Final Publishable JRP Summary for IND54 Nanostrain
Novel electronic devices based on control of strain at the nanoscale

Overview

The development of faster, smaller and more energy efficient computing is a technology goal that has far reaching consequences in every conceivable market sector. As current technology approaches the limit of processing power and size, innovative solutions are being developed by global leaders in semiconductor research. Novel electronic devices that exploit control of materials properties at the nanoscale via the application of strain, have the potential to be the next generation of processors. They are uniquely capable of generating precisely defined strains at very small scales, and as such are the technology driver for this new type of electronic switch. This project has developed new measurement tools and models to characterise strain at the nanoscale to aid in the understanding and development of these novel transistors.

Need for the project

Moore's Law predicts ever increasing processing power with the doubling of transistor density every two years, however traditional scaling trends of transistor miniaturisation that accompany Moore's Law have a physical size limit predicted to occur within the next decade. Meeting the need for faster and more compact computing needed for industrial competitiveness will therefore depend on developing new transistor and memory technologies.

Amongst the raft of new technologies fighting to supersede traditional complementary metal-oxide semiconductors (CMOS) is a novel concept in nanoelectronic device design based on the precise control of strain within nanoscale materials using piezoelectric materials. The active part of the transistor is achieved by electro-mechanical coupling in a piezoelectric material, i.e. the generation of a strain through the application of voltage to the device. In order to aid the design and manufacture of these devices, new characterisation and modelling tools are needed to measure and predict the strain within these materials and devices. However, there is presently no metrological framework or facilities for traceable measurement of the electro-mechanical coupling in piezoelectric materials at the required scale.

The project's scientific and technical objectives are intended to support the industrial development of new functional materials inspired devices and products by developing suitable metrological techniques for strain measurement. The measurement infrastructure is required to facilitate faster development of new materials and more rapid implementation into new devices, thus providing a competitive advantage to European industry.

Scientific and technical objectives

The aims of the project were to develop the metrological infrastructure and facilities within Europe for the traceable measurement of strain in piezoelectric materials for the semiconductor industry, including production equipment and instrument manufacturers.

The first three objectives examined and compared different measurement techniques; namely X-ray diffraction, optical microscopy and transmission microscopy. The fourth objective looked at modelling on the molecular level to facilitate the development of new materials. The final objective looked at extending digital image correlation as another possible measurement technique.

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EMRP
European Metrology Research Programme
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The specific objectives were to:

- Develop links between traceable strain metrology and crystallographic strain via in-situ interferometry and synchrotron X-ray diffraction. This enables a comparison of the intrinsic piezoelectric response (movement of atoms or ions) using X-ray diffraction, to the extrinsic response (movement and reordering of domains and grains), using interferometry.
- Develop ultra-high spatial resolution (100 nm or less) optical methods of strain measurements using infra-red scanning near field microscopy (IR-SNOM) using the PTB synchrotron radiation facility (MLS) in Berlin as an IR light source.
- Develop traceable validation of macroscale strain metrology in destructive methods including Transmission Electron Microscopy (TEM) and novel holographic TEM, to map intra-grain residual and active (electric field induced) strains. A particular issue with TEM measurements are the artefacts induced during preparation, so the uncertainty caused by the additional strain from the preparation of TEM slices was also investigated.
- Develop multiphysics materials modelling to underpin all the experimental activities described above, considering both residual, process-related strains in thin film and nano/micro-scale released structures, and electrically driven strains in active devices.
- Extend the use of Digital Image Correlation processing to nano-scale functional atomic force microscopy (AFM), scanning electron microscopy (SEM) and other strain mapping images.

Results

Develop links between traceable strain metrology and crystallographic strain via in-situ interferometry and synchrotron X-ray diffraction.

