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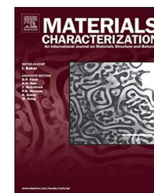

Advanced data mining in field ion microscopy

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ABSTRACT

Field ion microscopy (FIM) allows to image individual surface atoms by exploiting the effect of an intense electric field. Widespread use of atomic resolution imaging by FIM has been hampered by a lack of efficient image processing/data extraction tools. Recent advances in imaging and data mining techniques have renewed the interest in using FIM in conjunction with automated detection of atoms and lattice defects for materials characterization. After a brief overview of existing routines, we review the use of machine learning (ML) approaches for data extraction with the aim to catalyze new data-driven insights into high electrical field physics. Apart from exploring various supervised and unsupervised ML algorithms in this context, we also employ advanced image processing routines for data extraction from large sets of FIM images. The outcomes and limitations of such routines are discussed, and we conclude with the possible application of energy minimization schemes to the extracted point clouds as a way of improving the spatial resolution of FIM.

1. Introduction

Field ion microscopy (FIM), invented in 1951 by Erwin Müller [1, 2], is a high electric field technique which uniquely enables imaging of surfaces with atomic resolution. FIM is based on ionization of an imaging gas in the vicinity of a field-emitter tip as a consequence of the locally high electric field. The high electric field is achieved by applying a high voltage of a few kilovolts onto a very sharp needle-shaped specimen maintained at a temperature usually below 80 K. Specimens are either electropolished [3] or milled with a focused ion beam (FIB) [4] into a very sharp needle tip with an end radius below 100 nm. The advantage of using FIB for specimen preparation lies in its site specific application for extracting tips in microstructure regions of high interest such as across internal interfaces. An excellent review on using FIB for site specific specimen preparation can be found in reference [4].

Once the specimen is mounted an imaging gas is introduced. The introduced imaging gas gets attracted by the cold surface due to polarization forces. The gas atoms then thermally accommodate with the cold tip surface by performing a series of " hops". Surrounding the tip surface there exists a critical zone, where the maximum ionization occurs. This surface usually lies around 1–4 Å above the tip [5]. During the " hops", the ionization probability for the gas atoms can be considerable as they spend a significant amount of time in the critical surface. As a consequence an electron can tunnel from the imaging gas atom into the tip. The ionized gas atom is accelerated away from the positively biased tip and towards the detector, where gas ions contribute to image formation.

The surface is the intersection of the crystalline lattice with the imposed end shape, often approximated as nearly-spherical. Owing to the discreteness of the atomic arrangement at these scales the tip apex curvature is, in reality, made of atomic scale crystallographic terrace features where some of the top, edge and corner atoms are naturally protruding, producing local electrostatic field enhancement. This means that these exposed atomic terrace positions are sites of magnified electrostatic field strength and also of aberrated field direction. The amount of gas atoms ionizing depends on such a local enhancement of the electric field. This variation in electric field strength across the surface atoms gives the final contrast in the FIM image. The contrast in FIM also depends on the gas supply function and adsorption behavior [6-8]. Atomic resolution can be attained in some cases on certain high index facets where the surface field distribution is corrugated enough to give contrast in the image. By collecting the gas ions on a phosphor screen, an image is formed that reveals the distribution of the electrostatic field near the surface and the current created by the number of incoming imaging gas ions.

Historically, images were collected on a film in a dark room after sufficient exposure on the screen was achieved by field ionization [1]. Eventually, field ion microscopes were fitted with a stack of micro-

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channel plates (MCP) in-front of the phosphor screen. The image on the phosphor screen can be recorded with a high-resolution high-frame-rate camera. The MCPs act as a photo multiplier by creating an electron cascade in response to the gas ion impact. Another variant of FIM is referred to as eFIM™, which is performed on a local electrode atom probe (LEAP) [9] using the delay-line detector used in the atom probe mode.

The atomic resolution of FIM made it a popular technique for studying internal interfaces [10-12] and dislocations [13-15] at unprecedented atomic positioning resolution. When exposing the tip not only to the minimum field strength required for ionizing the imaging gas but also for evaporating the tip atoms themselves continually, the method is rendered depth sensitive. This means that the specimen can be investigated tomographically along the tip longitudinal axis, which has led to the development of 3DFIM [16]. The emergence of atom probe tomography (APT), which is additionally able to characterize the chemical identity of the imaged atoms, has led to some decline in the usage of the FIM technique by the materials science community. Nevertheless 3DFIM offers the important advantage over APT of a significantly higher spatial resolution with 100% positional detection efficiency in 3 dimensions in some cases. This high degree of positional accuracy allows characterization even down to single point defects in a material, a feature not offered by any other technique. This causes currently an increased interest in the 3DFIM technique.

