

Diploma Thesis

Kelvin probe force microscopy analysis of microfabricated ion traps

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Diplomarbeit

Kelvin Sonden Mikroskopie Analyse von mikrofabrizierten Ionenfallen

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Kurzfassung

Oberflächenbedingtes Rauschen ist nach wie vor ein Hindernis für skalierbares Quantencomputing mit Ionenfallen. Motiviert durch die immer noch unklaren Ursachen des Rauschens wird in dieser Arbeit eine Analyse der Oberflächeneigenschaften von industriell gefertigten Ionenfallen mittels Kelvin Probe Force Microscopy (KPFM) vorgestellt. Dabei KPFM wird als ortsaufgelöste Methode eingesetzt, um die Potenzialverteilung auf Aluminium- und Siliziumdioxidoberflächen zu untersuchen. Auf den Aluminiumoberflächen werden verschiedene statische Unregelmäßigkeiten im Potenzial beobachtet, darunter erwartete Merkmale wie Korngrenzen. Interessanterweise werden unerwartet große Abweichungen von bis zu 790 mV entdeckt, deren Ursachen jedoch nicht klar sind. Um die Auswirkungen dieser Potenzialabweichungen besser zu verstehen, werden Simulationen des statischen elektrischen Feldes anhand von Daten aus KPFM-Messungen durchgeführt, die mögliche Auswirkungen auf eingeschlossene Ionen aufzeigen. Außerdem werden Laserexperimente an einer Aluminiumelektrode beschrieben, bei denen während der KPFM-Messungen abwechselnd mit einem 405-nm-Laser beleuchtet und abgedunkelt wird. Diese Experimente ergaben jedoch keine signifikanten Ergebnisse. Zusätzlich zu den Untersuchungen an Metalloberflächen zeigt die Studie, dass mit dem verwendeten Versuchsaufbau eine Auflösung im Nanometerbereich auf einer Siliziumdioxidoberfläche erreicht werden kann. Das für diese Experimente verwendete Instrument ist ein Park NX20 Rasterkraftmikroskop (AFM), das bei Raumtemperatur in einer Luftumgebung betrieben wird.



Abstract

Surface related noise still remains an obstacle for scalable quantum computing with ion traps. Motivated by the still unclear origins of the noise this thesis presents an analysis of the surface properties of industrially fabricated ion traps using Kelvin Probe Force Microscopy (KPFM). KPFM is employed as a spatially resolved method to assess the potential distribution across aluminium and silica surfaces. Various static irregularities in the potential are observed on the aluminium surfaces, including anticipated features such as grain boundaries. Interestingly, unexpectedly large deviations of up to 790 mV are discovered, the underlying causes of them remain elusive. To further understand the impact of these potential deviations, simulations on the static electrical field are conducted using data obtained from KPFM measurements, revealing potential implications on trapped ions. Furthermore, laser experiments on an aluminium electrode are described, involving alternate illumination and darkening with a 405 nm laser during KPFM measurements. However, no significant results are obtained from these experiments. In addition to the investigations on metal surfaces, the study demonstrates that the experimental setup employed can achieve nanometer-scale resolution on a silica surface. The instrument utilized for these experiments is a Park NX20 Atomic Force Microscope (AFM), operated at room temperature in an air environment.

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Chapter 1 Introduction

The invention of ion trapping by Wolfgang Paul more than 50 years ago settled stage for experiments with confined atomic and molecular ions. Today, the trapping and cooling of ions to the motional ground state is a well-known routine [1]. One application of trapped and cooled ions is in the field of quantum computing. The original trap design was developed by Wolfgang Paul [2] and is called the Paul trap. This type of trap uses an RF oscillating voltage an static DC fields to create a three-dimensional potential minimum. This allows ions to be confined to a specific area [3]. Figure 1.1 shows a schematic cross section of a planar Paul trap [4].



inner DC loading slot inner DC

Fig. 1.1: Schematic cross section of a quadrupole surface Paul trap. The rectangular shapes in red and blue represent a cut of the RF and DC electrodes, respectively. When the RF voltage is positive, the curved arrows illustrate the direction of the electric field for a positive voltage [4]. (Figure taken from [4])

For the use in quantum computing these traps are operated in cryogenic environment (<20 K) and under ultra high vacuum ($\approx 10^{-11}$ mbar). This setup provides a very good isolation of the ions from their environment. Two states of an ion trapped in this way form a qubit. Trapped-ion qubits use the internal electronic states of the ion as the 0 and 1 qubit states. There are four types of trapped-ion qubits: hyperfine qubits, Zeeman qubits, fine structure qubits and optical qubits. Hyperfine qubits use hyperfine states of the ion with gigahertz energy splitting as the qubit states, while Zeeman qubits use magnetic sub-levels separated by an applied field with frequencies typically in the tens of megahertz range. Fine structure qubits use qubit states in the finestructure levels with separations typically in the tens of terahertz range, and optical qubits use qubit states are prepared by optical pumping. The individual operations of the qubits are performed by either optical or microwave addressing and the information is read by fluorescence detection [6].

Fig. 1.2 is a schematic representation of the preparation, control and readout of optical qubits. Panel (a) shows the preparation of state $|1\rangle$. To reach this state, the long-lived state $|0\rangle$ is



Fig. 1.2: Schematic preparation, control and readout of optical qubits. (a) preparation of state $|1\rangle$; the long-lived state $|0\rangle$ is coupled to a short-lived state $|e\rangle_{\rm SP}$. (b) qubit control; $|0\rangle$ is directly coupled to state $|1\rangle$ via a quadrupole transition. (c) readout process; the ion is irradiated with light to allow the transition $|1\rangle \rightarrow |e\rangle_{\rm R}$ and lead to fluorescence, which can be detected. If the state is $|0\rangle$, there is no transition [5]. (Figure taken from [5])

coupled to a short-lived state $|e\rangle_{\rm SP}$. The qubit control is displayed in (b), where state $|0\rangle$ is directly coupled to state $|1\rangle$ via a quadrupole transition. The readout process is shown in panel (c). Here the ion is irradiated with light of suitable wavelength that allow only the transition $|1\rangle \rightarrow |e\rangle_{\rm R}$ through emission of a photon, which can be detected. If the state is $|0\rangle$, there is no transition and therefore no fluorescence [5].

The potential use of ion traps for scaleable quantum computing and the associated desire for miniaturisation and scaling has led to rapid advances in the field of ion trapping. Planar microtraps, where fabrication is based on existing chip technology, made it possible to reduce the size of the trap from several centimeters to few millimeters [7, 8] and the distance of the ion from the surface from several hundred μ m to distances less 50 μ m [7, 9]. However, reducing the height of the ion above the surface also means that it is more susceptible to perturbations caused by fluctuating voltages at the electrodes. Such voltage fluctuations lead to higher heating rates of the ion, which is a problem for the use of ion traps in quantum computing [10].

These fluctuations in the potential at the surface of the electrodes have been associated in numerous studies with surface irregularities like adsorbate coverage and surface corrugation [11–14]. A distinction can be made between so-called "stray fields" and "surface electric field noise": (1) Stray fields are defined as phenomena that lead to the formation of a static electric field emanating from the surface. This static field is superimposed to the field that is used to trap the ions, affecting the position of the ion in the potential well [15]. (2) Surface electric field noise, however, is the variation in an electric field caused by the movement of charges on the surface of the trap. Ions are confined in harmonic potentials of the trap but resonances of the electric field noise with the motional modes of the trap can lead to ion heating and motional decoherence, both of which can be detrimental to applications of trapped ions [13]. More details on stray fields and fluctuating potentials are presented in the sections 2.1.1 and 2.1.2. Both types of noise, their origin as well as strategies in fabrication to prevent them, are of great interest to the ion-trap community, especially in relation to metal surfaces, which are used as electrodes to define the electric fields in an ion trap and are thus in close proximity to the trapped ions.

It is therefore necessary to understand these types of noise in order to be able to produce future generations of high performance chips. To gain direct insight into the processes taking place at the surface, Kelvin probe force microscopy is used in this work as a method of analysis. In this AFM-based method [16], the potential surface of the sample is imaged simultaneously with the topography with a lateral resolutions in the sub-nanometre range. Fig. 1.3 shows a schematic diagram of how KPFM works. A conductive AFM tip is moved across the sample and since measurements can also be made with high temporal resolution, the technique is suitable for investigating both static and dynamic potential deviations on the surface. This allows the direct study of surface processes such as scattering charges leading to scattered fields [16] but it can also be used to study processes such as adsorbate diffusion, which may be a cause of surface electric field noise [17].



Fig. 1.3: a) Schematic of a Kelvin probe force microscopy analysis. An AFM tip made of conductive material is moved over the sample surface. b) The surface potential is determined by the electrical forces acting on the tip, indicated by red arrows in a). The surface potential is independent of the topography [18]. (Figure taken from [18])

While this analysis technique is a common method in surface and interface related research fields, it is not yet a commonly used method in the ion trapping community. Therefore, a measurement setup for room temperature and ambient air measurements was developed and adapted within the scope of this Master's thesis using a commercially available Park NX20 AFM. The aim was to establish Kelvin Probe Force Microscopy as a method of analysis to characterise the quality, roughness and homogeneity of the surface potential of ion traps, thereby optimizing chip fabrication. Before the analysis of ion traps could begin, a suitable measurement setup had to be found. Different tips and contact options were tested. After an initial adjustment, the analysis focused on ion traps with aluminium surfaces. The most promising results were obtained from large area $(25 \times 25) \,\mu\text{m}^2$ scans which provided a basic understanding of the potential landscape. The scans revealed anomalies in the surface potential that were not known to exist on the chip surface. In addition, the influence of certain structures, such as grain boundaries, on the surface potential could be determined. Further details are given in section 3.3.

The chips investigated were manufactured in an industrial clean room using modified MEMS technologies. The chips were produced at 8 inch wafer level. As the chips were manufactured using established semiconductor processes, there should be no significant variations from chip to chip, but all results presented in this thesis are obtained on the same chip (unless otherwise

stated) to improve the traceability of the results. Chip fabrication and investigation was done at the production facilities of Infineon Technologies Austria AG in Villach.

This thesis is structured as follows: Chapter 2 presents the theoretical basis of surface electric field noise and stray fields. The difference between stray fields and surface electric field noise is explained. Possible origins of the different types of noise as well as their effects on the trapped ions are summarised. In the second part of Chapter 2, the concept and working principle of AFM and KPFM is explained. Chapter 3 discusses the experimental setup, the sample and the experimental results obtained in this Master's thesis. First the general setup of the AFM and its technical data are presented. Furthermore, the iontrap model investigated is shown. A series of experiments with large area $(25 \times 25) \,\mu\text{m}^2$ images of aluminium electrodes are presented. The results of these experiments, such as potential deviations and grain boundary effects, are discussed. A simulation is shown extrapolating the surface potential to different heights above the trap to investigate the impact on the trapped ions. Finally, the effects of direct laser irradiation on the sample surface was investigated and is summarized here. The thesis concludes with a summary of the main results and an outlook on possible future experiments that could be realised using Kelvin Probe Force Microscopy.

Chapter 2 Fundamentals

2.1 Surface related problems in ion traps

The assumption often made in electrostatics is that metal electrodes have an equipotential surface. This is an idealisation that applies to many applications, but this simplification cannot be made for surface sensitive applications and processes that take place in the close vicinity of the surface. Ion-trap technology falls into this category of surface sensitive applications, as the confinement of the ion by electric fields is sensitive to potential inhomogeneities [10]. Due to the high surface sensitivity, various types of perturbation mechanisms with different origins but also different impacts on the trapped ion exist. A distinction is made between perturbations due to static potential changes and perturbations due to fluctuating potentials. The majority of the literature uses, when discussing noise related to static potentials, the term "stray fields" . In the context of fluctuating potential the term "surface electric field noise" (SEFN) is used [15].

2.1.1 Stray fields

If a static field E_{DC} is added to the electric field used to trap the ion, the position of the trapped ion changes. In its original position, the ion, assuming its micromotion was properly compensated, was in the position called "RF null" and thus felt no forces caused by the AC field. Due to the change in position caused by E_{DC} , the ion is no longer at the RF null and therefore experiences forces induced by the AC field. This results in the so called excess micromotion. However, even in the RF null the ion is not completely motionless. The motion at the RF null is called "secular motion" and can be reduced by cooling. Micromotion however cannot be significantly reduced by cooling [15].

