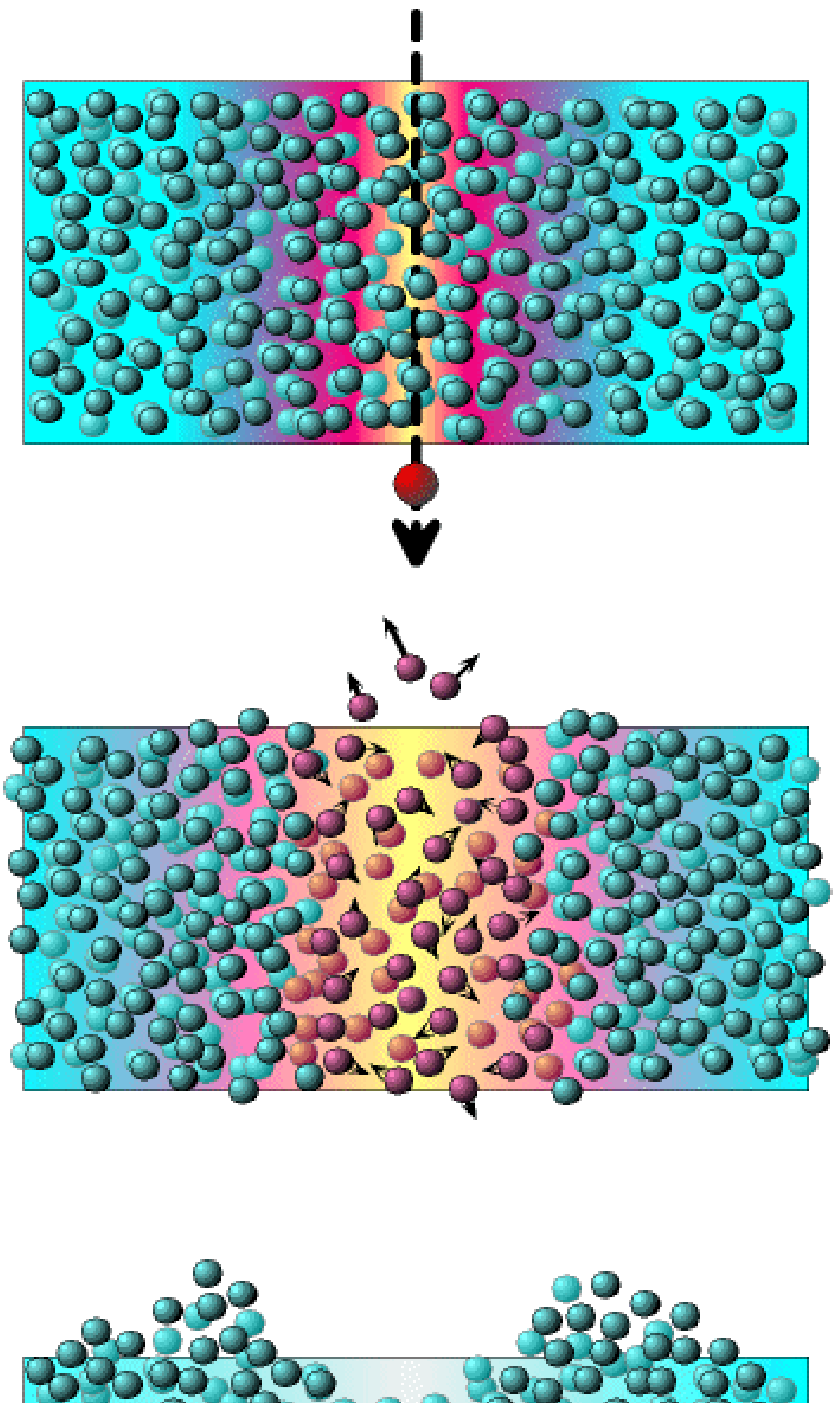
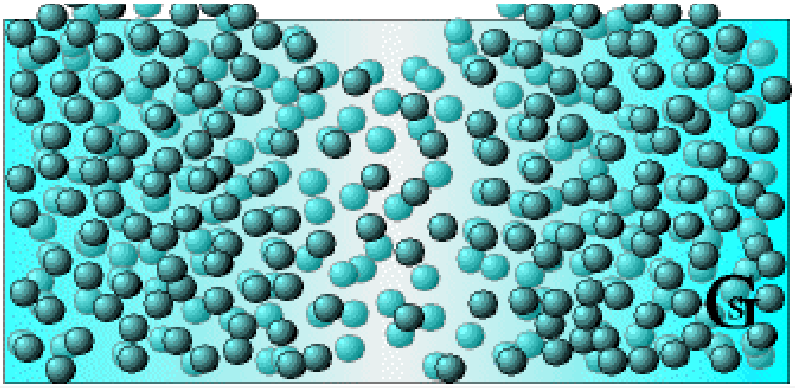
Structural Research Structure & Dynamics SF8

Ion-Surface Interaction - Matter Close to the Limit of Stability

Fast charged atomic particles (heavy ions) lead to extremely strong electronic excitations inside a narrow cylinder around each ion path. This causes a subsequent modification of the solid-state structure on a nano-meter scale (a millionth of a mm). Already nowadays these modifications, the so-called ion tracks, are used in different technical applications. Novel developments in nano-structuring of materials and medical applications, however, call for a sound knowledge on the *ultra-fast processes* during the evolution of ion tracks. An improved understanding will greatly simplify the treatment and selection of proper materials.





Time evolution of an ion track.
The initial excitation and ionization of atoms induces atomic motions, which freeze out and may lead to permanent modifications. As an example, this may lead to craters on an atomic scale.

The aim of this project is to uncover the nearly unknown track-formation mechanisms. Specifically designed experiments are performed and planned to unveil the mechanisms that couple the electronic excitations with atomic motions. Some of the experimental methods are world-wide unique and other techniques have not yet been applied to the investigation of *highly excited matter*.

These investigations of matter close to the limit of stability will yield information on the rapid transformation of a charged atom column into hot plasma inside the ion track, followed by *phase transitions on a nano-meter scale*. Thus, this project will be of significance for other fields such as

- *Radiation chemistry* and *biology*
- *Radiation dosimetry*
- *Tumor therapy* with high-energy ions.

Further information on short-time dynamics.

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Ion-Surface Interaction - Research Strategy

A consistent picture of the electronic and atomic processes induced by the passage of swift heavy ions in the bulk and at the surface of materials shall be developed. *Snapshots of the time evolution* of particle tracks will evolve within this project. This allows for qualitative and quantitative statements on the dominant *energy-conversion mechanisms* in matter. The excited electron system and the resulting atomic motions and rearrangements are monitored using complementary methods, such as

a) Spectroscopy of ejected Auger electrons and desorbed atoms to determine the short-time dynamics on a time scale of a *millionth of a billionth* of a second (10^{-15} s) and above.

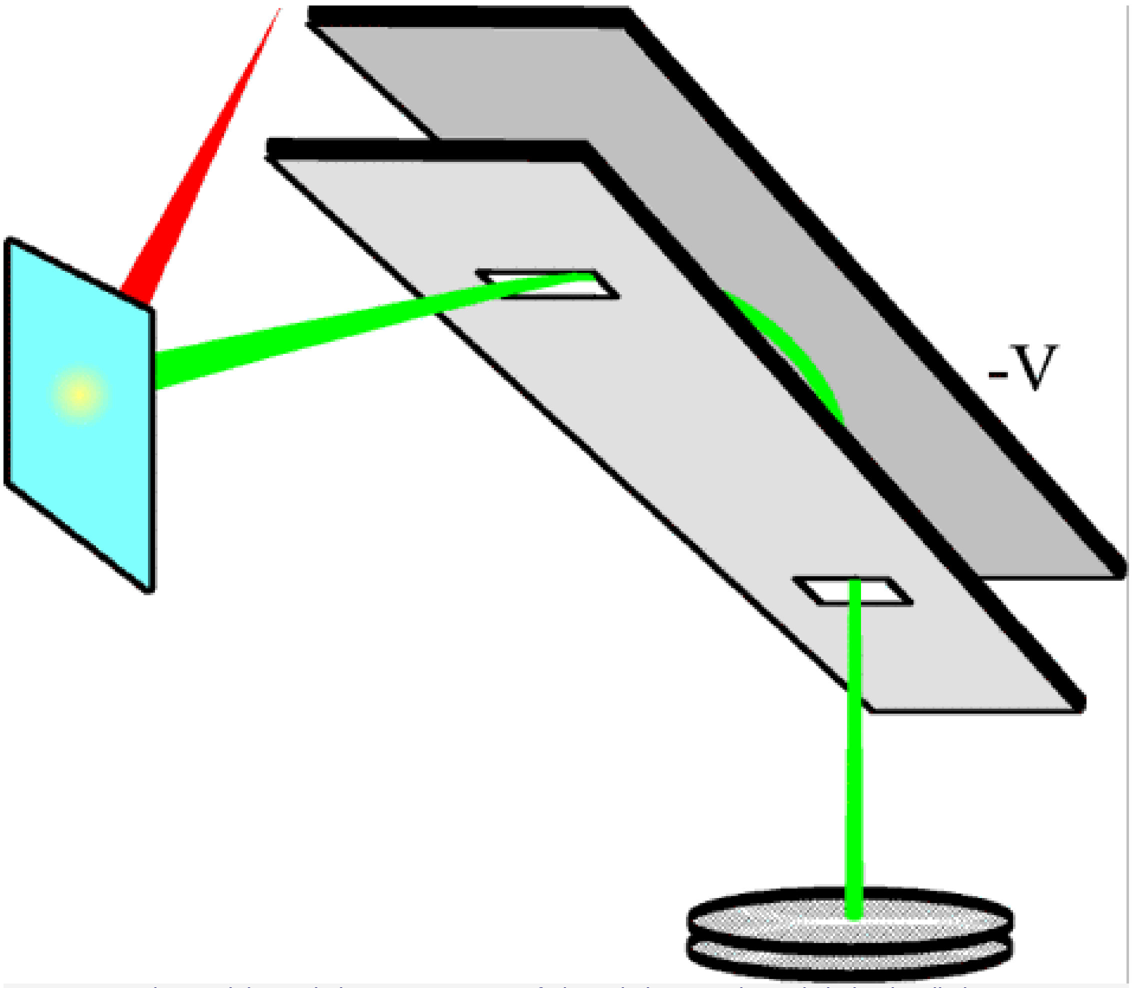

Fig. 1: High-resolution spectroscopy of ejected electrons (green) during irradiation of the sample (blue) with fast heavy ions (red)

b) On-line and off-line x-ray diffraction at HMI and BESSY II to investigate electronically induced phase transitions inside the bulk.

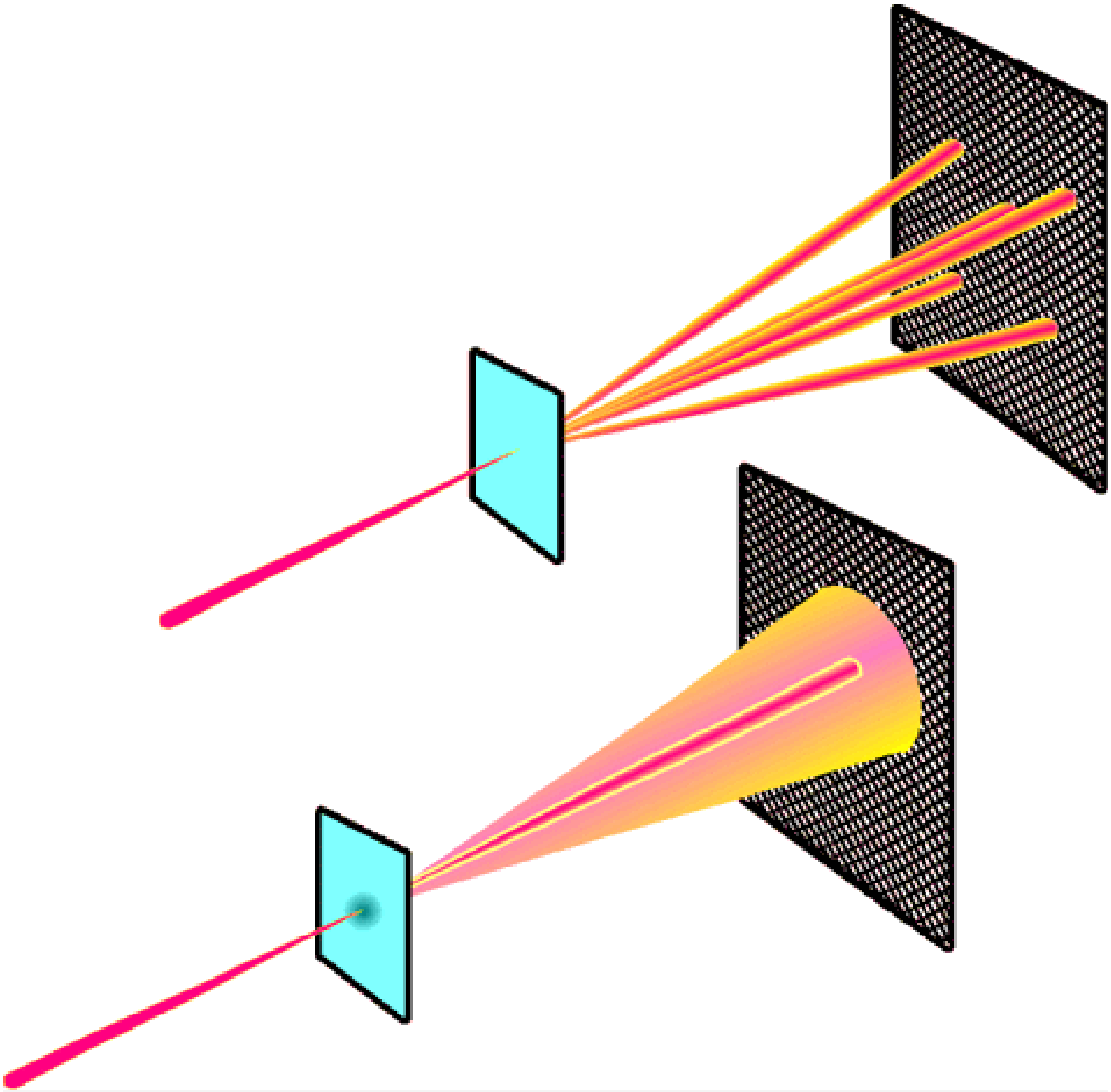

Fig. 2: X-ray analysis of a sample (blue area);
before (upper plot) and after the irradiation (lower plot) with fast heavy ions

c) Atomic-probe microscopy to investigate the specific structural modifications at the surface.