Ultimately, owing to all the advances in detector technology, 3DFIM is capable of producing large and accurate tomographic datasets containing information on sequential atomic positions. These large datasets lead to a new tremendous challenge of how to manage the data. Presently, there is a lack of efficient data handling and data treatment algorithms to extract pertinent information from these datasets in an (a) automated; (b) fast; (c) user-independent; (d) and error quantified manner. For instance, characterization of a volume of 0.001 μm^3(a typical sample size analyzed in 3DFIM) produces in the range of 2×10^5 images (assuming a constant field evaporation rate and capture speed). Hence, there is a great need for efficient algorithms and data mining routines to fully exploit the potential of 3DFIM. To this end, M. Dagan et al. [17] have proposed an atom by atom data extraction routine for reconstructing 3DFIM data. Building on their work we recently proposed a new method to extract atomic positions from 3DFIM datasets [18]. With this article, we focus our attention on using various modern image processing and machine learning algorithms for extracting information from 3DFIM.

The developments in Artificial Intelligence (AI), especially in computer vision have been explosive. Modern machine learning algorithms enable a fully automated detection and classification of objects in a picture. We give an overview about these advanced data mining tools and how they can be utilized to extract the wealth of information from 3DFIM images. We have implemented some of these concepts within a set of routines in Python™ (Python Software Foundation; Python Language Reference, version 2.7; Available at http://www.python.org) employing the SciPy package [19]. These routines allow us to extract the relevant information from a large number (order of several 10,000 s) of FIM images in very short computational times (order of minutes).

2. Existing Data Extraction Routines for 3D Field Ion Microscopy

A 3DFIM experiment produces a series of images of the continually field evaporating surface. A main challenge lies not in acquiring such large datasets but rather in analyzing them. The article by Vurpillot et al. [20] serves as an excellent review for the current state-of-the-art and the main issues associated with data extraction from large FIM datasets. We briefly review here the available analysis methods and also some recent developments. Broadly speaking the analysis methods can be categorized into an atom by atom approach and a geometrical approach.

The first approach towards advanced 3DFIM analysis was already developed in the early 70s for characterizing radiation damage in metals at the atomic scale [21, 22]. In these early approaches FIM images were captured on film which later were developed and manually analyzed individually. The captured FIM images were dissected atom-by-atom and the positions of atoms and defects were marked manually. Owing to the associated cumbersome analysis methods, systematic FIM studies of more complex atomic scenarios remained an exception. Taking the additional disadvantage of 3DFIM of being insensitive to the chemical nature, APT became gradually the more dominant technique. Yet, FIM's ability to characterize atomistic defects such as vacancies in three dimensions is still unparalleled with any other technique. In this context the drastic increase in computing power became an essential asset when Dagan et al. developed an automated method to reconstruct 3DFIM data atom by atom [20, 23]. The algorithm takes advantage of layer by layer evaporation and the atoms are identified based on a threshold intensity. The final coordinates are converted to real space based on theoretical nearest neighbor distances. This work led to a rise in interest around the physics of image formation in FIM and also in the use of the associated computationally enhanced analysis techniques.

The geometrical approach to 3DFIM atomic position reconstruction introduced by Vurpillot et al. consists in stacking the digital images obtained from a 3DFIM experiment [16]. The image stack is then corrected, assuming a known projection law, a specimen's geometry and a constant evaporation rate. The stacking approach does not provide atomistic precision but is rather used for investigation of segregation, clustering and fine scale precipitation studies [24-28]. This method can also be used to identify crystallographic planes and dislocations which are hard to spot in a 2DFIM image.

Both the atom by atom reconstruction approach and the geometrical method suffer from their own limitations. For instance, the atom-by-atom approach is limited to regions with atomic resolution, and thus a 3D reconstruction is only possible around certain high index facets. The geometrical approach looses the atomic positioning precision due to the simplistic geometrical assumptions of the tip shape. In the following sections we showcase how various data extraction methods can be employed to further improve the atom-by-atom analysis approach and recover as much positioning information as possible. In addition, the use of machine learning algorithms to extract the physics behind field ionization and evaporation is also explored.

3. Supervised and Unsupervised Machine Learning

Machine learning (ML) algorithms are currently exploited to derive systematic insights from very rich experimental datasets and for solving complex problems in various disciplines [29]. Progress in ML has led to decision rules that can in some cases be automatically derived by specific algorithms that are capable of learning, whilst exploiting the speed and the robustness of the available advanced computer infrastructure.

Machine-learning methods can be grouped into two major categories depending on the approach to a given problem viz. supervised and unsupervised learning [30]. Supervised learning algorithms try to identify the relationship between input and output. This dependency is learned as a function $f(x)$ by using a set of labeled data $\{X = [a_i,b_i]$, $i = 1,\ldots,N\}$ consisting of N pairs (a_1,b_1), (a_2,b_2) , … , (a_N,b_N), where the input variables a_i are D-dimensional vectors $a_i \in R^D$ and the output variables (or system responses) b_i are discrete values (e.g., Boolean) for classification problems and continuous values ($b \in R$) for regression tasks. Support Vector Machines (SVMs) and Artificial Neural Networks (ANN) are widely used techniques that fall in this category. Typical tasks that can currently routinely be carried out by a supervised machine learning algorithm are image segmentation and classification. In the computer vision community, semantic segmentation, which is an extremely challenging task, aims to partition the image into semantically meaningful parts (such as differentiating a cat, a car or Einstein in the same image), and to classify each part into one of the predetermined

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