This excess micromotion has a negative effect on optical manipulation processes like Doppler cooling, fluorescence collection. When several ions are lined up in a chain, excessive micromotion leads to changes in the spacing and reduces the stability of the entire chain. Because of these problems, it is necessary to understand the origins of excessive micromotion and how best to avoid it [19]. The static electric fields which deflect an ion from its proper position can come from a variety of sources. For example, the electrodes of the trap can get covered with an inhomogeneous layer of calcium, coming form furnace that emits calcium that later on gets ionized, which leads to a contact potential. There is also the possibility of stray charges present on such a Ca contamination layer (when oxidized) or the exposed dielectrics of the trap. Possible sources of implanted free charges are photoelectrons or electrons resulting from the ionisation of atomic flux when loading the trap. In addition to these effects, the surface of the trap itself can be a source of potential variations. Grains of different orientation can show potential variations in the range of 100 mV [15].

All of these sources of static potential changes have in common that they alter the work function of the electrode. Since Kelvin Probe Force Microscopy investigates the work function of a surface with spatial resolution, this method of analysis is suitable to investigate the causes of excessive micromotion in more detail. For example, KPFM analysis could be used to spatially visualise calcium contamination and determine the magnitude of the contact potential. The same applies to the visualisation of stray charges and different grain orientations. The knowledge gained by KPFM can then be used to modify the surfaces, and optimize post fabrication treatment to avoid these problems.

2.1.2 Surface electric field noise

The variation of an electric field caused by the movement of charges on the surface of a material is referred to as surface electric field noise (SEFN). The ion trapping community is particularly interested in noise arising from metal surfaces because these metal surfaces, which are used to apply the electric fields of an ion trap, are closest to the ions [13]. This noise generally has a large bandwidth ($\approx 100 \,\mathrm{kHz}$ -50 MHz) and frequencies resonant to the motional modes of the trap (0.1-10 MHz) can couple to the ion. As a result, the motional modes gain energy. This heating of the ions poses a problem for quantum information processes because the absorption of a phonon during a quantum gate operation reduces the fidelity of the computation [20]. The microscopic processes involved in the generation of surface electric field noise (SEFN) are still the subject of current research. However, the way in which the spectral density of the noise behaves with respect to the ion-electrode distance, the electrode temperature, the frequency, the adsorbate coverage and surface properties, and the electrode material suggests that this type of noise is due to processes at the surface [11]. Time dependent fluctuations (dynamic variations) of the surface potential can possibly be monitored by the use of KPFM. Yet there is no guarantee that this technique will help solve any problems related to SEFN, but it may help to better understand the mechanisms of SEFN. In the following chapters an overview of the current understanding of the origins SEFN is given. Here the approach of Brownutt et al. [10] is closely followed.

The below described origins of noise could eventually be studied in the future using KPFM. The fluctuations in the electric field have a large bandwidth, but for the trapped ions only fluctuations in the MHz range are of interest since they are able to disturb the ion [10]. Special KPFM measurement techniques can achieve extremely high temporal resolutions, suitable to study the fluctuations of the potentials. As already shown by Schumacher et al., a pump-probe approach can achieve a time resolution in the picosecond range [21]. Additionally and in contrast to in situ experiments with ions, KPFM investigates directly the surface of the ion trap but without the experimental effort that is necessary to actually trap ions. Thus, Kelvin Probe Force Microscopy is a technique that does not require extensive preparation and setup. Depending on the test design, only the desired surface parameters need to be met. The sample is then examined in a non-contact and non-destructive manner. As KPFM displays the surface potential spatially resolved, it is possible to investigate various surface influences quickly and easily. This could help to identify possible sources that contribute to the formation of SEFN. In addition, the rapid application of this AFM technique means that it can also be used to screen newly produced samples, which makes it suitable as a tool for post-production quality control.

In more specific experiments, adsorbates and their dynamics could be monitored. The study of adsorbates on different surfaces using KPFM has already been demonstrated [22–26] ;both the electrical behaviour of single adsorbed atoms [22] and the binding behaviour of complex molecules have been studied [24]. With high time resolution as already realised by Schumacher et al. [21], not only can adsorbates and their influence be represented in spatial resolution, but their possible movements on the surface can also be observed. In combination with other analytical techniques such as Auger microscopy, which can be used to quantitatively and qualitatively determine surface contamination, it would be possible to determine the influence of individual contaminants. It may also be possible to identify surface properties that enhance or attenuate certain behaviour of adsorbates, as suggested by Berlin-Udi et al. [13].

2.1.2.1 Calculation of heating rates

To quantify the noise in an ion trap, the so-called heating rate Γ_h is usually measured. The heating rate Γ_h can be approximated by

$$\Gamma_{\rm h} \simeq \frac{e^2}{4m_{\rm I}\hbar\omega_{\rm t}} S_{\rm E}(\omega_{\rm t}) \tag{2.1}$$

where $S_{\rm E}$ is the spectral density of the electric field fluctuations, $m_{\rm I}$ is the mass of the trapped ion, $\omega_{\rm t}$ is the trap frequency, e is the elementary charge and \hbar is the reduced Planck constant [10]. The spectral density $S_{\rm E}$ is further discussed and approximated in the following sections.

Current research has led to the emergence of several models to describe SEFN. A rough distinction can be made between models that describe noise without attributing it to a specific physical origin and models that describe noise originating from microscopic processes at the surface. Noise without any specific origin is described by fluctuating potentials and two-level fluctuators (TLF). Microscopic processes include fluctuating dipoles and adatom diffusion [10].

2.1.2.2 Patch potentials

A patch potential is generally understood as a spatial variation in the electrostatic potential of an electrode with an otherwise homogeneous potential. There are several reasons for such a variation in potential, most commonly variations in crystallographic orientation or surface adsorbates are responsible for the local change [27, 28].

Assuming a clean and regularly arranged metal surface, the properties of the surface change significantly in relation to the bulk. The homogeneous distribution of electrons in the bulk is disturbed at the surface and a dipole is formed at the metal-vacuum interface. The work function of the surface, ϕ , locally changes by

$$\Delta \phi = e \Phi_{\rm p} \tag{2.2}$$

where e is the elementary charge and $\Phi_{\rm p}$ is the patch potential. $\Phi_{\rm p}$ is given by

$$\Phi_{\rm p} = \frac{P}{\epsilon_0},\tag{2.3}$$

where P is the dipole moment per unit area. Due to the change in the work function $\Delta \phi$, small areas of deviating crystal orientation lead to local changes of $\Phi_{\rm p}$ on microscopic scale. Adsorbed atoms or molecules have a similar effect, becoming polarised as they approach the surface and thus forming an additional dipole layer [10].

Fig. 2.1 is a schematic representation of such a hypothetical surface. Here, an ion is trapped at a distance d above the electrode of dimension $R_{\rm el}$. It is assumed that the electrode represents an equipotential surface with a potential Φ_0 . This equipotential surface is interrupted by a surface imperfection where the potential is changed by $\Phi_{\rm p}$. The origin of the change does not matter here, it is simply assumed that the fluctuations of the potential are correlated over a distance of $r_{\rm c} \approx R_{\rm P}$ where $R_{\rm P}$ is the characteristic patch radius.

Assuming that there is no other free charge on the surface and that the potential difference $\Phi_{\rm P}(\mathbf{r}, t)$ exists only within a very thin layer compared to the distance d of the ion to the surface, the electrostatic potential at the position of the ion $\Phi_{\rm P}(\mathbf{r}_I, t)$ is given by eq. 2.4. It is a solution of



Fig. 2.1: Schematic of the patch potential model. Here, $R_{\rm el}$ denotes the characteristic dimension of the electrode, d the distance of the trapped ion from the electrode, $R_{\rm pl}$ the patch radius and $\Phi_{\rm p}(\mathbf{r}, t)$ fluctuations in the local potential. (Figure taken from Ref. [10].)

the Laplace equation with the boundary condition $\Phi_0 + \Phi_p(\mathbf{r}, t)$ on the surfaces. Setting $\Phi_0 = 0$ for simplicity results in

$$\Phi(\mathbf{r}_{\mathrm{I}},t) = -\int_{S} d^{2}r \frac{\partial G_{\mathrm{E}}(\mathbf{r}_{\mathrm{I}},\mathbf{r})}{\partial \mathbf{n}_{\mathrm{s}}} \Phi_{\mathrm{p}}(\mathbf{r},t).$$
(2.4)

Here $G_{\rm E}(\mathbf{r}_{\rm I}, \mathbf{r})$ is the electrostatic Green's function which satisfies the Dirichlet boundary condition $G_{\rm E}(\mathbf{r}_{\rm I}, \mathbf{r}) = 0$ for $\mathbf{r} \in S$, and $\mathbf{n}_{\rm s}$ is a unit vector normal to the surface. The electric field projected on the trap axis $\mathbf{e}_{\rm t}$ is given by Eq. 2.5.

$$E_{\rm t}(t) = -\mathbf{e}_{\rm t} \cdot \nabla \Phi(\mathbf{r}_{\rm I}, t) \tag{2.5}$$

The resulting spectrum of electric field is given by Eq. 2.6.

$$S_{\rm E}^{\rm PP} = \int_{\rm S} d^2 r_1 \int_{\rm S} d^2 r_2 \zeta(\mathbf{r}_{\rm I}, \mathbf{r}_1) \zeta(\mathbf{r}_{\rm I}, \mathbf{r}_2) C_{\rm V}(\mathbf{r}_1, \mathbf{r}_2, \omega), \qquad (2.6)$$

where $\zeta(\mathbf{r}_1, \mathbf{r})$ is a geometric factor indicating the electric field at the position of the ion created by a small patch at location \mathbf{r} on the electrode. The correlation function $C_V(\mathbf{r}_1, \mathbf{r}_2, \omega)$ of the fluctuating patches at points \mathbf{r}_1 and \mathbf{r}_2 contains the information about temporal and spatial correlations [10].

2.1.2.3 Two-level fluctuators

Two-level fluctuators (TLFs) are a special form of patch potentials. Lattice defects or surface irregularities cause local minima in the potential landscape. In a system with a high degree of disorder, such as amorphous materials, this can lead to the formation of TLFs when electrons, atoms or molecules are localised in two adjacent potential minima. Such a situation is shown schematically in Fig. 2.2(a). as point-like dipoles $\mu(\mathbf{r}_i, t)$ in a thin layer on a metal electrode. Such an arrangement can be used to describe the noise of an electric field generated by TLFs. Fig. 2.2(b) shows two adjacent potential wells as found in a two-state system where Δ is the classical energy difference between the two wells. Spontaneous transitions from one minimum to the next cause local fluctuations in the surface potential. The transition from one minimum to the other can occur either by tunneling through the barrier or by thermal activation across the



Fig. 2.2: Two-level fluctuators a) point-like dipoles $\mu(\mathbf{r}_i, t)$ in a thin layer on a metal electrode; b) two adjacent potential wells as found in a two-state system with the classical energy difference between the two wells Δ , the tunnel coupling Δ_0 and the depth of the potential well $V_{\rm b}$ [10]. (Figure taken from Ref. [10].)

barrier. In ion traps a possible source for TLFs are thin insulating layers covering the surface of the electrodes [29].

Since an ion trapped over a metal electrode is efficiently shielded from charge fluctuations within the electrode and the charges on the surface are compensated by their mirror charges, it can be assumed that the main microscopic noise processes on the electrode are sufficiently characterised by a collection of point-like dipoles $\mu(\mathbf{r}_i, t)$ [10]. These dipoles are located at positions \mathbf{r}_i within a thin surface layer where the layer thickness h is much smaller than the height of the ion above the surface d (see Fig 2.2). For a planar electrode and a homogeneous distribution of dipoles, the fluctuation of the electric field parallel and orthogonal to the surface can be given by equations 2.7 and 2.8.

$$S_{\rm E,\perp}^{\rm (TLF)} = \frac{3\pi}{2} \frac{\sigma_{\rm d}}{(4\pi\epsilon_0)^2 d^4} \bar{S}_{\mu}$$
(2.7)

$$S_{\mathrm{E},\parallel}^{(\mathrm{TLF})} = \frac{S_{\mathrm{E},\perp}^{(\mathrm{TLF})}}{2}$$
(2.8)

 $\sigma_{\rm d}$ is the surface density of the dipoles and \bar{S}_{μ} is the average dipole-fluctuation spectrum with a large number of fluctuators within a fixed range where $A \ll \pi d^2$ applies [10]. As shown in the previous sections, fluctuating potentials and TLFs lead to SEFN. These, in turn, lead to increased heating rates as shown in Eq. 2.1. There are already numerous studies on both models, including very elaborate in situ experiments [11, 13, 30, 31]. Such in situ experiments usually test the influence of different surfaces on the trapped ion. On the one hand, there is always the problem that the preparation of such an experiment is very time consuming and therefore different parameters can only be varied slowly. On the other hand, such experiments provide an understanding which surface parameters affect the ion, but do not allow direct conclusions to be drawn about the processes taking place on the surface since they provide no spatial information. This makes it difficult to identify the real causes of SEFN. In addition to in situ experiments, it is also possible to investigate various influences using simulations [12, 32, 33]. However, the accuracy of simulations is limited because the relevant surfaces are to complex to be modeled accurately. Furthermore, simulations, like in situ experiments, can never identify the fundamental origin of SEFN.