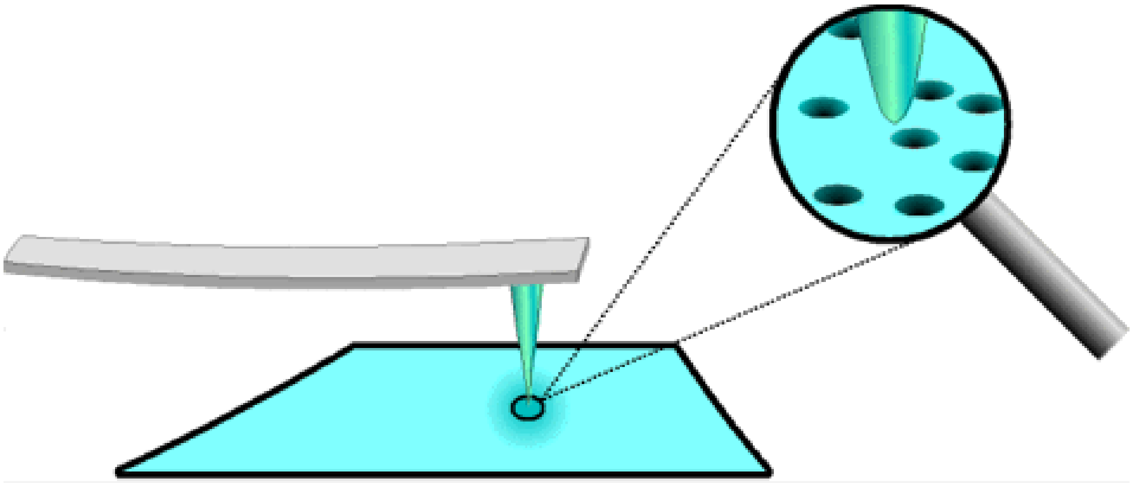

Fig. 3: Atomic-probe microscopy of an irradiated sample (dark blue area) with crater structures

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High-Energy Ion-Solid Interaction - Perspectives of Applications: Nano-Structures

Ion-track applications involve long-time detection of extra-terrestrial radiation and environmental investigations. Furthermore, etched ion tracks in micrometer-thick polymer films find use as membranes in the medical and biological field, and as particle filters in the electronic and automotive industry. The know-how gained in this project can directly be transferred to applications.

Novel applications are explored utilising the nanometer-sized feature of the tracks for electronic devices in organic and inorganic materials. Examples are nano-structured semi-conducting films for *pressure sensors* and *flexible electronics* and *electron field-emission* from irradiated amorphous carbon films for future displays. Collaborations with industrial partners provide additional important stimuli for basic research on ion tracks.

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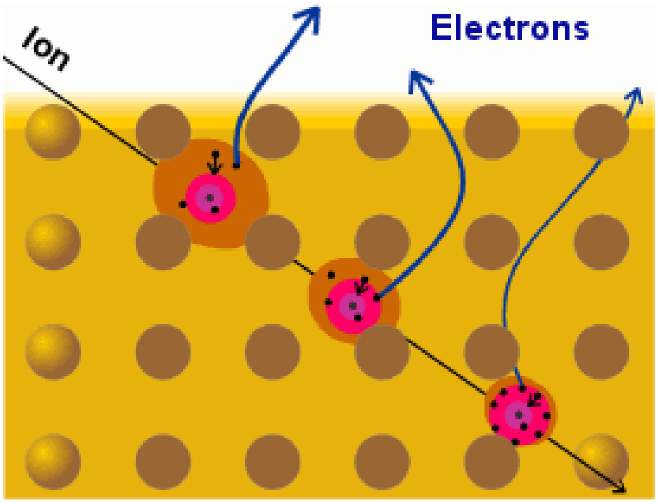
Ion-Surface Interaction - Highly Charged Ions Interacting with Surfaces

Studies at the ECR-Facility of ISL (the ISL operation ended Dec. 2006)



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Ion-Surface Interaction - Overview

The outstanding property of a multiply charged ion is its high potential energy. The removal of electrons from an atomic system requires energy, which remains as potential energy with the ion. For instance, for the production of an Ar^{18+} ions one needs about 10 keV. Note that the potential energy contained in a quantity of Ar^{18+} weighting one gram would be sufficient to provide electricity for a house for one year. Thus, a highly charged ion acts as a carrier of energy that can readily be transported and deposited at a specific location. In this work the injection of high energy spikes at the surface are of particular interest. The aim of the studies with slow and highly charged ions is the basic research on novel phenomena of condensed matter physics and possible application emerging from specific surface modifications associated with the high potential energy of hollow atoms.

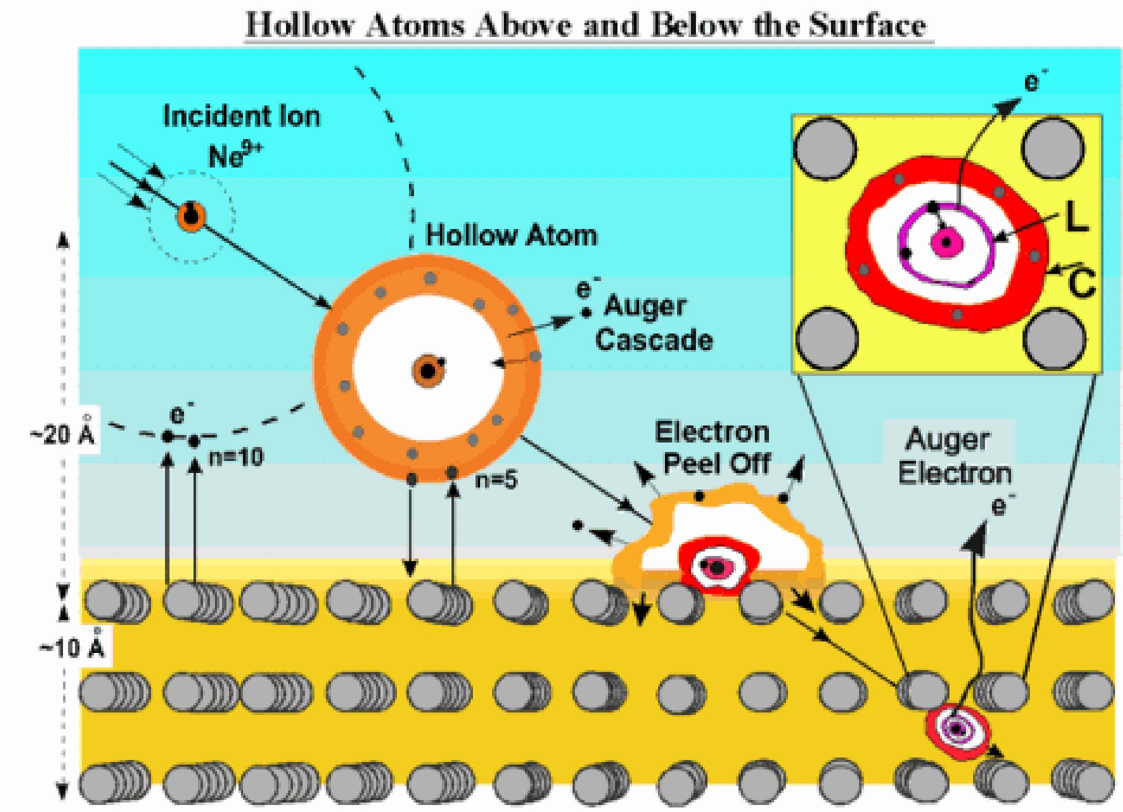

Fig. 1: Formation of hollow atoms at a surface

Fig. 1 provides an overview over the scenario of the mechanisms associated with slow highly charged ions interacting with surfaces. When such an ion approaches a surface, several electrons are transferred from the conduction band of the solid into high Rydberg orbitals of the ion. Thus, in front of the surface, a "hollow" atom is produced with many electrons in higher orbitals and empty inter-mediate shells. Hollow atoms undergo dielectronic processes such as autoionization, where the electron-electron interaction leads to the ejection of electrons and a relaxation of the electrons in the Rydberg orbitals. Another important reason for a shrinking of the electronic charge cloud is the flow of the Rydberg electrons back into the solid and the additional capture of electrons into lower orbitals. Hence, the diameter of the hollow atom decreases as it approaches the surface.

When the projectile hits the surface, the remaining Rydberg electrons are removed (peeled off) or enter into the solid together with the ion. Simultaneously, during the passage into the surface, the highly charged ion in-duces a negative charge cloud dynamically screening the nucleus. The appearance of an intense screening cloud, denoted C, is the outstanding property of a slow highly charged ion moving below the surface. The C cloud gives rise to hollow atoms of the second generation whose dimensions are much smaller than those produced outside the solid. Sub-sequently, as the hollow atom travels in the solid, Auger transitions and collisional charge transfer successively fill the inner shell orbitals.

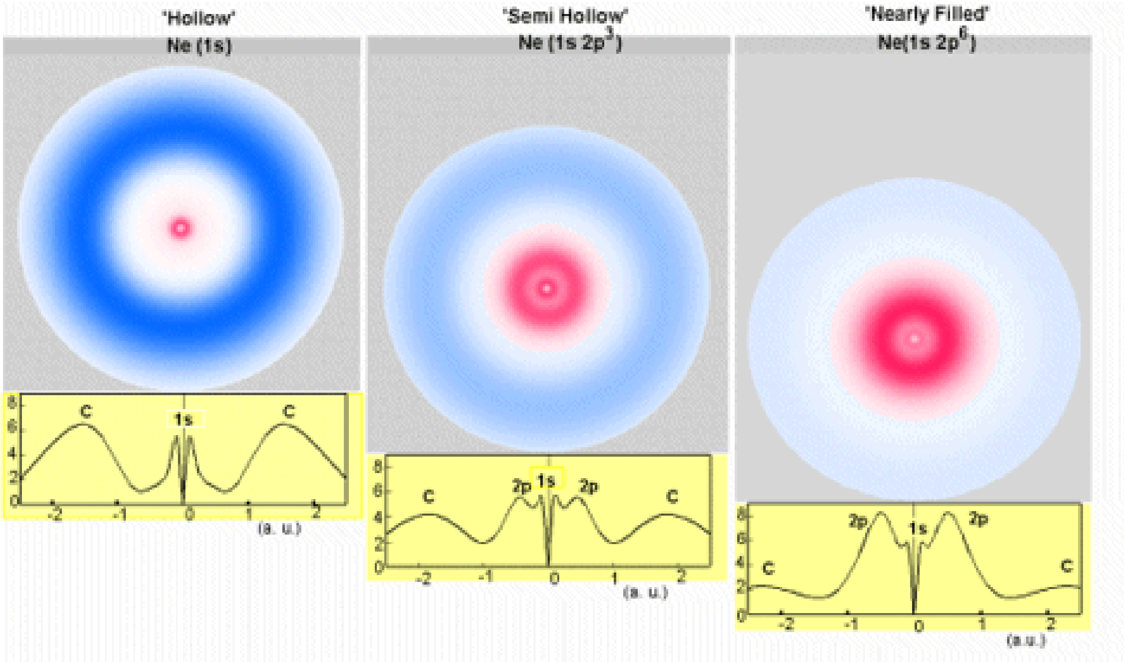

Fig. 2: Hollow atoms calculated using Density Functional Theory (DFT)

The structure of hollow atoms inside the solid can be visualized plotting the density of the induced charge cloud as shown in Fig. 2. The charge cloud was evaluated in a self-consistent manner within the framework of a Density-Functional Theory. The induced electron densities are relatively intense so that non-linear theories are required to describe their formation. Hence, the uses of non-linear (self-consistent field) methods are necessary in the present studies.

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Ion-Surface Interaction - Theoretical Work

Cascade Model for hollow atoms

To achieve a theoretical understanding for the dynamic properties of the hollow atom, a cascade model describing the filling of a hollow atom was developed. The filling sequence of the hollow atom is determined by expressions that are similar to those known from radioactive decay of nuclei. For Ne in Al the filling of the projectile L shell takes place via L-Auger transitions and collisional charge transfer both governed by the L-Auger rate Γ_L and the capture rate Γ^c_L, respectively.

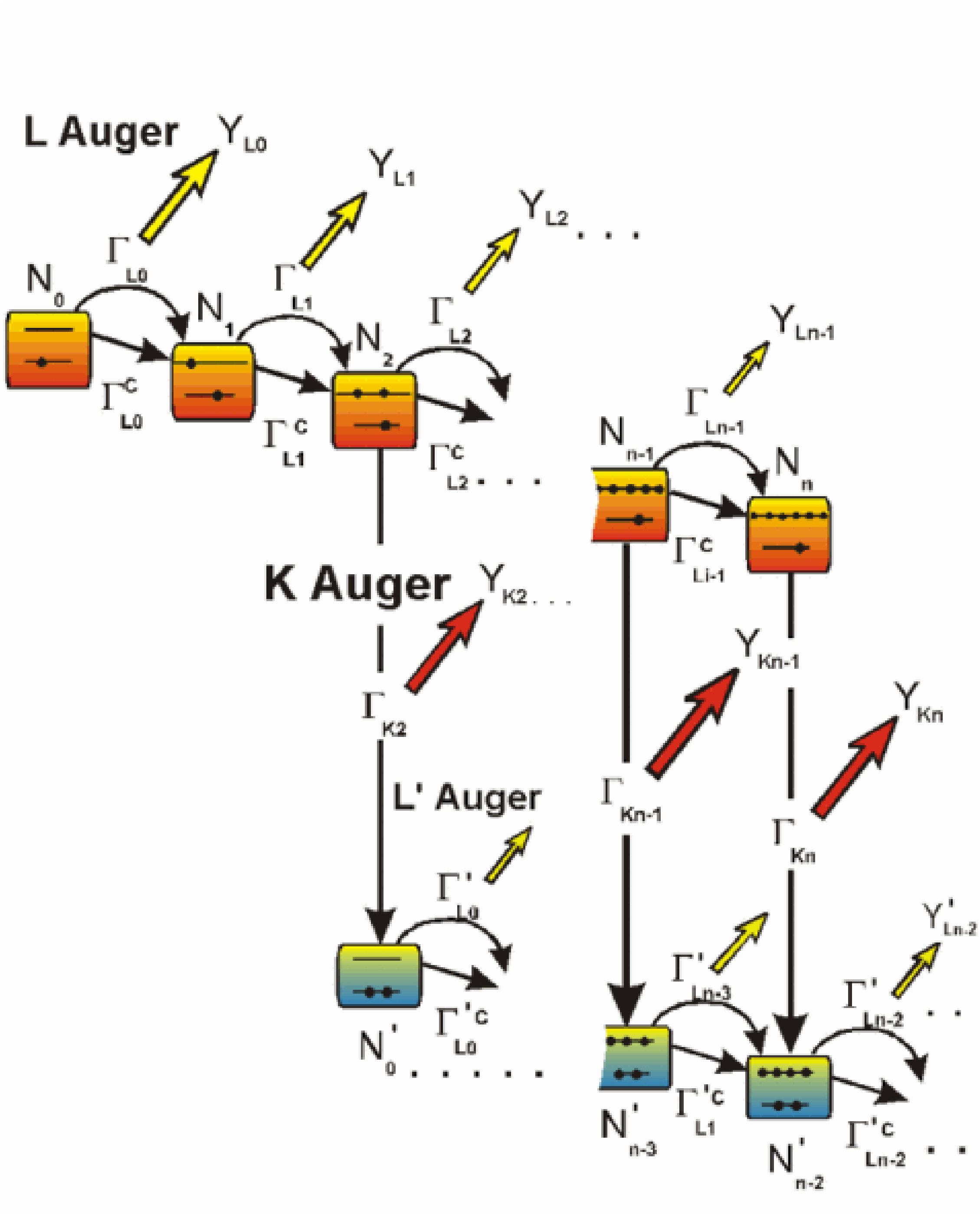

Fig. 1: The cascading decay of a hollow Ne atom

To calculate the time evolution of the system, we determined the time-dependent occupation number $N_\kappa(t)$ for the configuration $\kappa=(l,m)$ where l and m are the numbers of electrons in the L and M shell, respectively. For a given configuration, multiple paths correspond to several sources of ingoing flux. Similarly, the outgoing flux generally occurs via different paths. Thus, the quantities $N_\kappa(t)$ are obtained by solving the system of rate equations

$$\frac{dN_\kappa}{dt} = \sum_i N_{\kappa_i} \Gamma_i(\kappa_i) - N_\kappa \sum_j \Gamma_j(\kappa)$$

(1)

where $\Gamma_i(\kappa)$ and $\Gamma_i(\kappa)$ are rates for creation and loss of such configuration, respectively.

In general expression (1) has to be solved using numerical methods. With the assumption that the decay of the hollow atom can be neglected above the surface, the rate equation can be solved in closed form. After time integration one obtains the *intensity* of the Auger electrons in the elastic channel which may be evaluated analytically giving rise to the relatively simple expression

$$Y_{Kn} = \Gamma_{Kn} \frac{\prod_{i=0}^{n_L-1} \Gamma^f_{Li}}{\prod_{i=0}^{n_L} S_i}$$

(2)

with the L-shell filling rate $\Gamma^f_{Ln} = \Gamma^c_{Ln} + \Gamma_{Ln}$ and the sum rate $S_n = \Gamma^f_{Ln} + \Gamma_{Kn}$.

The closed form of the cascade model can be retained when electron attenuation effects are taken into account. (Also, electron diffraction effects can be included in the analysis.) When the Auger electrons are ejected below the surface, we assume an exponential attenuation law $a_K(t)$ = exp(-&Gamma^a_K t) where &Gamma^a_K is the attenuation rate. This time-dependent attenuation law follows directly from the well-known expression $a_K(l)$ = exp($-l/\lambda^a_K$) where l is the travel distance of the electrons in the sold, and $\lambda^a{}_K$ is the corresponding attenuation length. Attenuation effects are implemented into expression (2) by replacing the sum rate S_n through $S^a{}_{Kn} = S_n + \Gamma^a{}_K$.

Electron transport and emission spectra

As it was mentioned above, different mechanisms contribute to electron emission during the interaction of a highly charged ion with a solid: (i) removal of previously captured electrons by level shifting, (ii) autoionization of electrons captured in highly lying shells above the surface, (iii) electron peel-off at the surface, (iv) Auger processes filling low-lying orbitals of the hollow atom and (v) binary projectile-electron collisions below the surface.

The emission characteristics related to processes from below the surface are determined by the density of inner excited electrons at the surface $N(E',\Omega') = N(x=0, E',\Omega')$. The density $N(x,E',\Omega')$ can be determined by solving the transport equation or with a Monte-Carlo code taking into account suitable boundary conditions at the surface. The transport equation is expressed as

$$\frac{v(E')}{l(E')} N(x,E',\vec{\Omega}') + v(E')\cos\alpha' \frac{\partial N(x,E',\vec{\Omega}')}{\partial x} = S(x,E',\vec{\Omega}') + \iint_{E''} dE'' d\Omega'' W^{\sigma}(E',\vec{\Omega}';E'',\vec{\Omega}'') N(x,E'',\vec{\Omega}'')$$

(3)

The number of electrons in the state (E',Ω') at the depth x created by the moving projectile is given by the excitation function $S(x,E',\Omega')$. v(E') is the electron velocity. The number of electrons leave and entering the state (E',Ω') are given by the total mean free path of the electrons $l(E')$ and the transition function $Ws(E',\Omega';E'',\Omega')$, respectively. Both quantities are determined by elastic and inelastic scattering processes.

The escape process of excited electrons can be described using the standard model of a planar surface barrier and free electrons inside the target. From the conservation laws for energy and parallel momentum, we obtain the escape conditions: $E' > W$ (vacuum level: $W=E_F+\Phi$, E_F - Fermi energy, Φ - work function) and $\cos \alpha' > \cos \alpha_c = (W / E')^{1/2}$, &aplha;' is the angle between electron momentum and the outer normal. α_c defines the escape cone. Electrons with $\cos \alpha' < \cos \alpha_c$ are specularly reflected at the surface. After solving the transport problem the basic quantity for calculating the emission properties (energy spectra of emitted electrons *j(E)*, electron yield γ) is the energy-angular distribution of emerging electrons. Including the escape conditions this quantity can be written as

$$j(E,\vec{\Omega}) = \mathrm{v}(E')\left(1-\frac{W}{E'}\right)\sqrt{\frac{E'\cos^2\alpha'-W}{E'-W}}N(E',\vec{\Omega}')$$

(4)

where unprimed and primed parameters refer to quantities above and below the surface, respectively.

Application to Ne^{9+}-impact on Al: The above mentioned cascade model can be used for the description of the depth dependent excitation of electrons below the surface by different Auger processes (mechanism (iv)). Using a δ-function like ion density along the incoming straight line trajectory of the projectile ($x = \mathrm{v}_{ion}t$), the depth distribution of the K-Auger excitation in the specific case of Ne^{9+} impact on a metal surface is given by

$$Q^K(x) = \sum_{i=2}^{8} \Gamma_{K,i} N_i(x/\mathrm{v}_{ion})$$

(5)

where the index *i* labels the number of electrons in the Ne-L shell.

Together with the assumption of a Gaussian-like energy distribution of this excitation we obtain the depth and energy dependent excitation function $S^K(x,E')$. In order to calculate the emission properties related to the whole energy range as well as the spectral properties at low energies the excitation functions $S^K(x,E')$ and $S^L(x,E')$ related to K- and L-Auger transitions, respectively, can be used as the basic input quantities in the description of transport of excited electrons within the target. A Monte-Carlo code was developed to calculate the emission spectra showing the characteristic features of the K- and L-Auger transitions (Fig. 2).

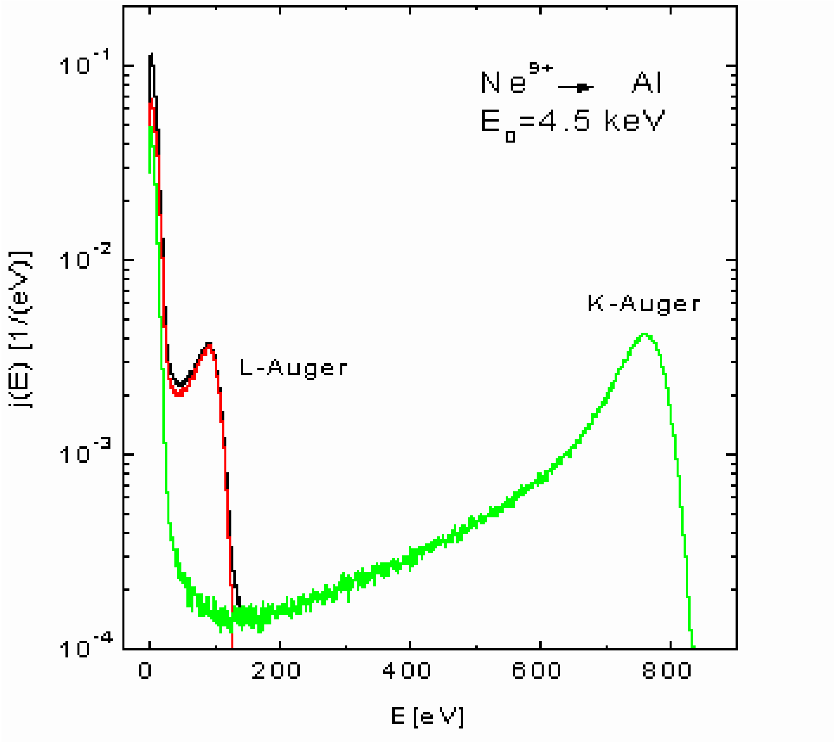

Fig. 2: Electron spectrum showing L- and K-Auger maxima
(work performed in collaboration with A. Dubus)

Furthermore, the data show the low energy maximum and the plasmon shoulder (Fig. 3).