2.1.2.4 Adatoms

Even under the optimal conditions of a very regular surface and ultra high vacuum adsorption of molecules and atoms occurs on the electrode surface. This results in the formation of a variety of defects from local contaminations or impurities to full layers of adsorbate. The particles that are originally in the atmosphere surrounding the ion trap are attracted to the surface of the trap by the van der Waals potential.

$$U_{\rm vdW}(z) \propto -\frac{C_3}{z^3} \tag{2.9}$$

Here z is the distance to the surface and C_3 is a function of the dynamic polarisability $\alpha_{p(\omega)}$ of a the particle. At small distances, the wave functions of the adsorbed atoms and the surface atoms involved begin to overlap and repulsion occurs. The resulting distance-dependent potential curve containing both Pauli repulsion and van da Waals attraction is shown in Fig. 2.3. The depth of



Fig. 2.3: Schematic display of the distance dependent adatom surface potential U(z) with $|n\rangle$ oscillation states with frequencies ν_n . The dashed lines indicate the energy levels $\hbar\nu$ of different vibrational states. The solid lines show the wave function and the characteristic frequency is given by the difference between the two lowest frequencies $\nu_{10} = \nu_1 - \nu_0$ [10]. (Figure taken from Ref. [10].)

the potential can range from a few meV to single digit eV.

The dipole moment μ_z generated by the adsorption is oriented perpendicular to the surface and depends on the distance of the adatom from the surface. If the distance is large compared to the wave function of the adatom, scaling of $\mu_z \propto \frac{1}{z^4}$ is expected. If the adatom and the surface are in contact, i.e., $\mu(z \approx z_0)$, the dipole moment can become several Debye large. From the diagram in Fig. 2.3 it can be seen that the potential U(z) allows several oscillation states $|n\rangle$ with frequencies ν_n . Due to the dependence of μ_z on the distance of the adatom from the surface, each oscillation state has a different average dipole moment $\mu_n = \langle n \mid \mu(z) \mid n \rangle$. Phonon-induced transitions between the different vibrational states and thus a fluctuation of the dipole moment μ_t are assumed to occur at temperatures above 0 K. For low temperatures the dipole fluctuation spectrum of the individual atoms S_{μ} can then be estimated using 2.10.

$$S_{\mu} \simeq (\mu_{n=0} - \mu_{n=1})^2 \frac{2\Gamma_0}{\omega^2 + \Gamma_0^2} e^{-\frac{\hbar\nu_{10}}{k_B T}}$$
(2.10)

Where Γ_0 is the decay rate at 0 K from the first excited state to the ground state, and ω is the trapping frequency. Eq. 2.7 is then used to calculate the spectral density of the electric field noise for planar electrodes. A homogeneous and independent distribution of adatoms is assumed and \bar{S}_{μ} is replaced by S_{μ} [10].

2.1.2.5 Adatom diffusion

Besides the noise caused by fluctuations in the induced dipole moment μ_t , adsorbed atoms and molecules can add to the noise of the electric field through their diffusion on the surface. The hypothesis here is that the change in the spatial arrangement of the dipoles over time contributes to the heating of the trapped ions.

The movement of individual atoms on a smooth surface can be described as a two-dimensional diffusion process with the diffusion constant

$$D = \frac{a_{\rm L}^2 \Gamma_{\rm hop}}{l},\tag{2.11}$$

where $a_{\rm L}$ corresponds to the lattice constant, $\Gamma_{\rm hop}$ is the hopping rate between adjacent adsorption sites separated by an energy barrier $V_{\rm b}$, and l is the coordination number determined by the lattice geometry. Adatoms can move either thermally activated $\Gamma_{\rm hop} \approx \tau_0^{-1} e^{(-V_{\rm b}/k_{\rm B}T)}$ or by quantum tunneling between adjacent minima of the surface potential. In the calculation of $\Gamma_{\rm hop}$ for the thermally activated process, τ^{-1} represents the frequency at which a change from one potential to the next is attempted. The resulting diffusion constant can be estimated by

$$D \simeq D_{\rm t} + D_0 e^{-V_{\rm b}/k_{\rm B}T}.$$
 (2.12)

Here the first term represents diffusion due to tunneling processes and the second term represents thermally activated diffusion. For most surface diffusion processes, D_0 is in the range of $10^{-7} \text{m}^2 \text{s}^{-1}$. This corresponds approximately to a τ_0 of $10^{12} - 10^{13} \text{s}^{-1}$ and a lattice spacing of a few Å. Assuming a typical barrier height of $V_{\rm b} = 150 \text{ meV}$ and a temperature range of 100 - 400 K, the result is $D = 10^{-15} - 10^{-9} \text{m}^2 \text{s}^{-1}$. At temperatures below several Kelvin, there is a plateau of $D \approx D_{\rm t}$ because thermally activated transitions are of course greatly suppressed at these very low temperatures.

As a model for the diffusing atoms, the surface polarisation density (Eq. 2.13) is now used.

$$P(\mathbf{r},t) = \mu \sigma_{\rm d}(\mathbf{r},t) \tag{2.13}$$

Here, $\sigma_{\rm d}(\mathbf{r}, t)$ is the surface density of the adatoms and μ is the dipole moment of the adatoms, which is assumed to be contant. A situation as shown in Fig. 2.4 is assumed. A small section of an electrode $A_{\rm el}$ with radius $R_{\rm el}$ and adatom occupation density $\sigma(\mathbf{r}, t)$ at position \mathbf{r} is shown.



Fig. 2.4: Configuration to assess the electric-field disturbance produced by the diffusion of dipoles on a flat electrode. A small section of an electrode $A_{\rm el}$ with radius $R_{\rm el}$ and adatom occupation density $\sigma(r, t)$ at position **r** is considered [10]. (Figure taken from Ref. [10].)

Such a setup is used to determine the possible influence of diffusing adatoms on the ion. The electric field noise spectrum resulting from such a setup is given by equation 2.14,

$$S_{\rm E}^{\rm AD} = \frac{\mu^2}{8\pi^2\epsilon_0^2} \int_{\rm S} d^2 r_1 \int_{\rm S} d^2 r_2 g_{\rm D}(\mathbf{r}_1) g_{\rm D}(\mathbf{r}_2) C_{\sigma}(\mathbf{r}_1, \mathbf{r}_2, \omega), \qquad (2.14)$$

where the $g_{\rm D}(\mathbf{r})$ are geometric factors describing the arrangement of the dipoles orthogonal or parallel to the electrode and C_{σ} is the correlation spectrum of the density fluctuation. If the adsorbate density at the surface is low, the diffusion of the individual dipoles can be assumed to be independent of each other [10].

2.2 Introduction to Kelvin Probe Force Microscopy

Due to the numerous uncertainties associated with surface processes in ion traps, analytical techniques that contribute to a better understanding of the surface processes are an important tool for the continuous improvement of the traps. In addition to existing analytical techniques such as SEM or TEM, which only allow topographical analysis of the surface, methods that provide insight about the static and dynamic electronic properties and behaviour of the surface are of key importance. Kelvin Probe Force Microscopy, KPFM for short, is an analysis technique derived from Atomic Force Microscopy (AFM) that measures the local contact potential difference between sample and tip. This allows the work function of the underlying sample to be determined with high spatial resolution [16]. The work function in solid state physics is defined as the minimum amount of energy required to move an electron from a solid to a point just outside the surface of the solid in vacuum. The final position of the electron is thereby far from the surface on the atomic scale, but still close enough to the solid to not be affected by electric fields in the surrounding vacuum. It is important to note that the work function is not a property of the bulk of a material, but rather a property of its surface. The work function depends on the crystallographic orientation of the surface (i.e., the arrangement and packing density of the atoms) and the chemical composition. Thus the work function is also sensitive to surface contaminations [34]. The work function of a surface is defined by

$$\phi = -e\phi_{\rm vac} - E_{\rm F,} \tag{2.15}$$

where ϕ_{vac} is the electrostatic potential of the vacuum (vacuum level) and E_{F} is the fermi energy. The work function is typically measured in electron volts (eV) and is in the range of 2-6 eV for metal surfaces. To understand the concept of the work function, it is easiest to consider a metal sample with a band diagram as shown in Fig. 2.5. The work function is the energy required to



Fig. 2.5: Schematic depiction of the work function of a metal.

remove an electron from the highest occupied Fermi level $(E_{\rm F})$ to a point outside the material, the vacuum level. At the vacuum level the electron has no kinetic energy. In the diagram, the work function is given by the difference between the Fermi level and the vacuum level. Prior to the introduction of the KPFM in 1991 by Nonnenmacher et al. [35], there was only one technique capable of measuring the work function spatially resolved, the so-called Kelvin method, in which two macroscopic capacitors are brought into close proximity [36].

Now days Kelvin Probe Force Microscopy is an established technique for the analysis of electronic surface properties. It has been widely applied in various fields due to its ability to directly and quantitatively measure the spacial surface potential distribution. In materials science, this technique is applied to the mapping of work functions [35], ordering measurements in III-V compound semiconductors [37], local surface and surface photovoltage spectroscopies [38], detection of surface states and defects under different environmental conditions [39], domain characterization in ferroelectric materials [40], measurements of organic and self-assembled films [41], and much more. KPFM is also a key tool for potential mapping of both passive and active semiconductor devices, including p-n junctions [42], resistors and n-i-p-i heterostructures [43], HEMTs [44, 45], LEDs [46, 47], solar cells [48, 49], and organic, polymer transistors [50, 51] and even characterising transparent conductors in microfabricated ion traps [52]. As the work function of a surface allows conclusions to be drawn about the chemical and physical properties of a surface, KPFM can be used to gain a deeper understanding of precisely these chemical and physical processes [16]. This, in particular, makes it an interesting tool in tackling the various surface bound problems found in ion traps.

2.2.1 Atomic force microscopy (AFM)

In the broadest sense, an AFM consists of a precisely defined tip located at the end of a cantilever that acts as a force sensor with a well defined spring constant. By scanning the surface while keeping the force acting on the tip constant, the topography of the sample can be measured. When using the AFM, a distinction can be made between different modes. (1) In contact mode (CM, Fig. 2.6) the tip is brought into direct contact with the sample surface and the topography is measured by the repulsive forces acting on the tip. (2) In non-contact mode (NCM, Fig. 2.6), the tip is oscillating, for example driven by a piezoelectric component. The excited oscillation frequency of the cantilever is either close to the resonance frequency (amplitude modulation, the change in oscillation amplitude is tracked at a constant oscillation frequency) or directly the resonance frequency (frequency modulation: the change in resonance frequency is detected; in addition the amplitude is kept constant). Changes in the topography lead to changing forces acting on the tip and thus to a shift of the cantilevers resonant frequency. This frequency shift is now used to keep the tip at a constant distance to the sample. Therefore a feedback loop monitors the frequency shift, and tries to minimise or keep it constant by adjusting the height of the tip. The change in resonance frequency, is measured using a laser aimed at the backside of the cantilever and a photodiode or a phase locked loop.

Figure 2.7 illustrates the basic operating principle of an AFM. The stage is movable in x-, yand z-direction. Also shown is the cantilever with tip and readout device consisting of laser and photodiode. The forces acting on the tip are visualized by arrows.

The forces acting on the tip in close proximity of the surface are of different origins. A distinction can be made between short-range repulsive and chemical bonding forces, van der Waals forces and long-range magnetic and electrostatic forces. The distance-dependent interaction of the tip with the short-range forces is described by the Lennard-Jones potential (Eq. 2.16), where σ_0 is the characteristic length, r the distance, and ϵ the depth of the potential well.

$$U_{\rm LJ} = -4\epsilon \left[\left(\frac{\sigma_0}{r}\right)^6 - \left(\frac{\sigma_0}{r}\right)^{12} \right]$$
(2.16)



Fig. 2.6: Simplified force-distance curve as measured with AFM. The noncontact (attractive) region of the scanning regime is highlighted. A defelction distance curve has a comparable shape and acts as raw data form which the force-distance curve can be measured. The bending of the probe in each regime is depicted on the right side [53].(Figure taken from Ref. [53].)