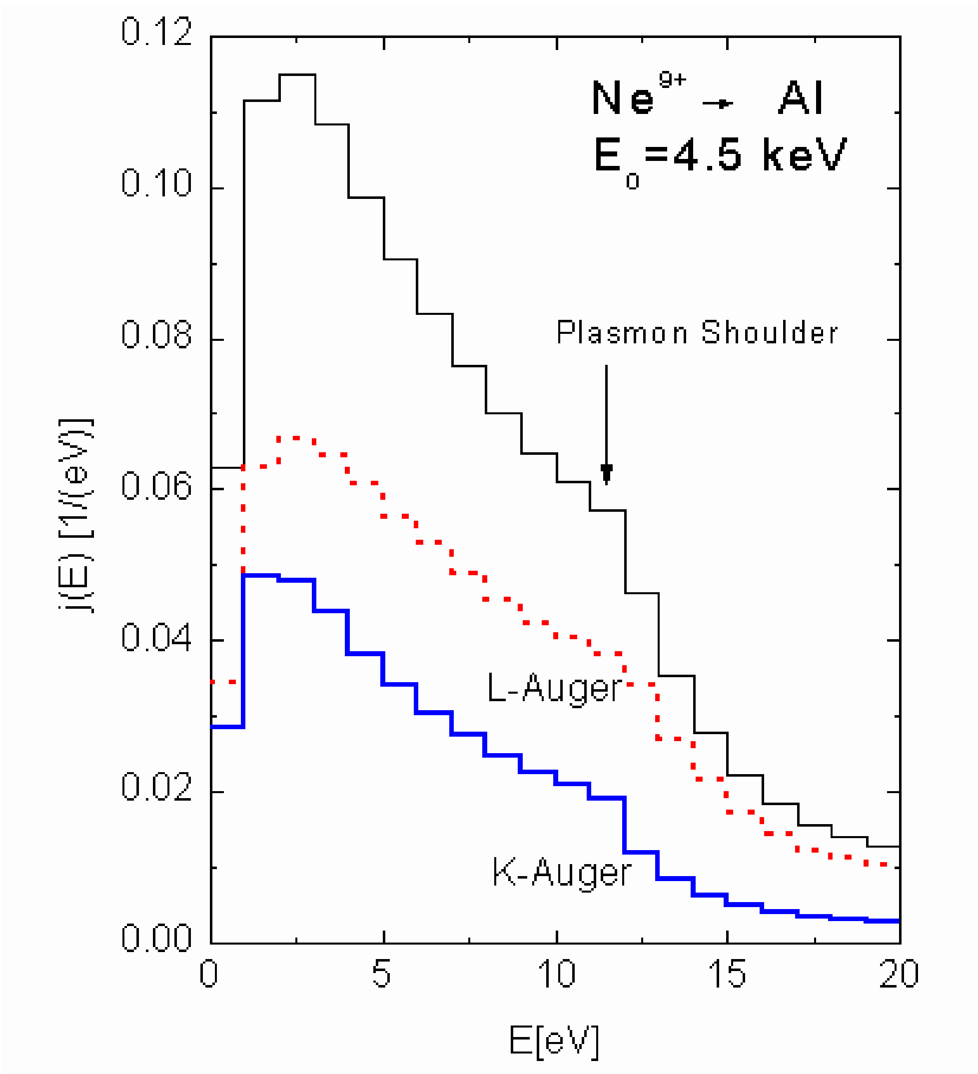

Fig. 3: Electron spectra showing the low-energy maximum including a plasmon shoulder (obtained in collaboration with A. Dubus)

The accumulation of electrons at low energies is determined by elastic and inelastic scattering processes of excited electrons within the target. The plasmon shoulder results from the decay of plasmons produced by K- and L-Auger electrons.

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Ion-Surface Interaction - Instrumental Methods

Highly charged ions of extremely low velocities are available at the 14.5-GHz Electron-Cyclotron-Resonance (ECR)-Source of the Ionenstrahl-Labor (ISL) as shown in Fig. 1. The ion source provides projectiles with energies up to 20q keV where q is the charge state of the extracted ions. The end of each beam line is equipped with a deceleration lens system to extract ions at energies as low as 1q eV. The beam line can be set on high-voltage so that the experimental apparatus can be operated on ground potential. This unique feature of the ECR-Facility at ISL makes it very attractive for external users to perform experiments with their own apparatus without much precaution for high voltage. Information about the activities of the external users during the last 3 years can be obtained from the User Activity Sheet.

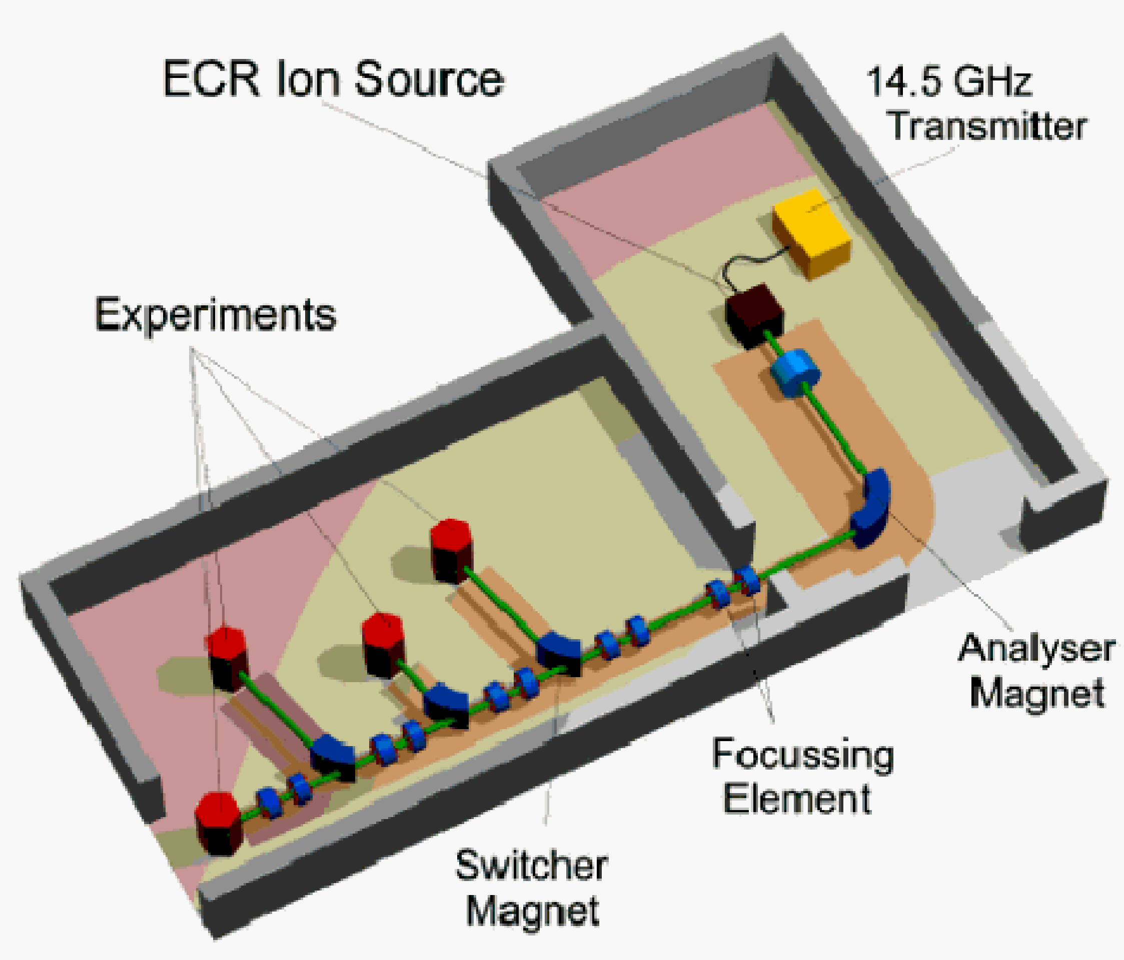

Fig. 1: The beamlines at the ECR-source

Fig. 2 shows the ultra-high-vacuum chamber used in the experiments including an electron spectrometer and facilities for surface examination. The base pressure during the measure-ments is a few 10^{-10} mbar. The upper part of the chamber contains equipment for surface preparation and analysis, i.e., an argon sputter gun and a LEED system. Auger electron spectros-copy is applied to verify the cleanness of the surface. After careful cleaning no measurable contaminations of the surface by C, N, and O can be detected at the target.

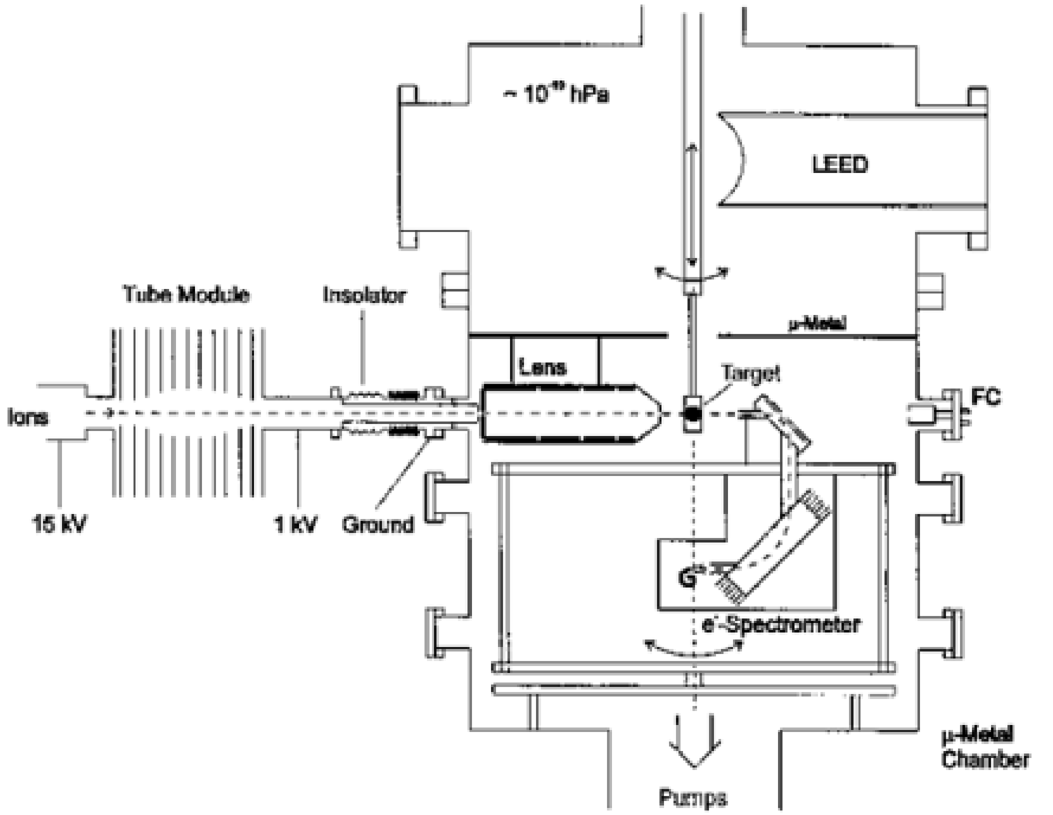

Fig. 2: The experimental set-up; note the deceleration system for the ions

In the lower part of the chamber the experiments are carried out. A beam of highly-charged ions (e.g. Ne^{9+} and Ar^{17+}) from the ECR-Source is used to bombard different targets such as Al and Si. After the ions are accelerated, they are magnetically analyzed and collimated to a diameter of about 1 mm at the position of the target. Since the beam can be put on high voltage the ions can be slowed down in deceleration systems (Tube Module and Lens). Electrons ejected by the interaction of the ions with the surface are measured with an electrostatic parallel-plate spectrometer whose observation angle can be varied in a wide range. The chamber is available to external groups.

It is planned to mount a combined STM/AFM system to the UHV chamber for in situ surface analysis. The bombardment with ions can produce local modifications in the morphology of the sample, reaching from the dislocation of single surface atoms to craters and hillocks up to a few 10 nm in diameter. Also, the electrical properties of the solid can be changed along the ion track. These alterations can be detected with the STM on conducting and semiconducting samples and the AFM on insulating samples. In order to examine the modification of the sample due to ion bombardment, the STM/AFM will be mounted to the upper part of the chamber. Using a set of manipulators the sample can be transferred between the STM/AFM stage, the preparation site, and the target region of ion beam. This allows the in situ control of the surface roughness after sample preparation and after the ion bombardment, without breaking the ultra-high-vacuum conditions. The measurements with the STM/AFM in air have already started.

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Ion-Surface Interaction - Experimental Results

Mechanisms for electron emission

In the experiments we measure absolute doubly differential yield $d^2 Y/d \bullet dE$ for electron emission. Fig. 1 shows a typical result for the collision system 4.5 keV Ne^{9+} on Al. The inset depicts the collision geometry, i.e., the incidence angle is $\psi = 45^0$ and the observation angle is $\alpha = 75^0$ relative to the target surface. The electron spectrum exhibits pronounced structures which can be associated with processes revealing information about the interaction of highly charged ions with the surface.

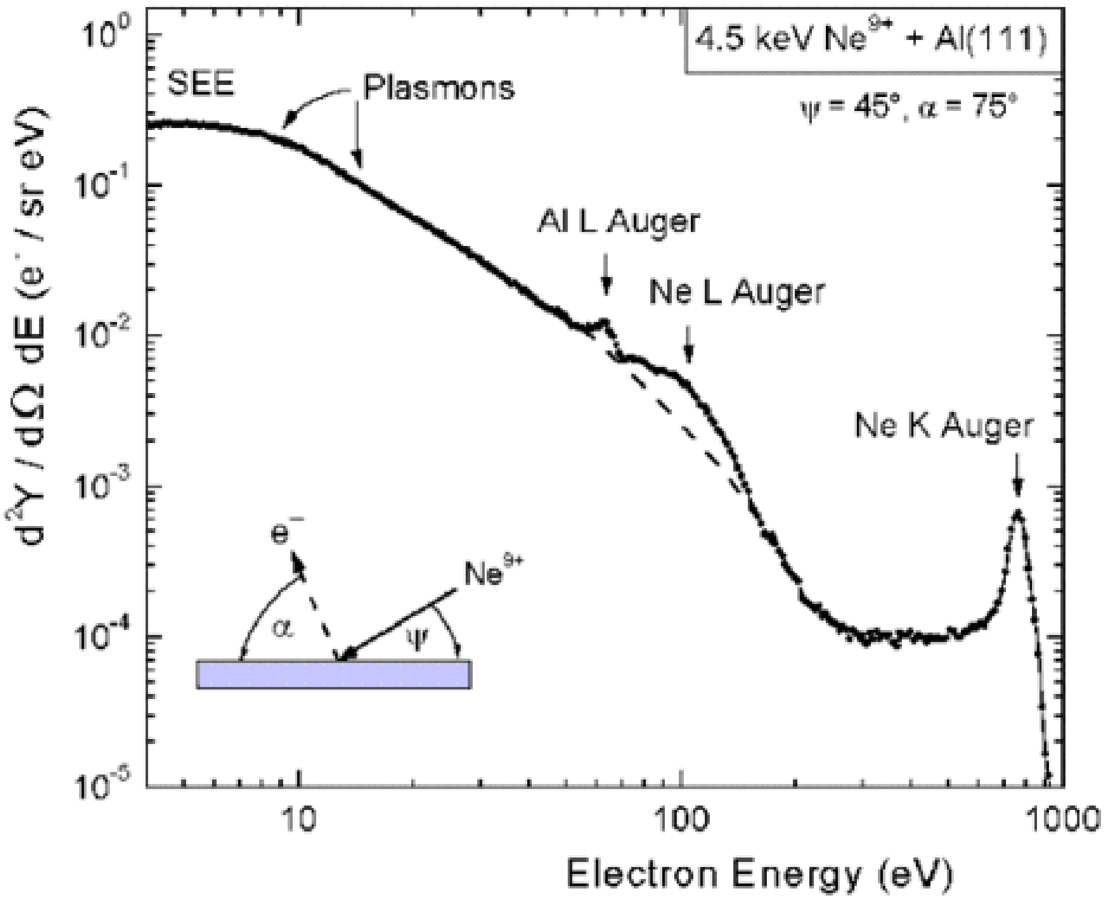

Fig. 1: Electron spectrum for 4.5 keV Ne^{9+} on Al

The spectral structures are primarily caused by dielectronic processes occurring above and below the surface. Above the surface, autoionizing transitions in higher Rydberg states give rise to electron energies as low as a few eV, whereas the L-Auger electrons originate primarily from below the surface. For instance, L-Auger transitions in the Al lattice atoms give rise to a pronounced peak near 63 eV {Benazeth78}. The vacancies in the Al L shell are produced in binary collisions with the hollow Ne projectile {Stolterfoht95}. Moreover, L-Auger electrons from the neon projectiles are seen near 110 eV. This energy stems from the energy liberated as an electron is captured into the L shell of the hollow neon.

In the energy range between 8 and 15 eV the spectrum contains electrons ejected from the decay of bulk plasmons. The electron structures due to plasmon decay are superimposed on an intense background from other processes and they can only be seen when the measured electron intensities are differentiated. In the following, examples for Auger electron emission and plasmon creation are given.

Auger spectroscopy

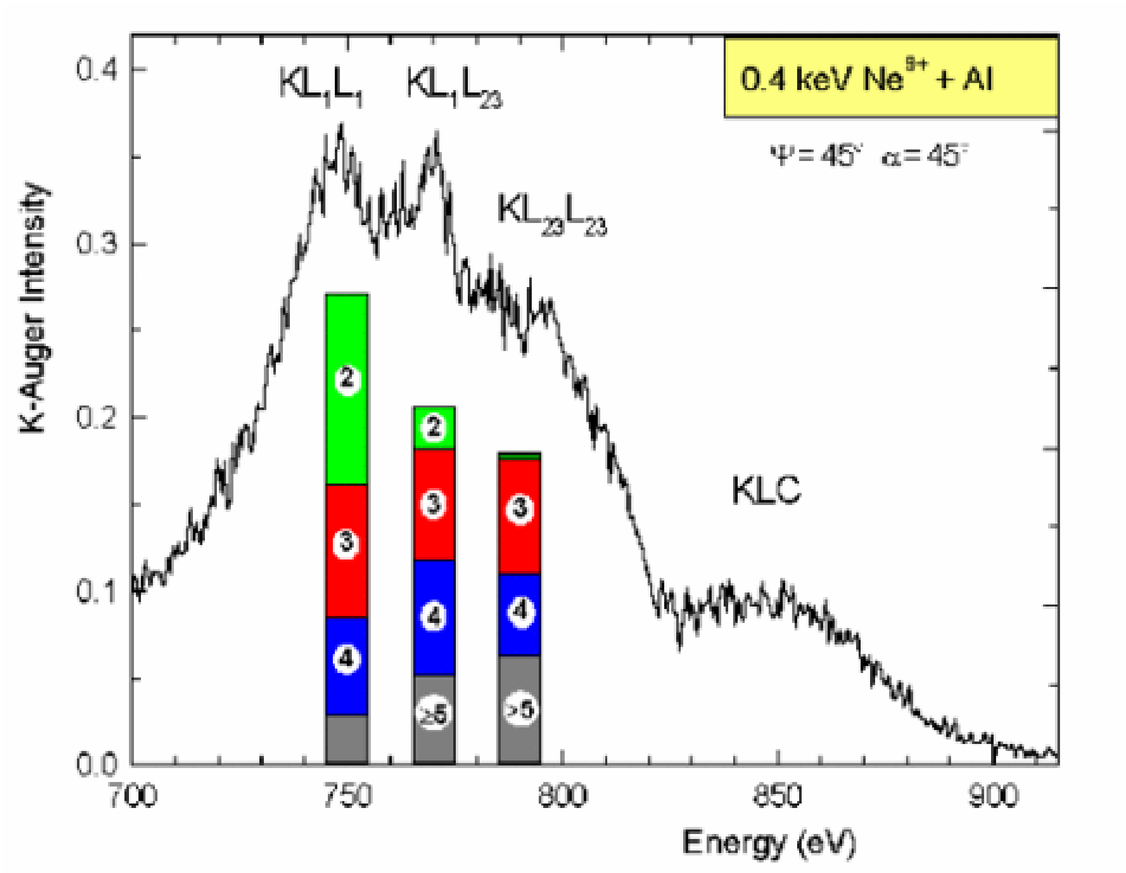

Fig. 2: Auger spectrum for Ne^{9+} incident on Al

Figure 2 displays a typical K-Auger spectrum for 0.4 keV Ne^{9+} incident on Al. The data show essentially 3 peaks that can be associated with *KLL* Auger transitions filling the K vacancy in hollow neon. The structure at higher energies labeled *KLC* is produced by Auger transitions where an electron from the induced electron cloud C is ejected. It is important to note that the relative intensities of the Auger peaks depend on the filling state of the hollow atom.

The experimental Auger structures are compared with theoretical data obtained using the cascade model as described in the theoretical section. The peaks of the *KLL* group are compared with a bar diagram which involves different contributions from Ne projectiles with different numbers *n* of electrons occupying the L shell. (Note the colored fractions with numbers representing *n*.) From the first bar one can see that a significant amount of neon atoms are still hollow during the Auger decay, see the relative large fraction with *n* = 2 (corresponding to 6 vacancies in the neon L shell).

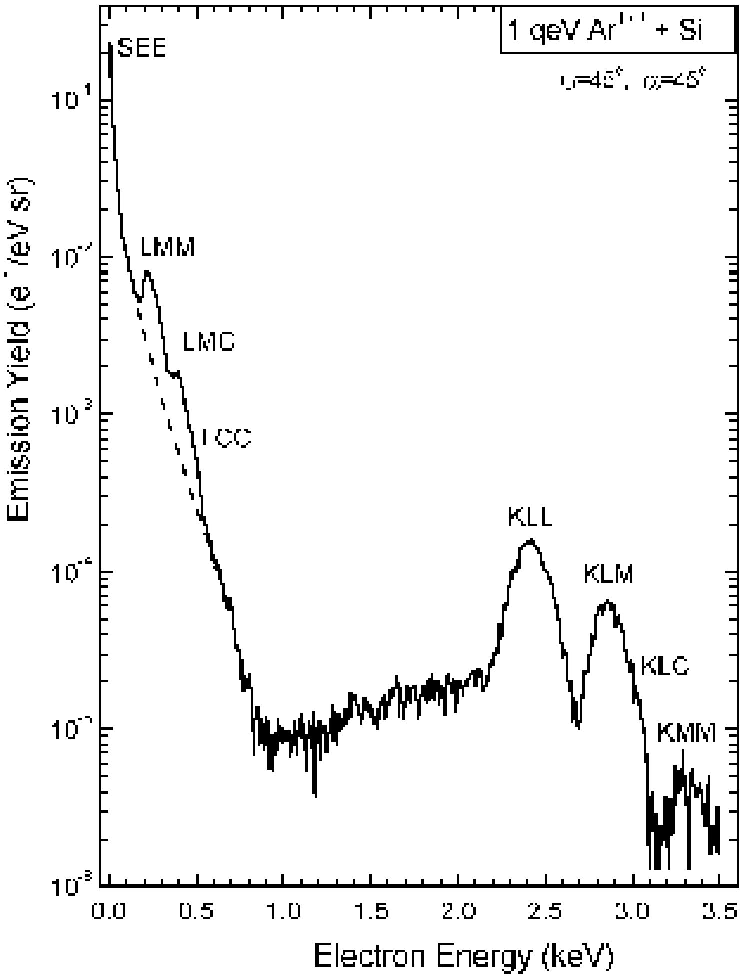

Fig. 3: L and K Auger Spectra from 17 eV Ar^{117+} incident on Si

Recently, hydrogen-like Ar^{17+} was produced at the ECR-source and extracted within a wide range of projectile energies from 170 keV down to extremely small values of 17 eV. Electron emission was measured to study the interaction of Ar^{17+} ions with a Si(111) surface. Moreover the angular dependence of the Auger electron intensities were measured and interpreted by means of model calculations using the cascade model described before.

Figure 3 shows a representative electron spectrum which exhibits various peaks attributed to the different Auger transitions in the projectile. The peak structures can be attributed to K- and L-Auger transitions in hollow argon. These peaks show that apart from the K and L shell, an M shells exist in hollow Ar atom when moving inside the solid. In addition, the highly charged Ar ion induces the negative charge cloud C, which coincides with the N shell. The experiment provides clear evidence for the C shell (see for instance the Auger transitions LMC and KLC).

Plasmon production by hollow atoms

The emission of low-energy electrons by 4.5 keV Ne^{q+} ion impact on an Al surface was measured for incident charge states q = 1 - 6. The electron spectra exhibit structures near 6.5 eV and 11 eV, which are attributed to the excitation of surface and bulk plasmons, respectively.