The term proportional to $-\frac{1}{r^6}$ approximates the long-range attractive interactions (London forces), while the Pauli repulsion at short distances is described by the term $\frac{1}{r^{12}}$. The force-distance curve plotted in Fig. 2.6 shows at small tip-sample distances an initial sharp drop due to pauli repulsion in the interaction potential. As the distance is further increased, attracting interactions take over, leading to the minimum in the potential, the interaction potential slowly increases again and asymptotically approaches zero. The force distance curve is caused by an interplay of attractive and repulsive forces, which have different effects depending on the distance [54].

In order to obtain topography and surface potential data in KPFM mode at the same time, the measurements are conducted in NC mode. Here, the tip oscillates close to its resonance frequency. The ability to reduce tip-sample forces and maintain a high sensitivity to sample topography is a significant advantage of the NC-modes of AFM. Therefore, the tip must be sufficiently close to the sample surface without snaping into contact or entering the repulsive regime. Non-contact AFM uses the attractive regime shown in Figure 2.6. If the tip approaches the surface, the oscillation is damped due to the forces acting on the tip. The change in amplitude and phase of the oscillation are due to the change of the cantilevers resonance frequency. The resonance frequency of the freely oscillating cantilever, ω_0 , is given by Eq. 2.17 where c is a function of the cantilever mass and k is the spring constant.

$$\omega_0 = c\sqrt{k} \tag{2.17}$$

When an additional force F is applied to the cantilever, the resonant frequency ω_0 changes and the changed resonant frequency ω_1 is given by Eq. 2.18. Here, F' represents the derivative of the force perpendicular to the surface.

$$\omega_1 = c\sqrt{k - F'} \tag{2.18}$$

In the feedback circuit, either the change in the amplitude or the change in the phase (which is actually caused by the shift in frequency) can be employed to maintain the position of the tip at



Fig. 2.7: Schematic of the key components of an AFM consisting of: a sharp tip mounted on a cantilever to scan the surface of a sample; the sample stage, a platform on which the sample is fixed in place during imaging; the laser and detector to measure deflections. As the tip moves across the surface, it measures the interaction between the tip and the sample caused by the forces $F_{\rm ts}$. The deflection of the cantilever can then be used to measure the interaction between the tip and the sample [54].(Figure taken from Ref. [54]

a constant distance from the surface of the sample. The change in oscillation of the deflected tip is measured and compared to the original frequency [53].

2.2.2 Kelvin Probe Force Microscopy

The KPFM image is determined by the contact potential difference (CPD) V_{CPD} between tip and sample. The V_{CPD} is defined via the formula 2.19.

$$V_{\rm CPD} = \frac{\phi_{\rm tip} - \phi_{\rm sample}}{e} \tag{2.19}$$

Here, ϕ_{tip} and ϕ_{sample} are the work function of the tip and the sample, respectively. In the following V_{CPD} is abbreviated as CPD. If the distance between sample and tip is sufficiently small, an electrical force will act on the tip due to different Fermi levels. This is illustrated in the schematic band diagrams of a sample-tip system of Fig 2.8. It is assumed that both the tip and the sample are metallic. Fig. 2.8 a) shows the state of the tip and sample at a large distance where only the vacuum levels are aligned. When the tip approaches the sample surface sufficiently for electrons to tunnel, the Fermi levels are equalised. This alignment occurs by the flow of electrons from the energetically higher Fermi level to the lower one, illustrated in Fig. 2.8 b). This leads to a charging of the tip and the sample, which, in turn leads to the build-up of a contact potential difference V_{CPD} between the tip and the sample. The force resulting from V_{CPD} can be balanced by applying an opposite DC voltage V_{DC} , which also cancels the local charging of the surface and the tip (Fig. 2.8 c). The voltage applied to equalise the charge (V_{DC}) corresponds to the difference in the work functions between the sample and the tip and thus to the CPD.



Fig. 2.8: Energy-level alignment of tip and sample with work functions ϕ_t and ϕ_s , respectively. a) Tip and sample are sufficiently separated and without electronic contact. b) Tip and sample are in electronic contact. The Fermi levels align, the difference between the vacuum levels of tip and sample (for $\phi_t \neq \phi_s$ is the contact potential difference (CPD). c) Applying a voltage $V_{\rm DC}$ to compensate the charge between tip and sample [16].(Figure taken from Ref. [16].)

To effectively determine the contact potential difference in KPFM mode, an AC voltage V_{AC} with the frequency ω_{AC} and a DC voltage V_{DC} are applied to the AFM tip. The alternating voltage V_{AC} causes the electrical forces acting on the tip to oscillate. V_{DC} is used to cancel the CPD and thus eliminate the electrical forces acting on the tip. Theoretically, the force acting on the AFM tip is described by

$$F_{\rm es}(z) = -\frac{1}{2}\Delta V^2 \frac{dC(z)}{dz},$$
(2.20)

where ΔV is the potential difference between $V_{\rm DC}$ and the voltage applied to the tip, z is the direction perpendicular to the surface and $\frac{dC(z)}{dz}$ is the gradient of the capacitance between the tip and the sample. Provided that the voltages $V_{\rm AC} \cdot \sin(\omega_{\rm AC} t) + V_{\rm DC}$ are applied to the tip, ΔV can be represented as follows:

$$\Delta V = V_{\rm tip} \pm V_{\rm CPD} = V_{\rm DC} \pm V_{\rm CPD} + V_{AC} \cdot \sin(\omega_{\rm AC} t)$$
(2.21)

The choice of sign depends on whether $V_{\rm DC}$ is applied to the tip (-) or to the sample (+). Combining 2.20 with eq. 2.21 leads to

$$F_{\rm es}(z,t) = -\frac{1}{2} \frac{\partial C(z)}{\partial z} \left[(V_{\rm DC} \pm V_{\rm CPD}) + V_{\rm AC} \cdot \sin(\omega_{\rm AC} t) \right]^2, \qquad (2.22)$$

which in turn can be split into three components [16],.

$$F_{\rm DC} = -\frac{\partial C(z)}{\partial z} \left[\frac{1}{2} (V_{DC} \pm V_{\rm CPD})^2 + \frac{1}{4} V_{\rm AC}^2 \right]$$
(2.23)

$$F_{\omega_{\rm AC}} = \frac{\partial C(z)}{\partial z} (V_{\rm DC} \pm V_{\rm CPD}) + V_{\rm AC} \cdot \sin(\omega_{\rm AC} t)$$
(2.24)

$$F_{2\omega_{\rm AC}} = \frac{\partial C(z)}{\partial z} \frac{1}{4} V_{\rm AC}^2 [\cos(2\omega_{\rm AC}t) - 1]$$
(2.25)

The three individual components represent different interactions of the tip with the sample. $F_{\rm DC}$ leads to a static deflection of the AFM tip and thus mainly contributes to the topographic

signal. $F_{\omega_{\rm AC}}$ is used to calculate the $V_{\rm CPD}$. $F_{2\omega_{\rm AC}}$ is not useful for imaging in KPFM mode, but is used in scanning capacitance microscopy [51]. The application of $V_{\rm AC}$ and the resulting forces acting on the tip result in additional vibrations of the cantilever, which are superimposed on the vibration of the AFM frequency. A lock-in amplifier is used to extract the part of the electrostatic force with the frequency $\omega_{\rm AC}$. $F_{\omega_{\rm AC}}$ is zero for the condition $V_{\rm DC} = V_{\rm CPD}$ and the CPD is directly derived [16].

The atomic forces can be detected either in amplitude-modulated (AM) or frequency-modulated (FM) mode. Frequency modulated mode has become the standard due to the higher lateral resolution that can be achieved [55]. In FM mode, the shift of the frequency, Δf_1 , is the quantity that is to be minimised by the applied voltage $V_{\rm DC}$. The signal obtained is proportional to the gradient of the force

$$\Delta f_1(\omega_{\rm AC}) \propto \frac{\partial F_{\omega_{\rm AC}}}{\partial z} = \frac{\partial^2 C}{\partial z^2} (V_{\rm DC} - V_{\rm CPD}) V_{\rm AC} \cdot \sin(\omega_{\rm AC} t).$$
(2.26)

The choice of ω_{AC} is critical to the quality of the signal. If ω_{AC} is too low, there will be an overlap with the topography signal as the tip will start to oscillate at the frequency ω_{AC} . The higher the frequency, the smaller the overlap between the signals. The frequency demodulator acts as an upper limit, since the limited bandwidth of the demodulator results in a loss of bandwidth as the frequency increases. Fig. 2.9 illustrates the relationship between these two parameters. The



Fig. 2.9: Frequency shift Δf versus piezo voltage V_z , at the frequency of V_{AC} , ω . The plot shows measurements with a silicon tip on a HOPG sample [51].(Figure taken from Ref. [51].)

graph shows the amplitude of Δf_1 and the oscillation of the piezo voltage V_Z , which controls the distance between the tip and the sample, at the frequency of the AC signal ω . It can be seen that V_Z decreases faster than Δf_1 with increasing frequency. This results in a smaller overlap between the topography and the CPD signal. It can also be seen that the signal intensity of Δf_1 also decreases with increasing frequency omega. This is due to the limited bandwidth of the demodulator. In addition to the appropriate setting of ω_{AC} , the choice of V_{AC} is important to achieve sufficient sensitivity in FM mode. Since V_{AC} , as shown in Eq. 2.23, also has a quadratic effect on the topography signal, the parameter should be chosen such that no noticeable influence can be detected. As the electrostatic interaction in FM mode is mainly with the tip apex due to the short-range nature of the force gradient, the lateral resolution is only limited by the tip radius when the parameter is set optimally [51].

2.2.3 Kelvin Probe Force Microscopy on dielectrics

Strictly speaking, equation 2.22 is only correct when both tip and sample are metallic. The theory is different for the system metallic tip/dielectric sample, but since such a system is investigated in the work, it will be discussed here, following Neff et. al [56].

In the following, the substrate is now a dielectric material with dielectric constant ε and band gap E_{ε} . This dielectric represents part of the gap of the capacitor formed by the tip and the metal back electrode as illustrated in Figure 2.10. The two metals have work functions ϕ_1



Fig. 2.10: Schematic for the KPFM analysis on dielectric materials. Here, the substrate is a dielectric material with a dielectric constant ε and a band gap E_{ε} . The dielectric is part of the gap of the capacitor formed by the tip and the metal back electrode. Back contact and tip have work functions ϕ_1 and ϕ_2 respectively. On the metallic back contact a dielectric containing an undefined number of charges q_i^{ε} is applied. Charges $q_j^{\rm g}$ and $q_k^{\rm t}$ can accumulate in the remaining gap and on a possible dielectric ε' on the AFM tip [56].(Figure taken from Ref. [56].)

and ϕ_2 , respectively, the CPD formation and measurement between them is explained in the previous section. The dielectric containing an undefined number of charges q_i^{ε} is in contact with the metallic back electrode. Charges q_j^{g} and q_k^{t} can also accumulate in the remaining gap and on a possible dielectric on the AFM tip with a dielectric constant of ε' . Possible sources of these charges are molecular or atomic ions and multipolar distributions. Considering the above described setup and following Neff et. al [56], the dependencies of the KPFM signal on dielectric materials is derived below.

The total electrostatic energy relevant for AFM measurements can be described by equation 2.27.

$$W_{\rm es} = -\frac{1}{2}C^{(0)}V_{\rm eff}^2 + \sum_{\rm i} q_{\rm i}\Phi^{(0)}(\mathbf{r}_{\rm i}) + \frac{1}{2}\sum_{\rm i} q_{\rm i}\Phi_{\rm im}(\mathbf{r}_{\rm i}) + W_{\rm Coulomb}$$
(2.27)

The effective voltage V_{eff} is defined by $V_{\text{eff}} = V_{\text{DC}} - V_{\text{CPD}}$, i.e, it includes not only the applied voltage V_{DC} but also the CPD of the metallic tip and back electrode. The first term of (2.27) describes the energy of the dielectric free capacitor with capacitance $C^{(0)}$, which depends on the geometry and material parameters. The second term contains the interaction of the point charges q_i (at the position \mathbf{r}_i inside the capacitor) with the electrostatic potential $\Phi^{(0)}$ of the

dielectric-free capacitor. The third term describes the interaction of each point charge with the image potential $\Phi_{\rm im}(\mathbf{r}_{\rm i})$. This image potential contains the sum of all image charges created at the point charges. The last term describes the Coulomb interaction between the point charges. Via the relations (2.28) and (2.29) where $\tilde{\Phi}^{(0)}$ represents the electrostatic potential at $q_{\rm i}$ (at position $\mathbf{r}_{\rm i}$), one comes directly to (2.30), which describes the forces acting on the tip.

$$\Phi^{(0)} = \tilde{\Phi}^{(0)} V_{\text{eff}} \tag{2.28}$$

$$F_{\rm es} = -\frac{\partial W_{\rm es}}{\partial z} \tag{2.29}$$

$$F_{\rm es} = \frac{1}{2} \frac{\partial C^{(0)}}{\partial z} V_{\rm eff}^2 - \sum_{\rm i} q_{\rm i} \frac{\partial \tilde{\Phi}^{(0)}(\vec{r}_{\rm i}) V_{\rm eff}}{\partial z} - \frac{1}{2} \sum_{\rm i} q_{\rm i} \frac{\partial \Phi_{\rm im}(\vec{r}_{\rm i})}{\partial z} - \frac{\partial}{\partial z} W_{\rm Coulomb}$$
(2.30)

In FM-KPFM mode, the frequency shift Δf is again minimised by the applied voltage $V_{\rm DC}$. At low frequencies, the frequency shift is related to the force gradient of the peak sample interaction $k_{\rm es}$ (Eq. 2.31) via Eq. 2.32

$$k_{\rm es} = -\frac{\partial F_{\rm es}}{\partial z} \tag{2.31}$$

$$\Delta f = \frac{f_0}{2k_0} k_{\rm es} \tag{2.32}$$

where f_0 is the oscillation frequency of the cantilever and k_0 is the spring constant. If this signal is to be minimised with respect to V_{es} , it can be represented as follows:

$$0 = \frac{\partial \Delta f}{\partial V_{\rm DC}} = \frac{f_0}{2k_0} \frac{\partial k_{\rm es}}{\partial V_{\rm DC}} = -\frac{f_0}{2k_0} \frac{\partial}{\partial V_{\rm DC}} \frac{\partial F_{\rm es}}{\partial z}$$
(2.33)

Combining Eq. 2.30 and Eq. 2.33 gives Eq. 2.34.

$$0 = \frac{\partial^2 C^{(0)}}{\partial z^2} V_{\text{eff}} - \sum_{i} q_i \frac{\partial}{\partial V_{\text{DC}}} \frac{\partial^2}{\partial d^2} \tilde{\Phi}^{(0)}(\vec{r}_i) V_{\text{eff}} - \frac{1}{2} \sum_{i} q_i \frac{\partial}{\partial V_i} \frac{\partial^2}{\partial z^2} \Phi(\vec{r}_i) - \frac{\partial}{\partial V_{\text{DC}}} \frac{\partial^2}{\partial d^2} W_{\text{Coulomb}}$$
(2.34)

Since neither the mirror charges nor the Coulomb interaction are affected by the applied voltage $V_{\rm DC}$, the third and fourth terms of equation 2.34 are omitted.

$$V_{\rm DC} = \frac{\Delta\phi}{e} + \frac{\sum_{\rm i} q_{\rm i} \frac{\partial^2}{\partial z^2} \tilde{\Phi}^{(0)}(\vec{r}_{\rm i})}{\frac{\partial^2 C^{(0)}}{\partial z^2}}$$
(2.35)

Since ideally $V_{\rm DC} = V_{\rm CPD}$ the surface potential can be calculated by Eq. 2.35 [56]. Regarding Eq. 2.35, single point charges in a dielectric have an impact on the KPFM signal. If the resolution of the KPFM measurement is sufficiently high, the slight alteration of the signal caused by point charges q_i can be detected. For ion trapping such analysis could lead to a better understanding of problems like charge implantation in dielectrics as stated by Harlander et. al [14].

Chapter 3 Results

Together with its academic partners, Infineon Technologies AG has set itself the goal of developing and manufacturing high-performance ion traps.

In order to build up a broad spectrum of know-how in the still young field of microfabricated ion traps and to find innovative designs and fabrication processes for future ion trap chips, Infineon is working on various implementation approaches. In addition to single-layer surface-electrode traps, which can be used to quickly and reliably test new surface designs and materials, multi-layer surface-electrode traps and 3D traps are also being produced in order to break new ground in the integration of optics and electronics, thus enabling the scalability of ion trap technology. The traps are manufactured at the Infineon chip fabrication facility in Villach. Together with experts from the various production areas, processes already established in other technologies are adapted or, if necessary, developed from scratch.

The focus of this work is the surface characterisation of existing trap types to improve future generations of ion traps. The surfaces of single-layer and multi-layer ion traps were investigated using KPFM, in order to gain a better understanding of the conditions at the surface, and thus possibly gain new insights into the problems described in section 2.1.

Kelvin Probe Force Microscopy is an analytical technique that is not widely used in industry. Since it could prove to be an important characterisation tool for ion traps, it was decided to establish this technique in the in-house "Failure Analysis" (FA) as part of this Master's thesis. The original purpose of the Failure analysis based in Villach, was to analyse failures and find weaknesses in the myriad products manufactured at the site, and to investigate customer returns for the cause of failure. As a result of the analytical expertise gained, the "Failure Analysis" Department has increasingly become a centre for analytical research at the Villach site. The department's extensive instrumentation includes an AFM as well as numerous other analytical methods like Auger electron spectroscopy and a TEM. The AFM, a Park NX20, which is a high resolution AFM designed mainly for industrial use, was used for all KPFM measurements.

3.1 The Park NX20 atomic force microscope

The standard measurement setup of the NX20 can be divided into four parts: the main system, the control electronics, a computer for data processing and monitors for data output. The main system is in turn divided into three separate components. Figure 3.1a shows these three parts, the XY stage, the Z stage and the focus stage. The Z stage controls the coarse adjustment of the Z scanner for example to bring the cantilever closer to the sample. The stepper motor of the Z stage has a maximum range of 25 mm. The actual component interacting with the sample is the head of the NX20, which is shown in Fig. 3.1b. It consists mainly of the cantilever holder, the so-called probehand, the Z scanner used for the exact height regulation of the tip during the measurement and the alignment knobs for the manual set-up of the laser and the position sensitive photo diode (PSPD). Furthermore, a super luminescent diode is built into the probe head, which generates the beam for the readout of the cantilever movement. Above the



Fig. 3.1: (a) The Park NX20 AFM main system, consisting of Z stage, XY stage and focus stage as they are placed in the NX20 housing. (b) Cross section of the NX20 probehead situated obove the sample on the XY scanner. The arrows pinpoint the most important parts such as the probehand that holds the cantilever, the Z scanner for the exact height regulation of the tip, the alignment knobs for for the manual set-up of the laser and the position-sensitive photo diode (PSPD), the super luminescent diode to generate the readout beam and optical microscope for rough orientation on the sample [18].(Figure taken from Ref. [18].)

probehand is a height-adjustable optical microscope used for coarse positioning of the cantilever above the sample. The probehand contains a bimorph to excite the cantilever oscillation, in NC mode, and a circuit to apply different voltages to the tip. The Z-scanner consists of a layered structure of piezoelectric materials and has a range of up to $15 \,\mu\text{m}$. The X-Y scanner shown in Figure 3.1b is used as the sample stage with a scan range of $100 \times 100 \,\mu\text{m}^2$. To move the sample on a larger scale, the X-Y stage with a range of $20 \times 20 \,\text{mm}^2$ is used. The whole setup is mounted on a vibration isolation system for vibration damping. To further shield the system from external disturbances, the entire system shown in Figure 3.1a is surrounded by an acoustic shielding enclosure [18].

The setup was operated at room temperature and in ambient atmosphere. Two different ion trap chips were investigated in depth.

- 1. Single-layer trap using aluminium as electrode material
- 2. Multi-layer trap with AlSiCu electrodes, AlSiCu is an aluminium alloy with 1% copper and 1% silicon added to the aluminium

The data presented here was acquired on each one specific, single layer and multi layer chip.

3.2 Sample preparation of single-layer aluminum traps

The ion trap analysed in this chapter was produced via commercial microfabrication processes. The stack cross section of the trap used is shown in Fig. 3.2.

The trap investigated here is fabricated on a standard silicon substrate (725 μ m thickness, 8 inches of diameter). A 1.3 μ m silicon dioxide layer was deposited on top for electrical insulation. This was done by chemical vapor deposition (CVD) using TEOS as precursor. On top of this oxide layer a 2 μ m thick aluminium layer was deposited using physical vapor deposition (PVD).



Fig. 3.2: Schematic cross section of the single-layer aluminium trap consisting of a 725 μ m thick silicon substrate; 1.3 μ m silicon dioxide layer deposited by a CVD process with tetraethyl orthosilicate (TEOS) as precursor and finally a2 μ m aluminium layer deposited using a PVD process.

The aluminium layer is then patterned using lithographic techniques. After the deposition and patterning processes, the chips are mechanically diced. This is done using rotating cutting wheels cooled by cooling water with additives. The cooling water has the additional effect of removing particles generated during the cutting process. After dicing, the chips were not subjected to any additional cleaning. The chip analysed in this work is shown in Figure 3.3. The layout of the chip was done by OxfordIonics, in a common project. After dicing the chip was stored for several months in the clean room of the facillity, after that the chip was transferred into a gel-box, supplied by "Gel-Pak". The gel-box was stored in an office. Between the first and the last measurement one month passed. During this time the ion trap was always stored in the same gel-box in the office. For the measurements, the chip was removed from the box and placed unprotected in the AFM without further cleaning or treatment.



Fig. 3.3: Top view of the investigated single-layer aluminum trap with a design from OxfordIonics. The figure is a microscope image of the actual chip, the wire bonding is indicated schematically. Each bonding pad is contacted and bonded to the printed curcuit board (PCB) (schematically displayed by the gray box in the background) that acts as electric ground. The area studied in this work is enlarged. The individual measurement sites are numbered and referred to in the main text by these numbers.

For further analysis the chip was bonded to a printed circuit board (PCB) shown schematically in Figure 3.3. The electrical contacting by means of wire bonds is necessary to ensure a sufficient contacting of the chip. If the contacting is inadequate (e.g. by using silver conducting glue), no meaningful KPFM images can be taken. The regions where measurements were taken are numbered, in the highlighted and enlarged area. The data presented in the following section refer to this numbering.

3.3 Kelvin Probe Force Microscopy analysis of aluminium electrodes

In this section KPFM images of aluminum electrodes will be presented and different types of surface potential deviations will be encountered. Since this chapter only investigates metal surfaces (with a thin layer of oxide and various types of adsorbates originating from the environment), the measured contact potential differences can be understood as deviation in the work function of the metal surface. It has to be kept in mind that in all displayed images, only the CPD between tip and sample is displayed and never the absolute work function of the material. According to Eq. 2.19 and the used measurement setup $V_{\text{CPD}} \propto -\phi_{\text{sample}}$ applies.

Figure 3.5 shows a typical topography image and the corresponding KPFM signal, of the aluminium electrode at position 1. In the topography scan the grain structure of the aluminium can be seen, the individual aluminium grains are clearly separated by grain boundaries (GB). The size distribution of the grains ranges from the sub-micron range to diameters >5 μ m. The surface texture of the grains is also clearly visible and two types can be easily discerned. (1) stepped structures are seen on the majority of the grains, an example is marked in blue in Fig. 3.5a. (2) flat terrace structures are only occasionally found. These grains (2) feature wide flat terraces separated by abrupt steps. An example for a terraced grain texture is framed in red in Fig. 3.5a. A close-up of a stepped grain next to a terraced grain is shown in Fig. 3.4. Here the corrugated/smooth surface of a stepped/terraced grain can be distinguished easily. Both stepped



Fig. 3.4: Grain morphology of a stepped and terraced grain.

and terrace-like topographies always extend over the whole grain but do not form structures or patterns that extend across grain boundaries. To compare the corrugations of both types of grain structure, height profiles are taken across the grains highlighted in red and in blue, respectively (the arrwos in Fig. 3.5a indicate where the profiles were taken). Fig. 3.5c displays the height of the "flat terrace" grain and panel (e) that of the "stepped" grain. In each panel the topography and the corresponding contact potential difference (CPD) are plotted. The terraced and stepped structures visible in the topography are also visible in the KPMF signal. The potential changes due to the step structures are around 30 mV. In the case of the stepped structures, the potential curve usually follows the topography, so that the valleys have a lower potential than the crests. The difference between peak and valley is around 40-50 mV.