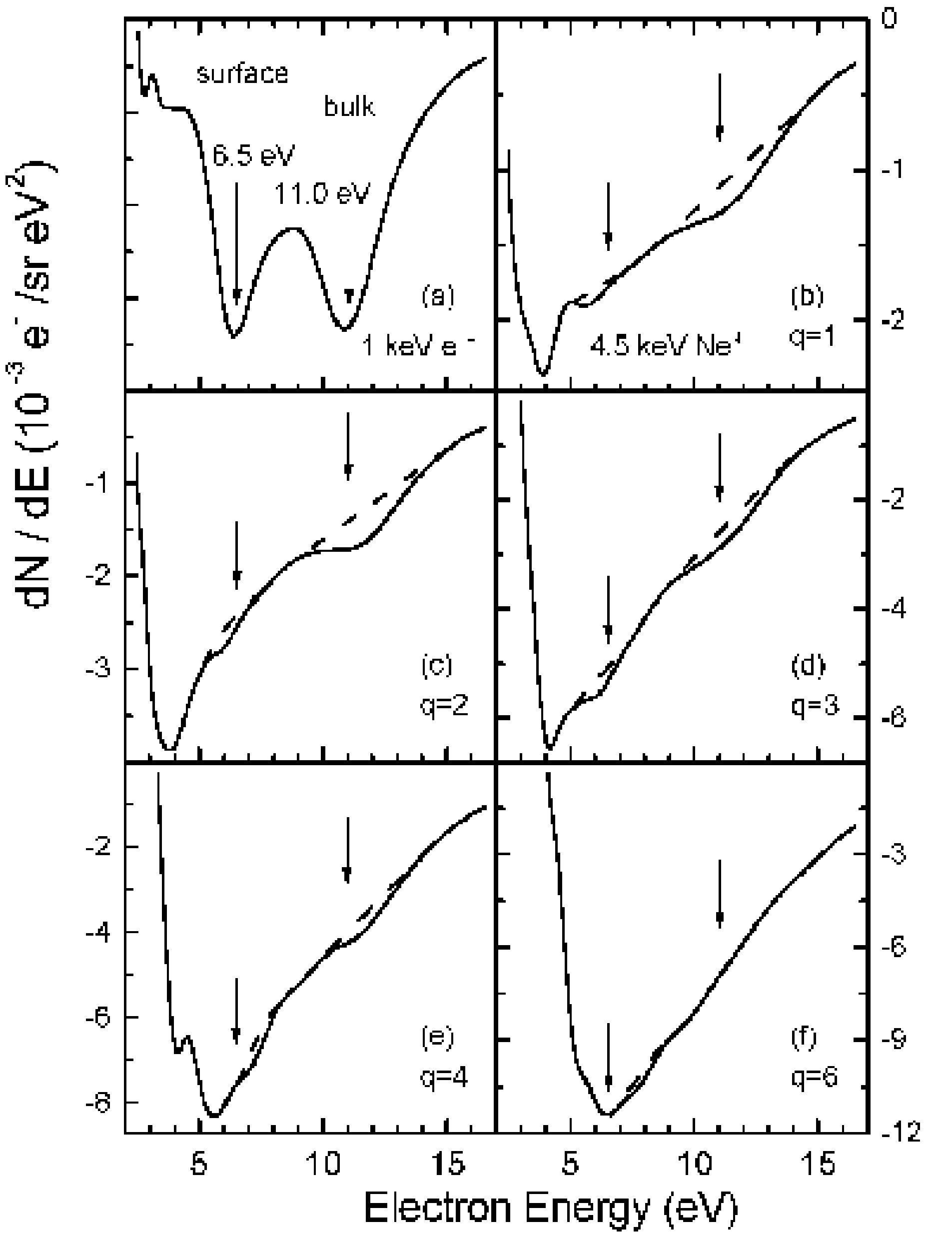

Fig. 4: Differentiated electron spectra showing structures due to plasmon decay

Examples for the differentiated electron spectra are given in Fig. 4. In Fig. 4 (b) – (f) the data for 4.5 keV Ne^{q+} impact with q= 1 - 4 and 6 are presented. The expected energy position for the plasmon decay are for surface plasmon at 6.5 eV and for bulk plasmon at 11 eV (see arrows). Figure 4 (a) shows the well-known spectrum for 1 keV electron impact, which exhibits the typical signatures for plasmons, i.e., a minimum in this first derivative. The curves for q = 1 - 4 in Fig 4 (b) – (e) reveal similar structures associated with the creation and the decay of plasmons. The derivative for q = 1 clearly shows a structure near 11 eV which is commonly attributed to bulk plasmons. This structure is enhanced for q = 2 but becomes less pronounced in comparison to the background as the charge state increases further. Finally, the bulk plasmon structure seems to disappear for q = 6.

As a primary mechanism for plasmon excitation by slow heavy ions, we propose that the capture of a conduction band electron into the L shell of the Ne projectile provides the excess energy. However, this process of plasmon-assisted electron capture is resonant only for the case of one or two vacancies in the L-shell. Therefore, a Ne^{q+} ion with q > 2 impinging on the solid has to be successively filled (see Cascade Model) before it is able to excite a plasmon. Hence, for the higher charge states the bulk plasmons are selectively created below the surface when the resonance conditions for plasmon-assisted electron capture is achieved. This plasmon-assisted electron capture is similar to those considered by Baragiola and Dukes [1996]. However, we note that the projectile enters into the solid and the capture into the L-shell occurs primarily below the surface.

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Ion-Surface Interaction - Collaborations

In the following, representative examples are given for experiments performed at the ECR-facility by external groups in collaboration with the local group. The work concerns primarily ion-solid interactions. In specific cases, the experiments were extended using a gaseous target.

Universität Bremen, Fachbereich Physik, Kufsteiner Strasse 1, D-28359 Bremen

Thomaschewski and J. Bleck-Neuhaus

Hollow nitrogen atoms probing the jellium edge in front of a Au(111) surface

The deexcitation of slow, hydrogen-like nitrogen ions through interaction with a Au (111) surface is studied by *KLL* Auger electron spectroscopy. Special emphasis is given to processes occurring above the first atomic layer in projectiles that graze the electron gas at different depth. It is found that the increasing electron density around the jellium edge causes acceleration of L -shell filling. No difference is seen for projectiles that do or do not penetrate the first atomic layer. A cascade model of hollow atom deexcitation at the border of the electron gas is presented. The model includes a depth dependence of the L shell filling rate caused either by interaction with the electron continuum or by a violent collision with a single target atom. Good agreement with experiment is found, along with some evidence for transfer of electrons from states below the Fermi level.

Institut für Allgemeine Physik, TU Wien, Wiedner Hauptstr. 8-10, A-1040 Wien, Austria

M, Sporn, G. Libiseller, T. Neidhart, M. Schmid, F. Aumayr, HP. Winter, and P. Varga

Potential Sputtering of Clean $Si0_2$ by Slow Highly Charged Ions

The recently discovered phenomenon of *Potential Sputtering*, i.e., the efficient removal of neutral and ionized target particles from certain insulator surfaces due to the Potential rather than the kinetic energy of impinging slow highly charged ions, has now also been observed for stoichiometric $Si0_2$ surfaces. Using a sensitive quartz crystal microbalance technique, total sputter yields induced by Ar^{q+} (q = 5 - 14) and Xe^{q+} ($q \leq 27$) ions have been determined for LiF and $Si0_2$ surfaces. The primary mechanisms for *Potential Sputtering* (defect mediated sputtering) and its considerable practical relevance for highly charged ion-induced surface modification of insulators are shown.

Department of Atomic Physics, Stockholm University, S-10405 Stockholm, Sweden

W. Huang, H. Lebius, Z. Pešic, G. Vikor, R. Schuch

Energy Loss in Large-Angle Scattering of Slow Highly Charged Ar Ions from a Au Surface

Energy loss of slow (v = 0.06 a.u.) highly charged Ar^{q+} (q=7 - 15) ions scattered from a Au(111) single crystal surface has been investigated for different incident angles ($\psi = 5^0$ - 37.5^0) and a fixed scattering angle of 75^0. The energy position of the elastic peak seems to agree well with the value expected for the binary elastic scattering. At small incidence angle (5^0) an additional inelastic energy loss besides the elastic energy loss was identified in spite of the large scattering angle. This additional energy loss is found to compare well to a combination of a modified Firsov model with processes of electron capture, recapture, Auger transitions, and image charge acceleration during the ion-surface interactions.

Centre Interdisciplinaire de Recherche Ions Lasers, CEA-CNRS-ISMRA et
Université de Caen, F-14070 Caen Cedex, France

J.-Y. Chesnel, H. Merabet, C. Bedouet, F. Frémont, and X. Husson
Institute of Nuclear Research of the Hungarian Academy of Sciences, P.O.B. 51, H-4001 Debrecen, Hungary

B. Sulik

Enhancement of dielectronic processes in Ne^{10+} +He collisions at energies as low as 1 keV.

The method of high-resolution Auger spectroscopy was used to study mechanisms for double electron capture producing the projectile configurations *3lnl'* and *4lnl'* in Ne^{10+} + He collisions. Emphasis was given to slow collisions with projectile energies as low as 1 keV. At low collision energies the production of the configurations *3lnl'* of non-equivalent electrons is found to become dominant. It is shown that dielectronic processes produced by the electron-electron interaction play a major role in the creation of the Ne^{8+} 3lnl' states.

In addition collaborations exist with the

Universität Osnabrück

GANIL in Caen

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Analysis

The accelerators at ISL were used for basic research, for the modification of materials and for the analysis of matter. The objects under examination vary from complicated layer structures of semiconductor devices to those of art historical nature. The following methods were available also for external customers:

ERDA	(Elastic Recoil Detection Analysis)
PIXE	(Proton induced X-ray emission)
RBS	(Rutherford Backscattering with helium or heavy ions)

Here, you will find a summerizing overview of sensitivities, resolutions, etc. for the different methods.

Team

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Strukturforschung Struktur & Dynamik SF8

ERDA

(Elastic Recoil Detection Analysis with high energetic heavy ions)

For the ERDA-method the samples are irradiated with high energetic heavy ions under grazing conditions. The energy as well as the number of the outscattered atoms (recoils) of the sample components are measured at a fixed angle relative to the beam direction. At ISL the element - respectively mass identification is done by means of the time-of-flight method (TOF), i.e., the coincident measurement of energy and flight time for each recoil. Owing to the element specific energy loss in material it is possible to calculate from the measured energy spectra the depth dependent concentration distributions for all components of a sample.

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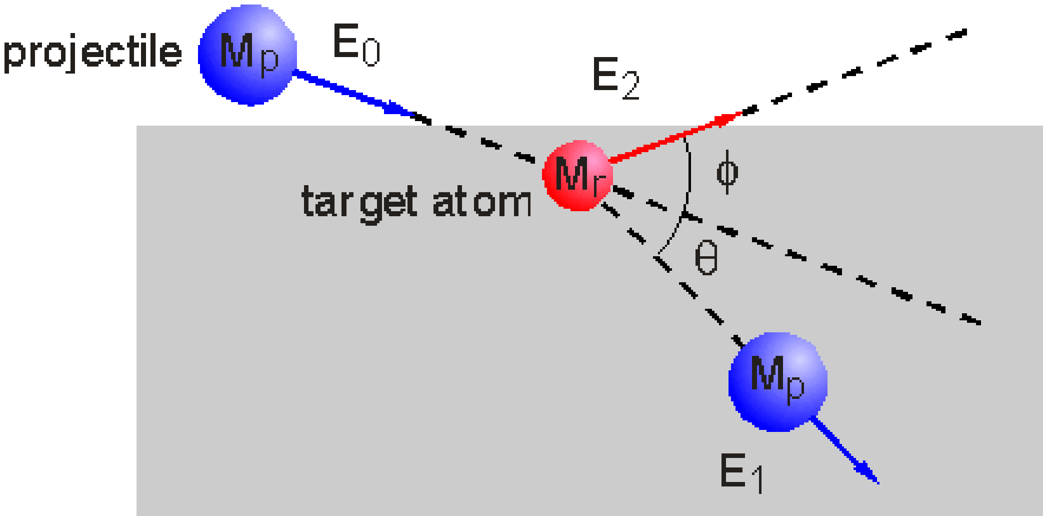
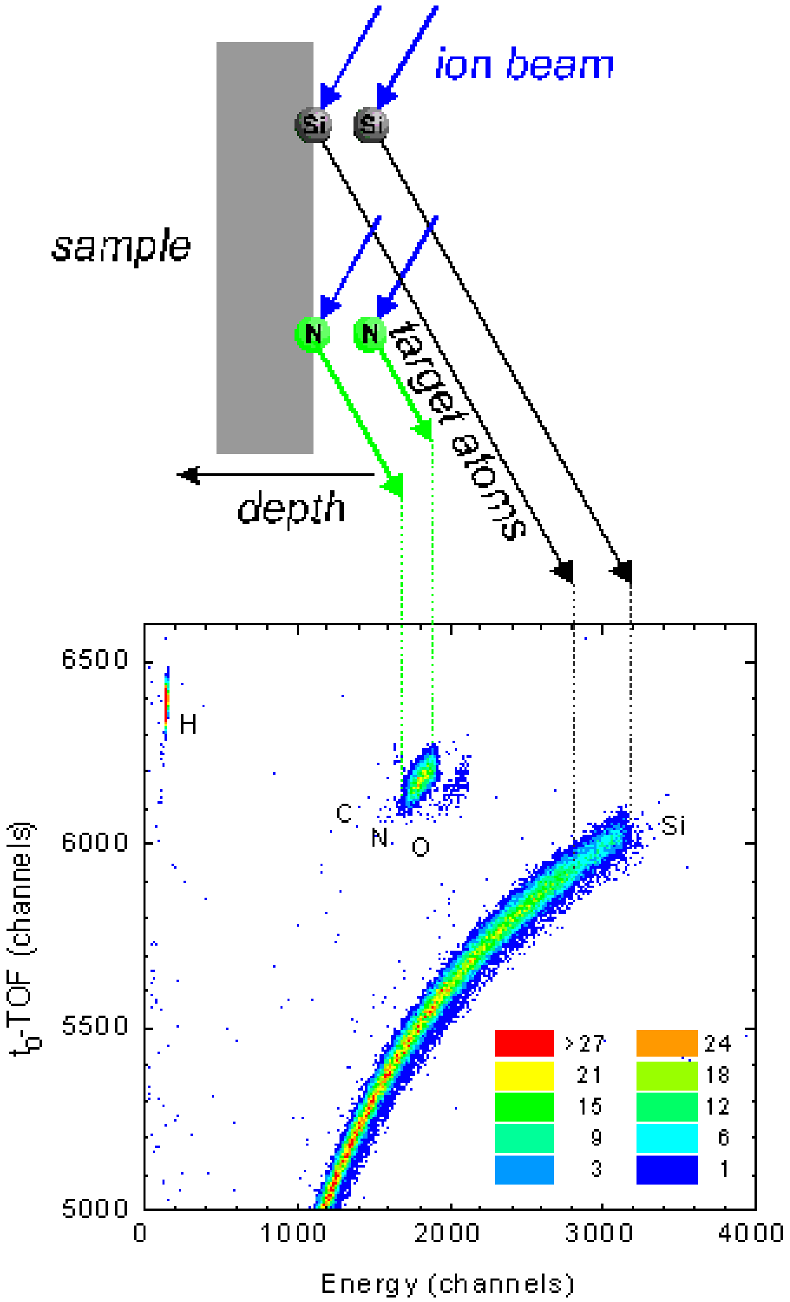
ERDA - Measuring Principle