In addition to the small scale structures within the grains, there are topographic differences between grains. The peak-to-valley distance over the whole area is 483 nm and the root mean square roughness (Rq) is 34.8 nm. A slight but abrupt disturbance in the signal can be seen at the top of the image. The exact cause of this transient change in contrast is unknown and is most likely due to momentary poor contact between the tip and the sample. Figure 3.5b shows the potential surface simultaneously acquired with the topography channel of Fig. 3.5a. The KPFM scan also clearly shows the grain structure of the aluminium surface and the individual grains image can be assigned to the corresponding grains in the topography image. The Peak to valley potential in Fig. 3.5b is 1.1 V and the Rq is 69 mV. The clear separation of the grains by grain boundaries in the CPD is due to the structural difference and thus the different local work functions of grain and grain boundaries.



Fig. 3.5: Topography and contact potential difference of the single-layer aluminum chip, position 1 (see 3.3 a) for reference $25 \,\mu \text{m}$ topography image showing the grain structure of the aluminium. Both the grain boundaries and the texture of the grains is clearly visible. The majority of the grains show a stepped structure (blue frame). Some grains feature a terraced structure (red frame).b) Corresponding KPFM image showing variations of the work function of the aluminium surface and a clear separation of the grains due to the structural differences between grain and grain boundaries [57]. Areas of "large potential deviations" are enclosed with rectangles and discussed in the text. (c,e) Show topographic height profiles of a "terraced" and a "stepped" structure. The line profiles were taken along the red and blue arrows indicated in panel a). The white arrows mark the grain boundaries used to determine potential differences between boundary and surrounding surface summarized in Tab. 3.2. d) Comparison of the pixel density at a given CPD of the two grains marked in panel b) in red an blue, respectively. The grain enclosed in red has an on average 115 mV higher work function compared to neighbouring blue grain. e) Potential along the blue arrow. f) Line profile plotting the CPD across an area with "large potential deviation" (black arrow in Fig. 3.5b). Resolution of 512×512 pixel, scan speed of 0.15 Hz, acquisition time ≈ 1 hour. During every measurement the forward and backward signal was recorded to gain a better estimation on possible artefacts, the images presented here show the forward trace only.

In an idealized picture (see Fig. 3.6), a GB is the interface between different crystallographic or rational lattice orientations of a material.



Fig. 3.6: Schematic of a grain boundary at the atomic scale. In this example grains have identical lattices, but they are rotated with respect to each other (indicated by the blue lines).(Figure taken from Ref. [57].)

At the boundary the lattices are not aligned, resulting in sub-optimal atomic arrangement and unfavourable distances between individual atoms that can lead to compression or expansion of the lattice. These lattice defects affect the local properties with respect to the undisturbed surface or bulk [57]. The discontinuation of the regular lattice at the grain boundary together with unfavourable atomic arrangements often leads to atomic sites with enhanced reactivity. Therefore, grain boundaries are usually very attractive to adsorbates from the surrounding vacuum or gas phase or segregation from the bulk. Both phenomena – the initial lattice distortion and the passivisation of reactive sites – affect the work function at and in close vicinity of a grain boundary [58, 59]. Thus, it is fully expected to see the grain boundaries in the KPFM signal. The deviations in the surface potential at the grain boundary are not identical. For a more precise determination of the effect of grain boundaries on the surface potential see Table 3.2.

In addition to the effect of GB on the local work function, there are also other types of irregularities in the potential. The most prominent irregularities are the local "large potential deviations" of the potential (see boxes in Fig. 3.5b). There the surface potential deviates by several hundred mV from the surrounding surface. As can be seen in the image, these extreme deviations are found on parts of grain surfaces (1, 4, 6) or only at the grain boundaries (2, 3, 5). In Fig. 3.5f, such a "large potential deviation" is shown. This particular "large potential deviation" with a peak-to-background potential of ≈ 0.7 V is labelled in Fig. 3.5b and the arrow indicates where the potential of the CPD has been taken across the image. Possible origins for such local inhomogenities can be very diverse and could not be clarified within the scope of this Master's thesis. Local impurities in the aluminium, different orientations of the grain structure or local irregularities in the adsorbates are possible causes.

In addition to these "large potential deviations", there are also more subtle deviations. The area of such a minor deviation is outlined in red in Fig. 3.5b. The grain located in this area shows a difference of about 115 mV compared to the neighbouring grain marked in blue. This difference has been determined by comparing the average contact potential differences of the encircled grains ($\overline{CPD}_{red area} - \overline{CPD}_{blue area}$). Again, the origin of these differences is not yet known. Different crystallographic orientations could be the reason similar work function differences for different grain orientations have been reported in the literature [60, 61].

To learn more about the grain structure and the corresponding irregularities in the potential, several $25 \times 25 \,\mu\text{m}^2$ scans were then taken. Figures 3.7 and 3.8 show more images from this series. They where acquired with the same settings and in the same environment as the first data set presented in 3.5. For better visibility and optimized contrast, the topography and CPD images of Fig. 3.8, Fig. 3.7 and 3.8 have all different scales. Figure 3.7a shows the topography and 3.7b the corresponding potential landscape. The images were taken from position 2.



Fig. 3.7: Topography and CPD images taken at position 2. (a) The topography and the grain size distribution is similar Fig. 3.5a with a peak to valley distance of 421 nm and a Rq of 32 nm. (b) The KPFM signal is also similar to Fig. 3.5b with a peak to valley distance of 0.86 V and a Rq of 63 mV. Some grains with higher potential are marked in red (R1-R6), some with lower potential in blue (B1-B4). Panel (c) compares the potential distribution of the marked grains. The average CPD difference between red and blue grains is ≈ 100 mV.

The topography in Fig. 3.7a is not significantly different from the AFM image of position 1 shown in Figure 3.5a. The peak to valley distance is 421 nm and the Rq is 32 nm. Both "steps" and "terraces" can be seen on the grains. In the KPFM signal the features already described in Figure 3.5b, such as GB and corrugations, are again observed in Fig. 3.7b. Here the peak to

valley potential is 0.86 V and the Rq is 63 mV. Areas with higher potentials are marked again in red (R1-R6) and those with lower potentials in blue (B1-B4), most of them represent a whole grain. The grains marked in red and blue, respectively, have similar average potentials. The potential distribution is shown in Fig. 3.7c. The average CPD difference between the grains is calculated as

$$\Delta \overline{\text{CPD}} = \overline{\text{CPD}}_{\text{red}} - \overline{\text{CPD}}_{\text{blue}}$$
(3.1)

with

$$\overline{\text{CPD}}_{\text{red}} = \frac{1}{n} \sum_{i=1}^{n} \overline{R}_i$$
(3.2)

$$\overline{\text{CPD}}_{\text{blue}} = \frac{1}{n} \sum_{i=1}^{n} \overline{B}_i$$
(3.3)

resulting in a $\Delta \overline{\text{CPD}}$ of $\approx 100 \text{ mV}$. In comparison to the surface area of pad 1 shown in Fig. 3.5b, more grains of different potential are found in this area of pad 2. Furthermore, they appear in clusters, where neighbouring grains have similar work function. Irregular, extremely strong deviations in the local CPD are also observed in this surface area. They are again found on grain boundaries, parts of grains and whole grains. There is no correlation with topographical conditions, i.e., steep or corrugated grains (or the opoosite), cannot be identified by their CPD.

The third example of an aluminum electrode in shown in Fig. 3.8. The AFM data (same parameters an sizes as before) was acquired on position 3 of the chip. Figure 3.8a shows the topography and 3.8b the corresponding potential.



Fig. 3.8: Topography and CPD of an aluminum surface taken at position 3 of the chip (see Fig. 3.3. (a) Topography: grains in the area enclosed in red are significantly smaller than in the rest of the image and as in the other images acquired on different positions on the chip. The roughness in this area is increased with a Rq of 47 nm in the red area compared to 38 nm for the whole $25 \times 25 \,\mu\text{m}^2$ area. Grains marked in green feature a peculiar topography, where a large terrace turns into an area, with high step density. (b) KPFM signal of the same surface area as marked in (a). In the red areas a high density of "large potential deviations" is found. The green marked structures lead to deviations in potential between 50-350 mV. c) . (c, d) Line profiles along the yellow arrows 1 and 2, respectively, showing the topography and the corresponding CPD.

The topography shows similar structures as those described in Figure 3.5a and Fig. 3.7a, with a peak to valley of 478 nm and a Rq of 38 nm. However, there is a difference in grain size compared to the other investigated areas. The grains in the centre of Figure 3.8a are smaller than usual. This is also reflected in the significantly increased roughness of this surface area, with a Rq of 47 nm, compared to a Rq of the total area of 38 nm. The potential surface also shows similar characteristics to the previous positions with a peak to valley of 1.1 V and a Rq of 63 mV. In addition to the "terraces" and "steps" on the surface, which can be seen in all images both in the topography and in the potential landscape, a topographic feature that has a clear influence on the potential is observed here. The grains of interest are outlined in green. These grains feature a combination of large, flat terraces (which is often tilted with respect to the macroscopic surface, see AFM image in Fig. 3.8a and the height profiles in Figs. 3.8c and 3.8d) with regions of high step density. The surface orientation is thus the terrace orientation (probably a close packed surface with low miller indices) on one side of the grain and the stepped surface

on the other side. It is known for aluminum single crystals that the work function decreases with increasing packing density therefore increasing step density [62]. This change is not equally evident in all grains and the changes compared to the rest of the grain range from 50-350 mV. Exemplary, two line profiles are shown in Fig. 3.8c and Fig. 3.8d where the topography and the CPD are both plotted. They where taken along the yellow arrows labelled 1 and 2 in Fig. 3.8a. The topography in Fig. 3.8c shows two large flat terraces of two neighbouring grains (inclined with respect to the macroscopic surface). In the corresponding CPD curves, the potential is almost constant all over the terraces, and also remarkably constant in the adjacent regions. The decrease in CPD is in agreement with a lower work function on a surface with high step density. The same explanation can be applied to Fig. 3.8d. The the-peak-to-valley potential distance for the grains in Fig. 3.8c is 330 mV and for the grains in 3.8d 240 mV.

In both the KPFM image and in the topography, the area with predominantly small grains is marked. It is noticeable that in this area "large potential deviation" occur more frequently compared to an equally sized area in the other two regions on the chip. Furthermore, in the two examples already described, the irregularities are always distributed over the entire surface and cannot be clearly assigned to a topographical feature. This is not the case in Figure 3.8b. Furthermore, the "large potential deviation" are concentrated in the grain boundaries: whole grains are hardly affected, only in box (4) and (9) a small partial area is affected. On close inspection, many of these "large potential deviations" are located at grain boundaries, where grains with a (partial) "terrace" topography meet (e.g. box 2, 3, 6, 7, 8). In these examples, the neighbouring grains are situated such that the terraces face each other with a strong tilt or a steep edge. The flat terraces have CPDs above the average of the image, and the grain boundaries in between them feature even more enhanced CPDs.

In order to provide a better overview on the "large potential deviations" present in all three KPFM images, these are marked by white boxes and numbered. The size of the box is chosen such, that the "large potential deviation" is enclosed completely. To determine the magnitude of a single "large potential deviation", the maximum potential in the enclosed area was determined, CPD_{max,enclosed}. From this maximum the average potential of the whole $25 \times 25 \,\mu\text{m}^2$ area was subtracted.

$$\Delta \text{CPD} = \text{CPD}_{\text{max,enclosed}} - \text{CPD}_{\text{avg}}$$
(3.4)

Table 3.1 summarizes all areas where the deviation from the average potential is above the threshold of >230 mV. The threshold for the change in work function was set to be above the deviation that can be expected from the variation in the crystallographic orientation.

Tab. 3.1: "Large potential deviations" from Figures 3.5b (data set 1), 3.7b (data set 2) and 3.8b (data set 3). The values where determined by subtracting the average potential of the respective image from the maximum potential of the marked area.

Nn	"large potential devia-	"large potential devia-	"large potential devia-	
INT.	tions" data set 1 (mV)	tions" data set 2 (mV)	tions" data set 3 (mV)	
1	630	300	270	
2	390	480	340	
3	300	520 (max.)	410	
4	380	470	370	
5	710	430	<u>610</u> (max.)	
6	790 (max.)	370	240	
7			330	
8			380	
9			300	

When looking for comparable features that lower the CPD, nothing was found. To determine the changes directly at the grain boundary, again data from all three positions was used. This was done by selecting five GBs in each image they; are marked by arrows in the topography images of Figs. 3.5, 3.7 and 3.8. Fig. 3.9 shows one of these grain boundaries (number 2 from Fig. 3.5a). The plot in Fig. 3.9c shows topography (dashed) and potential (continuous) profiles taken along the arrows a) and b). As a guide to the eye the background color of the graph matches the color of the arrow in Fig. 3.9a. As it can be seen in the diagram, the two grains have slightly different potentials. The CPD of the left grain is lower by $\approx 30 \text{ mV}$ compared to the right one. Therefore not a single potential deviation is calculated but two. To determine the deviation at a GB relative to its neighbouring grains the CPD at the shaft (CPD_{shaft}) was subtracted from the maximum CDP of the grain boundary CPD_{GB} leading to

$$\Delta CPD_{shaft} = CPD_{GB} - CPD_{shaft}.$$
(3.5)

The same was done for the values at the tip yielding

$$\Delta \text{CPD}_{\text{tip}} = \text{CPD}_{\text{GB}} - \text{CPD}_{\text{tip}}.$$
(3.6)

The calculated values for all investigated grain boundaries are shown in 3.2.

Fig. 3.9: (a) Topography and (b) CPD of a grain boundary between two grain with the "stepped" topography (see Fig. 3.5b). (c) height an CPD profiles along the arrows in panels a) and b). The pink and blue background color refer to the left an right grain respectively, The width of the grain boundary is highlighted in yellow.

Tab. 3.2: Potential deviations caused by grain boundaries. The values where determined following Eq. 3.5 and Eq. 3.6.

	potential deviations of		potential deviations of		potential deviations of	
	GB in Fig. $3.5 (mV)$		GB in Fig. 3.7 (mV) $$		GB in Fig. 3.8 (mV) $$	
Nr.	ΔCPD_{shaft}	ΔCPD_{tip}	ΔCPD_{shaft}	ΔCPD_{tip}	ΔCPD_{shaft}	ΔCPD_{tip}
1	63	43	15	14	81	131
2	100	78	22	112	48	77
3	47	29	25	61	84	45
4	32	18	24	62	90	95
5	45	29	54	108	32	88
average GB deviation: 58; RMS: 33 mV						

As can be seen in Tab. 3.2, the deviations caused by GBs have quite different values, ranging from 14 mV to 131 mV. They all have in common that they are positive, meaning, that they lead to a higher CPD. A similar effect, only of bigger scale was observed at the "large potential

deviations". When looking at Eq. 2.19, one can see that an increase in CPD is caused by an decrease in the work function of the sample. Thereby we can conclude that both, "large potential deviations" and GB lower the work function of the the analysed sample. On aluminum it is actually a known phenomena that grain boundaries lower the work function by inducing lattice distortions and the accumulation of defects and impurities [63]. Since "large potential deviations" also lead to a lower work function, they might have the same origins. The larger deviation compared to GBs may then be caused by a higher concentration of defects.

As it was shown in this chapter, there can be various types and reasons for deviations in the surface potential. On the one hand, there are deviations like, "stepped" and "terrace" topographies and grains with steep edges that lead to pronounced potential deviations. These differences between grains are most likely caused by changes in the lattice structure of the surface. On the other hand deviations at GBs appear, which seem to originate from lattice distortions and defects.

3.4 Simulating the E-field away from the surface

In the previous chapters it was shown from KPFM data that there are various deviations in the potential on metal surfaces. Such deviations will affect the electric field at the position of the ion. In particular, the ion may be moved out of the zero of the RF field, leading to excess micromotion [15]; the secular frequencies of the ion may be affected as well.

In order to estimate how the potential inhomogeneities described in the previous chapters affect the electric field, simulations of the generated electric field as a function of the distance above the surface of the electrodes were conducted. In these simulations, the electric field caused by the potential distribution at the surface was calculated at different ion heights $(z = 1 \,\mu\text{m}; z = 20 \,\mu\text{m} \, z = 100 \,\mu\text{m})$. Based on the obtained fields, the theoretical secular frequency of a ${}^{40}Ca^+$ ion was calculated. The measurement data chosen for this calculation is the "dataset 2" shown in Fig. 3.7b. The individual steps performed to calculate the field and the secular frequency are explained in the following.

The first step was to determine the mean value of the potential of the whole data set. The calculated mean value was then subtracted from each individual data point so that the mean potential of the surface was zero. Fig. 3.10a shows the data after this offset subtraction. The next step was to embed the data set in an environment of potential. To do this, the measured square potential surface of $25 \,\mu m$ side length was symmetrically surrounded by a zero potential surface, resulting in a total square potential surface of $250 \,\mu m$ side length. This procedure is called zero padding. This resulting area was Fourier transformed. Using Eq. 3.7 the data was translated to the heights z,

$$\tilde{V}(\mathbf{k}, z) = e^{-k|z|} \tilde{V}_{\text{surf}}(\mathbf{k}), \qquad (3.7)$$

where $\tilde{V}(\mathbf{k}, z)$ is the Fourier transformed potential of the potential at height z and z is the height respectively the distance from the surface/the x-y plane, and $\tilde{V}_{surf}(\mathbf{k})$ is the Fourier transform of the surface potential at z = 0 [64]. As we can see from 3.7 only deviations on the length scale of the distance are visible, due to the exponential suppression

After calculating the Fourier transform of the potential at given height z, the data was transformed back to obtain the potential $\bar{V}(x, y, z)$. The electrical field at a given height z can then be calculated by $\mathbf{E} = -\nabla \bar{V}(x, y, z)$. Figs. 3.10c and 3.10d show the calculated electrical field from the used data set at the heights of 20 μ m and 100 μ m, respectively. One can see that in both images the field strength is the strongest near the center gradually decaying in the direction of the edges. At the heights of 20 μ m the maximum of the field is 74 V/m and the minimum is 22 V/m. At 100 μ m the field is significantly lower than at 20 μ m having its maximum at 0,050 V/m and its minimum at 0.043 V/m. Besides the two images showing the E-field at 100 μ m and 20 μ m also the E-field at 1 μ m of surface distance is shown. Although such a distance is by far a unrealistic distance for trapping ions, it shows the major contributors for the E-field. The "large potential deviations" have by far the greatest contribution to the E-field at this distance.

When looking at the farther distances, the E-field of the single contributors add up and merge to a single maximum, as it can be seen in Figs. 3.10c and 3.10d. At this point it has to be mentioned that the area of $25 \times 25 \,\mu\text{m}^2$ used to calculate the E-fields is to small for calculating exact E-fields especially for larger distances, e.g. 100 μ m. Acquiring areas of the size needed for exact calculation using KPFM is a very tedious challenge and was out of the scope of this thesis. Nevertheless the calculated fields should be in the right order of magnitude, giving a qualitative estimation of the effect of potential deviations on the E-field. From the E-fields in Fig. 3.10 it is hard to tell, if and how other deviations in the potential may have effects on the static E-field since the deviations, especially the large ones, are spread quite evenly in these images. To get

a better understanding how an unevenly distribution of "large potential deviations" affect the E-field an additional data set (data set 1) was used to simulate the corresponding E-fields. The procedure to simulate the images in Fig. 3.11 was the same as in Fig. 3.10. Fig. 3.11a shows an image of the data set gained from position 1. As above the offset was changed to yield an average potential of 0. Figs 3.11b, 3.11c and 3.11d show the E-fields at $1 \,\mu\text{m} \, 20 \,\mu\text{m}$ and $100 \,\mu\text{m}$, with maxima (minima) of 68 V/m / 6 V/m at $20 \,\mu\text{m}$ and $0.033 \,\text{V/m}$ / $0.028 \,\text{V/m}$ at $100 \,\mu\text{m}$, respectively. In 3.11 the potential deviations are less evenly distributed than in Fig. 3.10. Especially the "large potential deviations" are concentrated on a small area in the upper right corner. The E-fields on the corresponding images are also strongest in the same area.

For this electrical field the curvature in terms of the secular frequency of a ${}^{40}\text{Ca}^+$ ion was calculated ¹ Therefore the Hesse matrix \mathcal{H} of the energy potential was calculated, receiving the eigenvalues λ_n with n = 1, 2, 3 that can be used to calculate the secular frequency ω_n with Eq. 3.8

$$\omega_n = \frac{1}{2\pi} \sqrt{\frac{e}{m} \lambda_n} \tag{3.8}$$

where *m* is the mass of the ion. For further explanation see reference [65]. Figures 3.10e, 3.10f, 3.11e and 3.11f show the field curvature in terms of secular frequencies calculated for the E-fields at ion heights of 20 μ m and 100 μ m. The highest calculated frequencies for data set 1 and 2 are in the same range. At 20 μ m the maximum is roughly at 0,9 MHz and at 100 μ m at 10 kHz.

Considering these findings, potential deviations on the surface of metal electrodes could have effects on the secular frequency of trapped ions. A relevant effect of the potential deviation on the surface of material electrodes on an ion cannot be excluded. Nevertheless it has to be mentioned that these simulations do not resemble a realistic environment as the ions are exposed to. As stated earlier, the data sets were embedded into an area of homogeneous potential before doing any calculations. Especially at greater distances, this leads to errors since potential deviation from neighbouring areas may lead to an averaging effect decreasing the E-field or on the other hand adding up and thereby causing greater fields. Furthermore, possible long-range deviations over several 100 μ m may be present, which are not taken into account here. Therefore, more studies in these direction have to be made to get a better understanding. Of great interest would be studies in which the results of the simulations are tested in situ with trapped ions. For this purpose, a trap could be designed, precisely characterised using KPMF and then used to trap ions.

¹In an ion trap set up where not only the DC field but also the RF field causes motion of the ion the overall secular frequency is calculated by $\hat{\omega}_n = \sqrt{\omega_{\rm RF}^2 + \omega_n^2}$ where $\omega_{\rm RF}$ is the secular frequency caused by the RF-field and ω_n is the secular frequency of the static electrical field.

Fig. 3.10: a) Image of the CPD at position 2 (data set 2) with an average of zero CPD. b-d) Electrical fields calculated with Eq. 3.7 from data set 2 at heights of $1 \,\mu\text{m}$, $20 \,\mu\text{m}$ and $100 \,\mu\text{m}$. e) and f) show the corresponding field curvatures expressed as secular frequencies at $20 \,\mu\text{m}$ and $100 \,\mu\text{m}$ calculated with Eq. 3.8.

Fig. 3.11: a) Image of the CPD at position (data set 1) with an average of zero CPD. b-d) same analysis as it was done in Fig. 3.10 for dataset 1.

3.5 Laser Experiments on aluminum and AlSiCu electrodes

Several experiments were carried out to test the effect of light exposure on the electrical potential of the aluminium surface. Two types of experiments were conducted: (1) the sample was first illuminated and then mounted to the KPFM. (2) the sample was irradiated with laser light during a running KPFM measurement (in situ experiment). The light source used was a commercially available laser pointer with a wavelength of 405 nm.

In the first set of laser experiments the sample was first illuminated and afterwards analysed. The laser beam was directed onto the surface from as distance of 20 cm. The spot on the surface was roughly $1 \,\mathrm{mm^2}$. The sample used in these measurements was different than the samples described in previous chapters. Instead of an aluminum surface, the top most metal was AlSiCu. Furthermore, the sample was not electrically contacted via wire bonds but with silver conducting paste. Fig. 3.12 shows four KPFM maps of the AlSiCu surface. The reference measurement of the pristine surface shown in panel a). The KPFM maps in panel b) were acquired after illuminating the sample with the 405 nm laser for 60 s. The image acquired is $1 \times 1 \,\mu \text{m}^2$. The data presented in Fig. 3.12 c) and d) were measured consecutively afterwards. The measurement of panel c) was started 55 minutes after laser exposure, d) after 110 minutes. As can be seen from the fixed colour range of the images, the CPD does not deviate a lot in each measurement but overall it decreased after laser exposure. For a better comparison Fig. 3.12e shows the surface potentials of panels a)-d) taken along a horizontal line from each panel. The CPD curves and panels a-d) are color coded. Due to the noisy signal, the line profile was averaged over 125 nm (length delimited by colored lines). The potential difference between the reference measurement and the measurement immediately after the laser irradiation is about 250 mV. This difference decreases after approximately 2.5 hours of measurement time the difference has decreased to $\approx 200 \,\mathrm{mV}.$

This charging and decharging effect was also observed on other surfaces such as pure aluminium and TiN on both surfaces with a similar timescale for charge decay as on AlSiCu. In following experiments, however, it was found that the charging was absent when contacting the samples with wire bonds instead of the silver-filled conductive paste that did not ground the sample sufficiently. One explanation for the build up of the charge is that the electrode material emitted photo electrons. The generated charge could not be compensated because of some kind of diode effect caused by the silver conducting paste. Such a diode effect could arise either on the intersection between electrode and silver conducting paste due to the presence of surface oxides, or inside the silver conducting paste because of improper contact between the silver particles or organic residues. Such a charging effect is not expected in a real ion trap set-up since here the sample (ion-trap) is grounded by wire bonding. For this reason, the unintended charging was not investigated further.