- irradiation of the sample with high energetic heavy ions at grazing incidence



schematically description of the scatter geometry

- coincident measurement of energy and time-of-flight with fixed flight path for the outscattered atoms of the sample
- according to $E=M/2\ v^2$ it is possible to identify and separate the various masses in the two-dimensional scatterplot time vs. energy



scatterplot (time vs. energy) of atoms from a SiN_x:H layer on Si scattered to 60° relative to the direction of the irradiating beam of 230 MeV ^{129}Xe-ions

- the concentration of each element is calculated from the measured number N_r' of the corresponding forward scattered atoms from the sample

$$N_r = \frac{N_r'}{\sigma_r \, \Delta\Omega \, N_0}$$

- the solid angle ΔΩof the setup is known
- N_0 the number of the incident projectile ions is measured without any disturbance of the beam using the residual-gas-ionization
- the differential Rutherford cross section for the forward scattering of the sample atoms with mass M_r and nuclear charge Z_r can be calculated exactly

$$\frac{d\sigma_r}{d\Omega} = \left(\frac{Z_p Z_r e^2}{2E_0} \right)^2 \left(\frac{M_p + M_r}{M_r} \right)^2 \frac{1}{\cos^3 \phi}$$

- no free parameter is left, i.e., ERDA is a standard free, absolute method
- the thickness of a layer and the concentration profiles are calculated from the measured energy difference of the forward scattered sample atoms relative to the maximum possible energy of an atom scattered to the detection angle, which is given by the kinematical factor

$$E_2 = k_r E_0$$

$$k_r = \frac{4 M_p M_r \cos^2 \phi}{(M_p + M_r)^2}$$

- the detection sensitivity is almost the same for all elements
- only for hydrogen the sensitivity is enhanced by a factor of four
- when using heavy projectile ions no restriction of the detectable mass range exists
- possible uncertainties of the used stopping cross sections result in uncertainties of the calculated depth distributions

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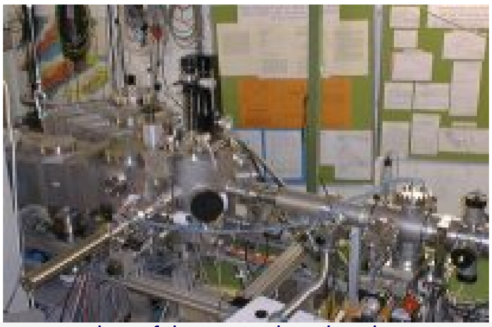
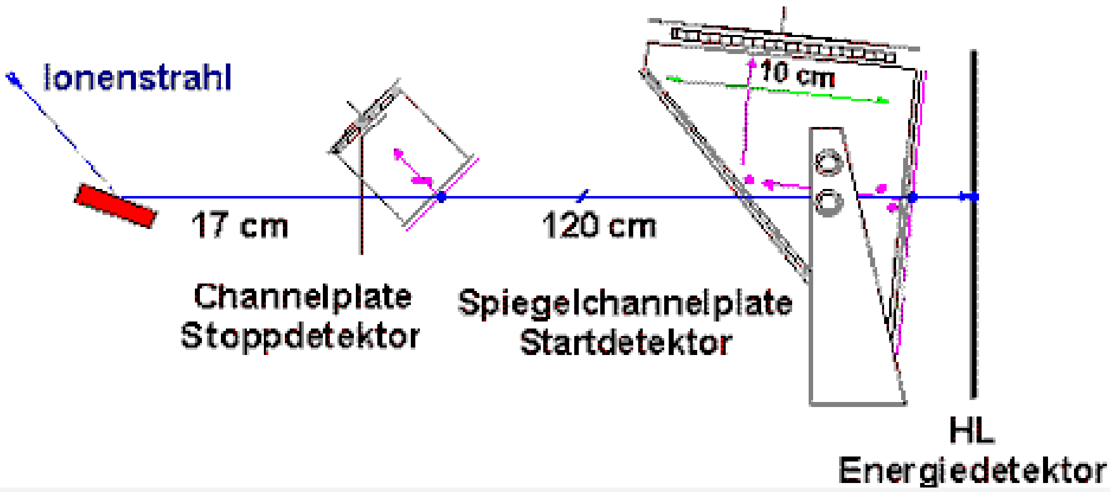
ERDA - Setup

Scattering chamber:



view of the scattering chamber
(enlarged picture (159 kB))

Flight path:



schematically description of the flight path

Parameters:

Sample dimensions:	1 cm x 1 cm
Sample lock:	6 samples per ladder
Scattering angle:	Φ = 15° - 45°
SB-detector:	72 mm x 60 mm, 24 stripes each 3 mm wide
Detector opening:	Δ&Phi = ±1,45° (24 x 0,12°)
Solid angle:	$\Delta\Omega$ = 2,1 msr

Flight path:	d = 120 cm
Time resolution:	Δt = 150 ps
Typical ion beam:	230 MeV $^{129}Xe^{17+}$, ca. 0,3 TnA
Measurement time:	10 - 100 min
Sensitivity:	some ppm for H and heavy elements, maximum 10 ppm for the others, depending on the sample structure
Depth resolution:	about 10 nm close to the surface, decreasing with increasing depth
Maximum depth:	about 2 µm, depending on the material

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PIXE (Proton Induced X-Ray Emission)

The object, that is to be analyzed, is irradiated by high energy protons. They excite the atoms, to emit characteristic X-rays, which identify the chemical elements in the probe. Very low proton currents are needed, and the studied objects are in normal atmosphere. Therefore highly sensitive and large objects, as objets d'arts, can be studied without any damage.

Analysis of the gilding of a 3600 year old egyptian coffin.
(enlarged picture (146 kB))

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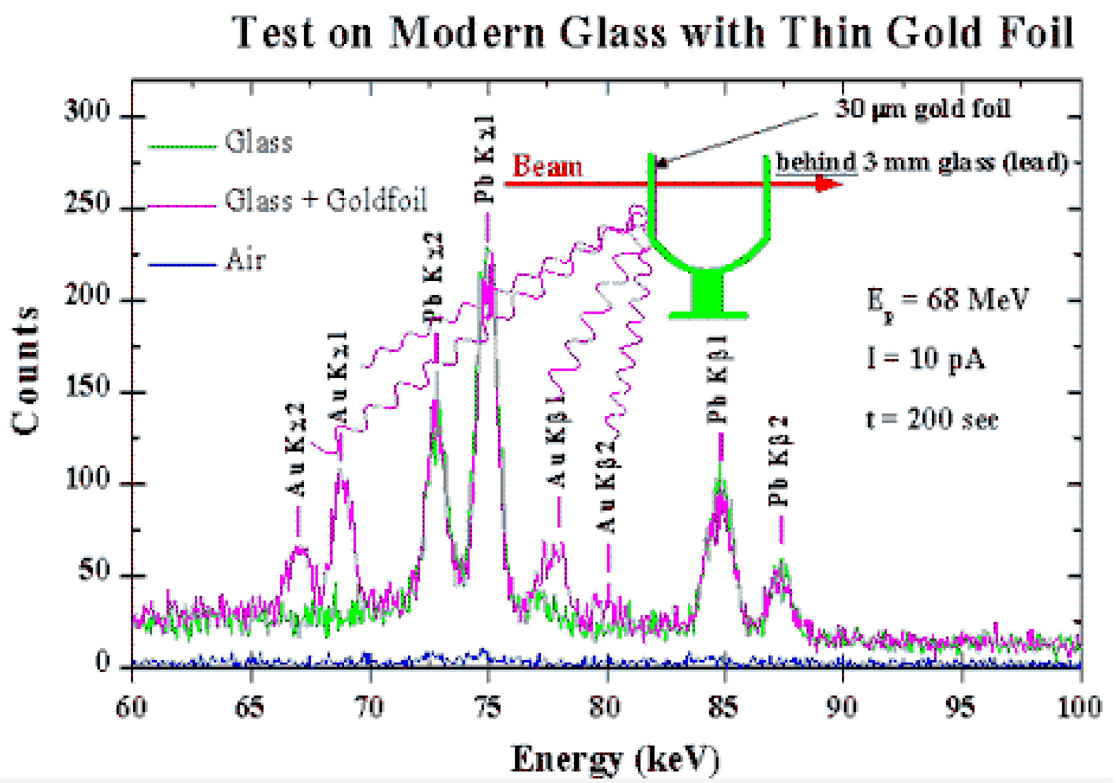
PIXE - Measuring Principle

Irradiation of any material with a proton beam induces the emission of characteristic X-rays, that identify the elements in the material, independent of their chemical bonding. Only X-rays above about 2 keV, i. e. from elements heavier than phosphorous, can be detected with the object in air due to the absorption of the X-rays in the air and the vacuum window of the detector; often the pieces to be analyzed would be damaged, if brought into vacuum. PIXE is performed at many places with protons of about 3 MeV. Here 68 MeV protons are used. With low energy protons the analysis is limited to a depth of around 0.25mm by the range of the protons. The range of 68 Mev protons is roughly a few centimeters, offering the fairly unique possibility of a nondestructive analysis to this depth. 68 MeV protons induce also for the heaviest elements the emission of K X-rays with good cross sections. These high energy X-rays are little absorbed and can therefore also be detected from deep inside of any test piece. The spectrum of K X-rays is also much less complicated than that of L X-rays, which have to be used with the usual low energy protons. The absorption of the X-rays on their way out from deep inside of the studied object, that depends on the composition and any layer structure of the probe, makes a fully quantitative analysis of the elements difficult. Some information on the depth, in which an element is present, can be gained from the measured intensity ratios of the various K and L lines of this element. Their absorption in the probe differs markedly because of their different energy and depends therefore on the depth.