Fig. 3.12: KPFM of an AlSiCu surface. The series of measurments is intended to illustrate the influence of laser exposure (405 nm) on a surface contacted with silver conductive paste. (a) Serves as a reference of the non-exposed sample. b) Potential map after exposing the sample one minute. (c) and (d) subsequent measure b) but without additional light exposure. Each measurement took about 55 minutes. (e) Potential curves of panels a-d) along the x-axis. To reduce local influences on the potential, the mean values of a range were used as indicated.

To prove that there is no long lasting charge buildup caused by laser illumination another set of experiments were conducted. Unlike in the experiment described before, the sample was not electrically contacted with silver conducting paste, but with wire bonds. In these experiments the sample was illuminated in situ. In the in situ measurements however, where the sample was illuminated during the ongoing measurements, eventually occurring short lasting phenomena during and short after laser illumination could be tracked. In addition to that the measurements can be conducted faster, since the measuring process was not interrupted by every illumination. The sample used was the same single layer aluminium chip as described in section 3.2. The laser used was the same commercially available laser pointer with a wavelength of 405 nm as used before on the AlSiCu chip. In all experiments, the laser was manually aimed at the sample from a distance of about 20 cm. No changes in potential were observed during laser exposure in any of the experiments performed. A representative experiment is shown in Figure 3.13.

Fig. 3.13: Topography of a CPD map of aluminum before an after laser exposure. The data was taken at position 4 (see Fig. 3.3). (a,c) Are the AFM topography images of the aluminium surface before (a) and after (c) illumination. The exposure was repeated 17 times for one minute each with two minutes breaks, using a 405 nm laser and during the AFM/KPFM measurement. There were always two minutes of darkness between the exposures. The black frame indicates the overlap of the images. (b,d) are the corresponding KPFM images.

The images presented in Fig. 3.13 were taken at position 4. They are all acquired the same $4 \times 4 \mu m^2$ large area of a single grain with "stepped" topography. At the edges of the image grain boundaries can be seen. There was a slight thermal drift between the images, the overlapping area is outlined in black. Panels a) and b) show the simultaneously obtained topography and potential, respectively, prior to the laser illumination. During the acquisition of the images displayed in panels c) and d) the surface was exposed to the laser. The aim of this procedure was to measure possible effects during exposure and to observe possible decay effects. Therefore, a cycle with short periods of irradiation was established. First, the sample was measured 2 minutes without irradiation, afterwards the sample was irradiated for 1 minute while continuing

the AFM/KPFM measurement. This was repeated until the measurement was finished. Since one measurement took 55 min the sequence was repeated 17 times until the measurement was completed. As mentioned before the measurement started with 2 minutes of darkness.

Fig. 3.14: Schematic of the irradiation cycle during data acquisition. The image shows the KPFM image already shown in Fig. 3.13d. The unmarked areas were measured without laser exposure, the red areas indicate when the sample was exposed to the laser. The fast scanning direction is horizontal, this image is recorded from bottom to top.

However, no relevant change could be detected during or after the light exposure. When compared with the reference sample, no significant changes were observed in the overlapping areas at all. The only difference is the resolution of the KPFM signal. Panel b) has a slightly better lateral resolution than d). A possible reason for this is the process of laser irradiation. For this the AFM shielding had to be partially opened to provide access with for laser. In addition, reflections of the laser from the sample surface could have disturbed the signal readout by the SLD.

The slow scanning direction of the images presented in Figs. 3.13 is the Y direction. If the potential were to change due to the exposure of the laser, it would be possible to detect this by repeating sequences in the Y direction.

The fact that no effects occur due to laser illumination can be deduced from the plot of the surface potential along the slow scanning direction (Y direction 3.15). To reduce the influence of local potential deviations, the signal has been averaged over a distance of $1 \mu m$ alog the x-axis (red frame in Fig. 3.13d). In Fig. 3.14 and the plot of 3.15, the brackets mark the individual sequences. Sequences 1-5 and 9-13 are highlighted. If laser exposure would cause any significant effects, a regular pattern in potential would be detectable, i.e.by comparing the average potential measured in the absence of light to the average CPD during irradiation. This comparison is shown in Fig. 3.15 Within these sequences, however, no regular, or repeating potential change can be detected.

Fig. 3.15: Plot of the potential of the area marked by the red frame in Fig. 3.13.

Tab. 3.3: Average CPD of the segments of the illumination cycle highlighted in color in Fig. 3.15.

Nr.	Avg. CPD dark (mV)	Avg. CPD irradiated (mV)
1	286	287
2	293	284
3	292	287
4	289	288
5	276	280
9	288	293
10	290	287
11	284	282
12	283	277
13	274	292

From these experiments it can be concluded that the irradiation of an aluminum surface with a laser of the wavelength of 405 nm causes no detectable effect on the surface potential even though emission of photo electrons cannot be excluded.

3.6 Analysis of silicon dioxide

In addition to the investigations on metals, also the analysis of dielectrics with KPFM was done. The focus was on silicon dioxide (SiO₂), which is the material of the layer underneath the topmost metal in ion traps used here. On all surfaces where the topmost metal is removed by lithographic patterning, such as the electrodes, SiO₂ is exposed to the environment. As dielectrics are considered to be a possible source of increased heating rates [14, 32], this Master's thesis also attempted to investigate dielectrics using KPFM. The focus was on the development of a process to provide high-resolution images as the first step. Carrying further experiments was out of the scope of the thesis. Nevertheless, the knowledge gained here can be used to assess what kind of measurements should be pursued in the future.

As explained in Chapter 2.2.3, KPFM measurements on dielectrics require a specific measurement setup. In order to contact the SiO_2 surface, it needs to be applied to a metallic backside contact. In the analysed trap a metal layer below the SiO_2 acted as the backside contact. Vertical interconnect accesses (vias) were used to contact this backside contact and connect it to the KPFM, as shown schematically in Fig. 3.16. The device was used as fabricated.

Fig. 3.16: Schematic of the trap and set up used for the KPFM measurements on SiO_2 . Silicon was used as the carrier substrate with a metal layer deposited on top, and the SiO_2 layer deposited on the metal. As electrode material AlSiCu was used. In order to be able to connect the AlSiCu to the measurement setup, vertical interconnect accesses (vias) were inserted into the SiO_2 to enable contacting. In this setup the metal layer acts as back contact for the KPFM measurement.

Fig. 3.17 shows AFM and KPFM images of the SiO₂ surface. As the SiO₂ is amorphous, no grain boundaries are visible. In the topography (panel (a)) the $1 - 5 \mu$ m sized smooth structural features are result of the deposition method, which is CVD using TEOS as a precursor. Apart from this underlying structure many small objects are observed. These structures are aluminum containing impurities according to TEM investigations, their origin has not yet been conclusively determined. The peak to valley distance is 205 nm and the Rq is 20 nm. The corresponding KPFM image, like the topography, shows no significant features related to the SiO₂ surface. Same as in the topography, the impurities are visible in the KPFM. With a small lateral extent of about 50 nm and a potential difference between 50 and 100 mV, they are a good way of checking the resolution of the KPFM. The peak to valley distance in the KPFM signal is 1.02 V and the Rq is 67 mV.

Fig. 3.17: Amorphous SiO₂ investigated with AFM and KPFM. (a) Topography showing the basic structure of SiO₂. Furthermore, with a diameter of $\approx 50 \text{ nm}$ impurities can be seen, the origin of which is not clear. (b) shows the corresponding KPFM image. The impurities are also clearly visible here.

Chapter 4 Conclusion

In conclusion, this thesis has successfully introduced KPFM analysis as a method for characterizing ion traps in an industrial environment. The study utilized a commercially available AFM to investigate the surface properties of both single-layer and multi-layer ion traps, focusing on the aluminum and silicon dioxide surfaces. Through the simultaneous acquisition of topographic and potential maps, several factors influencing the surface potential of the electrodes were identified.

The findings revealed that grain boundaries play a significant role in determining the potential changes, with an average potential change of 57 mV attributed to grain boundaries. The presence of specific surface structures, such as "terraced" and "stepped" mythologies on the grains, was found to influence the potential of the aluminum electrode, leading to potential variations in the range of 30-250 mV. Moreover, variations in potential between different grains were observed, with deviations of up to 115 mV extending over multiple grains.

Notably, localized potential deviations of up to 790 mV were detected at both grain boundaries and within individual grains. While one instance of these fluctuations could be linked to topographical conditions, the majority of variations were found to be statistically distributed. To further investigate the impact of surface potential deviations on the electrical field and the secular frequency of trapped ions, a series of simulations was conducted, confirming that "large potential deviations" have a significant effect on both parameters.

Furthermore, the thesis explored the influence of laser exposure on the aluminum surface. Experimental results indicated that laser irradiation caused a significant charging effect, resulting in a 250 mV potential change. However, this effect was attributed to the use of silver conducting paste for electrical contacting. In contrast, when wire bonds were employed for electrical contacting, no charging was observed.

Additionally, an attempt was made to characterize silicon dioxide surfaces using the measurement setup. The study demonstrates the feasibility of obtaining high-resolution images of dielectric surfaces through KPFM analysis. Surface impurities on the silicon dioxide were successfully identified in the KPFM signal, exhibiting a lateral extension of approximately 50 nm and a potential deviation of about 115 mV compared to the surrounding potential.

Chapter 5 Outlook

In the present investigations AFM and KPFM have been found to be very useful techniques to investigate simultaneously topographic properties and local contact potential. Thus, possible future experiments of interest can be derived. As the experiments on aluminium have shown, there are various causes that can lead to local deviations in the surface potential. There is an opportunity here to look more closely at the origin of the different potential deviations. It would be interesting to find out whether there are structures that lead to a defined deviation of the potential. It would also be interesting to find out how such structural deviations can be avoided in the fabrication process or afterwards. It would also be of interest to investigate the influence of grain boundaries in more detail in future experiments. In the figures presented in section 3.3, which are used to determine the potential grain boundary distortion, large area $(25 \times 25 \,\mu m^2)$ images are used which allow only an approximate assessment of the influence. For a more accurate determination, several small area images $(4 \times 4 \,\mu m^2)$ could be taken focusing on GB. This would not only allow a better assessment of the effect of GBs on potential, but would also allow any differences between individual GBs to be determined. It would also be interesting to investigate the origin of the "large (CPD>230 mV) potential deviations". Combined analyses to determine possible structural or qualitative differences of these regions would be of interest. Experiments aimed at eliminating these fluctuations are also possible.

In addition to the proposed experiments, which are ex situ surface analytical experiments, more elaborate experiments investigating the influence of different surface parameters on a trapped ion would be of interest. For this purpose, identical ion traps could be fabricated, differing only in parameters such as grain size, potential roughness etc. The respective heating rates could provide information about the influence of the different surfaces. A systematic study of laser illumination is also worth an attempt, despite the unpromising results so far. Since the laser was only a laser pointer and the setup itself was not very professional, it is possible that different results could be obtained by improving the measuring device. Furthermore, the potential change of the ion trap, which was contacted with silver paste and illuminated with a laser, is an indication that laser exposure can have significant and long-lasting effects under certain circumstances.

In addition to further experiments on metallic surfaces, experiments on dielectrics are also possible. In this paper, it is only shown that the described experimental setup allows high resolution images. The setup could be used for experiments on charge dynamics in dielectrics. Similar to the laser experiments on aluminium surfaces, experiments on the influence of lasers on dielectrics are also conceivable. It would be interesting to see how different deposition parameters and dielectrics affect the residence time of charges in the dielectric. Finally all the experiments shown have been carried out in air and at room temperature, but ions are trapped in (ultra-) high vacuum and cryogenic environments. Thus, it would be of interest to carry out all the experiments under such conditions.

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