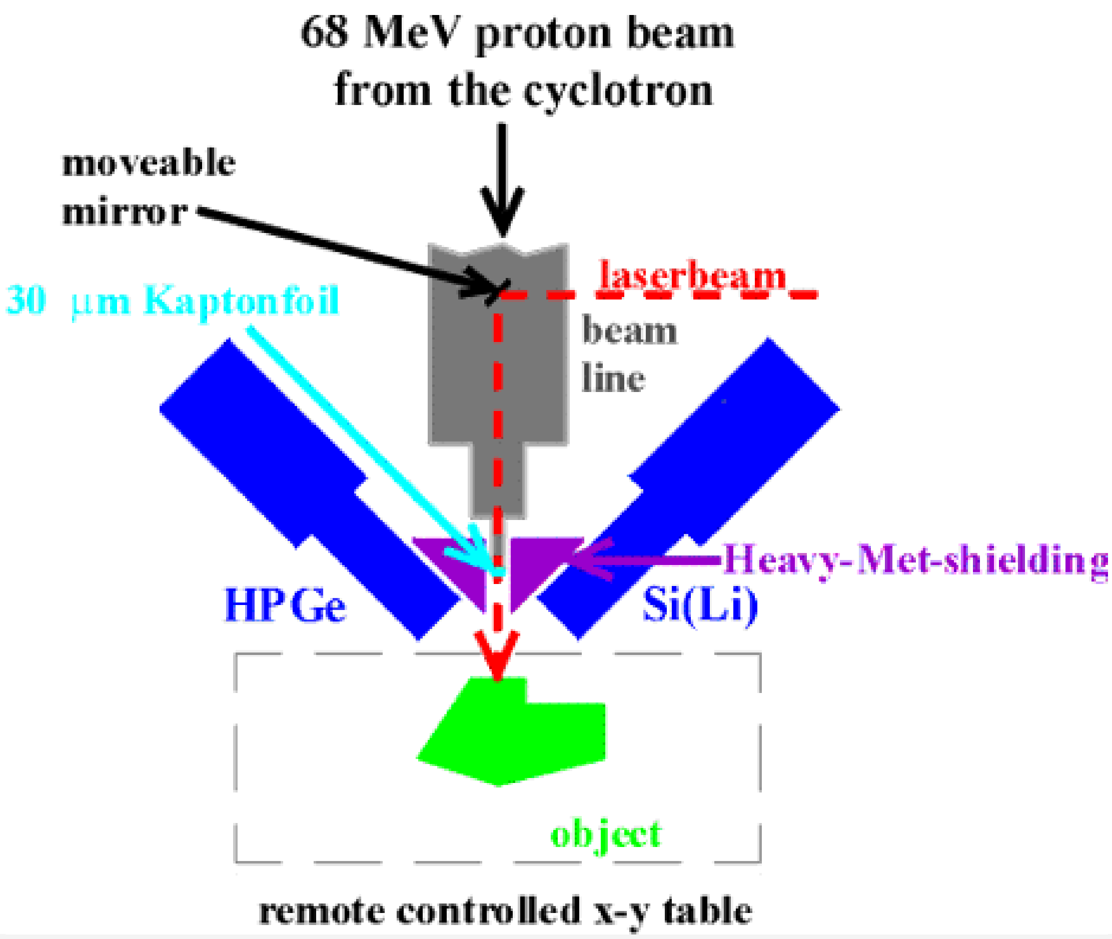


Non destructive detection of a thin gold foil behind 3mm of lead glass

PIXE - Setup

The simple measuring set up is placed at target location TW. The proton beam exits through a thin Kapton foil into the atmosphere. The item to be tested is placed about 10 cm behind the foil on a remote controlled x-y-table. Also bulky and heavy (50kg) pieces can be positioned to 0.1 mm. The measured spot can be marked and documented by taking and storing a digital image with a TV-camera. The beam is first focussed on a luminescent screen with an intensity of 1 nA to a diameter of 0.1 mm or more. Then the beam current is reduced to < 1 pA, before the object and the Ge- and Si(Li)-detector for the X-rays are put into place. Typically one measurement takes 3 min.

Setup:



schematically description of the setup

Parameter:

size of object	1 mm to 1m

distance beam exit to object	10 cm
distance detector to object	5 cm
detector HPGe	180 eV @ 5.9 keV
detector Si(Li)	155 ev @ 5.9 keV
Beam	68 MeV Protons, below 10 pA
measuring time	200 sec bis 0.5 h
Sensitivity	1 ppm for elements with Z around 50 in a light matrix, decreasing 0.1% in unfavourable cases
depth resolution	ca. 10 µm
possible depth of analysis	depends on element and matrix, up to some cm

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RBS (Rutherford Backscattering with helium or heavy ions)

For the RBS method a sample is irradiated with light energetic ions, typically hydrogen, helium or neon of a few MeV. At a backward angle, close to 180° relative to the beam direction, the number and the energy of projectile ions backscattered from the target are measured. Since these values are dependent on the mass respectively on the nuclear charge of the scattering atoms and because the projectiles sustain an energy loss in the material it is possible to determine the elemental composition as a function of depth.

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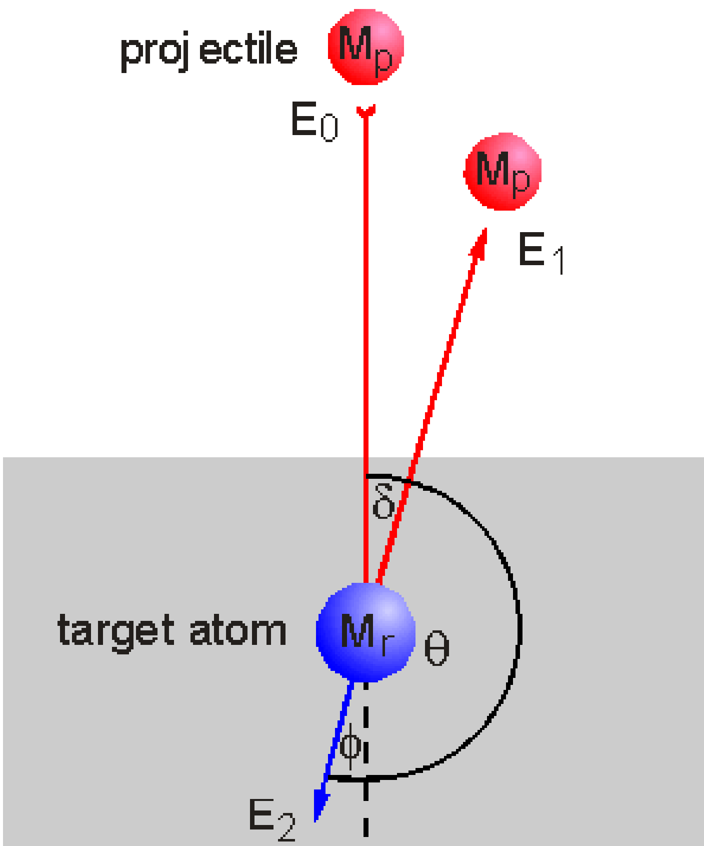
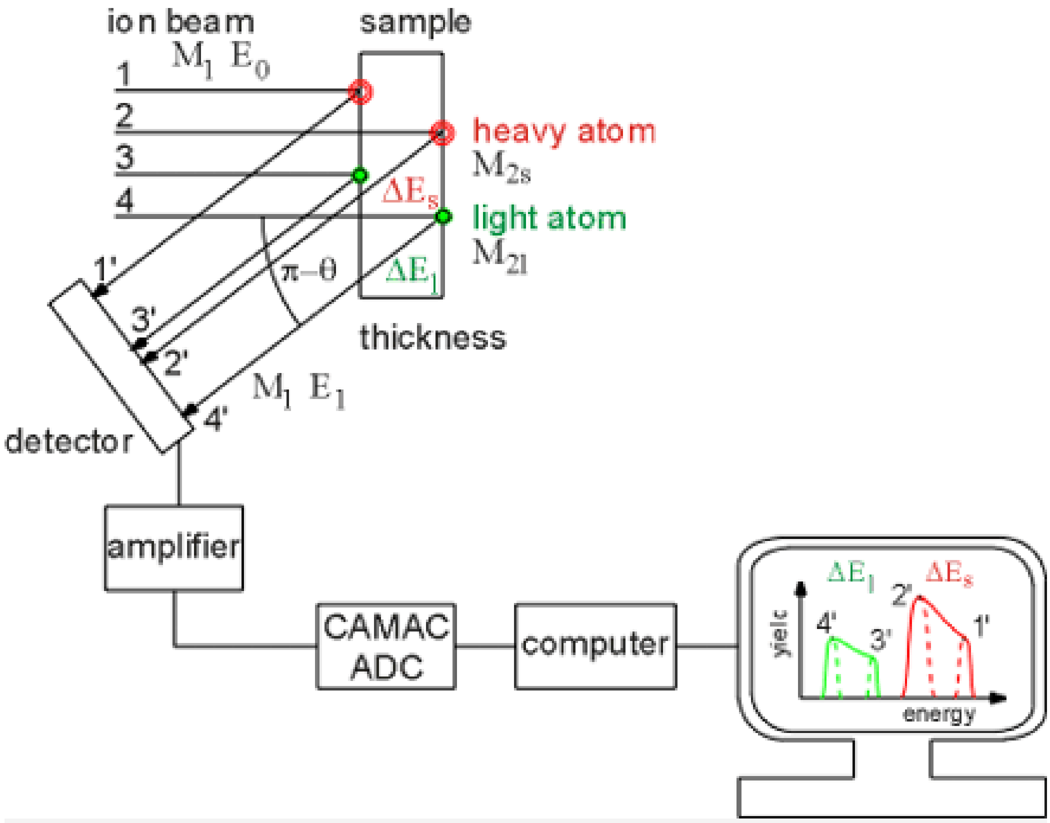
RBS - Measuring Principle

- irradiation of the sample with light ions and detection of the elastically backscattered projectiles at large angles



schematically description of the scatter geometry

- the mass identification of the target atoms results from the energy of the backscattered projectile, typically measured by means of a surface-barrier detector



schematically description of the measuring principle

- using heavier ions e.g. ^{14}N allows a better mass separation compared to so called standard RBS using H- or He-ions as projectiles
- the thickness of the layer respectively the concentration profile is determined from the energy difference of the backscattered projectile referring to the corresponding maximum energy for the scattering at a surface atom, given by the kinematical factor

$$E_1 = k_p E_0$$

$$k_p = \left(\frac{M_p / M_r \cos\theta + \sqrt{1 - (M_p / M_r)^2 \sin^2\theta}}{1 + M_p / M_r} \right)^2$$

- in the case of thicker samples the mass identification may be complicated due to the superposition of the spectra originating from the various sample components
- the number N_p of the measured backscatterd projectile ions gives the concentration of the corresponding element

$$N_r = \frac{N_p}{\sigma_p \, \Delta\Omega \, N_0}$$

- the solid angle $\Delta\Omega$ for the setup is known

- N_0 the number of the incident projectile ions is measured without any disturbance of the beam using residual-gas-ionization
- for the energies used, the differential Rutherford cross section for the scattering of a projectile with the nuclear charge Z_p from a target atom with the elemental number Z_r can be calculated exactly

$$\frac{d\sigma_p}{d\Omega} = \left(\frac{Z_p Z_r e^2}{2E_0}\right)^2 \frac{1}{\sin^4\theta} \frac{\left(\cos\theta + \sqrt{1-(M_p/M_r \sin\theta)^2}\right)^2}{\sqrt{1-(M_p/M_r \sin\theta)^2}}$$

- no free parameter is left, i.e., RBS is a standard free, absolute method
- since the scattering probability increases with Z_r^2 RBS is more sensitive for heavier components of the sample
- scattering to large angles from atoms with masses close to or even below the projectile mass is not possible, therefore, these light elements are not detectable
- possible errors in the used stopping cross section result in errors of the calculated depth distributions

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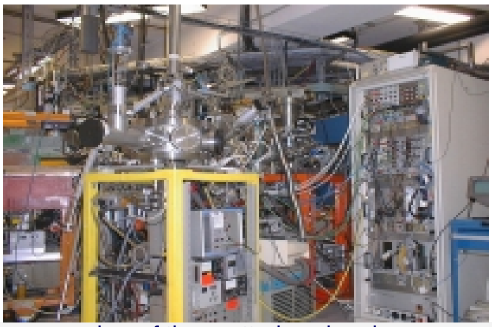
RBS - Setup

Scattering chamber for heavy-ion RBS:



view of the scattering chamber
(enlarged picture (203 kB))

Parameters:

Sample dimensions:	1 cm x 1 cm
Sample lock:	7 samples per ladder
Scatter angle:	$\theta = 165°$
Distance between detector and sample:	d = 10 cm
Detector opening:	$\Delta\theta = \pm 1.2°$
Solid angle (4 detectors):	$\Delta\Omega = 22.2$ msr
Typical ion beam:	15 MeV $^{14}N^{4+}$, about 5 TnA
Measurement time:	10 - 100 min
Sensitivity:	ppm for heaviest elements in light samples down to 0.1% for light elements
Depth resolution:	about 10 nm close to the surface, decreasing with depth
Maximum depth:	about 2 µm, depending on the material

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Selected Publications: Defects in Semiconductors

The Behaviour of ^{12}B in CdTe Studied with ß-NMR Techniques
Oldekop, E.; Eyert, V.; Niedermeyer, F.; Wienecke, M.; Zeitz, W.-D.
Mat. Sci. Forum Vols. 248-249 (1997) 267

Pd-defect-complexes in ZnTe and CdTe and interaction with group-V-elements
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