The main objective here was to add an in situ interferometer to the diffractometer at project partner XMaS's X-ray beamline at the European Synchrotron Radiation Facility (ESRF) in Grenoble. This was a challenging task considering the mechanically and electrically noisy environment of the beamline, as well as the multiple rotation axes of the diffractometer goniometer. The system was built in collaboration with SIOS, a leading interferometer manufacturer, and tested on single crystal bulk piezoelectric samples. These tests showed excellent agreement between the overall changes in length of the sample measured using the interferometer compared with the intrinsic atomic movements as measured by X-ray diffraction. This links atomic movements with the real world physical movements that are required for a working device.

Much of the work involved upgrading and extending the XMaS X-ray beamline at the ESRF in Grenoble. Although other beamlines have since developed similar capabilities, it is the only beamline worldwide to include simultaneous interferometric measurements. The measurements on bulk samples showed excellent agreement between interferometric data and X-rays. However for thin film samples the results showed that a better understanding was needed of the strain state in thin films in order to carry out piezoelectric measurements.

This work has stimulated other collaborations, not originally part of the project plan. In collaboration with the Diamond Light Facility at Oxford, NPL developed a new method for discriminating thin film and single crystal piezoelectric strain using Diffuse multiple scattering, providing full field imaging advantages. There was also a follow-on project to add magnetic capabilities to the beamline. A magnet assembly was designed and implemented allowing DC magnetic fields to be applied simultaneously with the in-situ interferometry, X-ray and polarization measurements. Experiments on a multiferroic BiFeO3 thin film, supplied by a collaborator, have shown differences to the strain response with and without magnetic field.

The final improvement to the XMaS capability involved extending the measurement frequency of the system into the MHz range. The original intention of this upgrade was to investigate the effect on the piezoelectric response of increased frequencies, but in fact the unforeseen advantage of the new setup was the faster turnaround of data output and quality at the lower frequencies.

This objective was completed successfully, an interferometer was installed on an X-ray beamline for the very first time, and measurements have shown the importance of comparing the change of lattice plane spacing measured by X-ray diffraction with the actual change of length of the sample.

Develop ultra-high spatial resolution (100 nm or less) optical methods of strain measurements using IR-SNOM,

Two high lateral resolution optical techniques were developed for the characterisation of materials and strain: confocal Raman spectroscopy and near-field infrared microscopy (IR-SNOM), as well as nano-Fourier transform infra-red spectroscopy (FTIR).

Confocal Raman spectroscopy is a non-destructive laser based technique able to provide information about material composition, crystallinity and strain fields with a lateral resolution of several 100 nm. Micro Raman spectrometry was used to characterise piezoelectric thin films with respect to their composition and lateral homogeneity, but low Raman activity in these materials meant that quantification of strain with this method was difficult. As a consequence the quantification of strain could only be carried out on non-piezoelectric materials with a higher Raman activity. Bulk silicon carbide and graphene films were investigated, mapping the strain produced as a result of nanoindentation, and graphene was found to have a very high strain sensitivity making it a candidate for an ultra-low strain sensor.

IR spectroscopy is also an optical method and provides complementary chemical information of a sample. In combination with near-field approaches IR-SNOM was able to circumvent the optical diffraction limit, providing a spatial resolution below 40 nm. The group at the PTB low-energy storage ring, used the Metrology Light Source (MLS) as an ultra- broadband IR synchrotron source to increase the accuracy of the technique taking advantage of the higher source brightness. This enabled the acquisition of the full photon resonance in silicon carbide samples, thus enabling a more accurate determination of the spectral bandshifts than previously possible.

This objective was largely completed, and both methods were used to characterise strain at the nanoscale. However because of the low Raman activity of the available piezoelectric materials it was not possible to measure the strain as a result of the piezoelectric effect.

Develop traceable validation of macroscale strain metrology in destructive methods including TEM and novel holographic TEM, to map residual and active (electric field induced) strains.

TEM offers the ability to image down to the nanoscale, and although chemical and crystallographic information are routine the techniques to measure and quantify strain are less common. The objective was to apply novel TEM based holographic methods to the measurement of piezoelectric strain. Successful in-situ electron microscopy experiments for measuring strain, rely on optimising the process: thin lamella preparation, electrical contacting, observation and analysis. The production of TEM samples free from preparation induced defects has been a concern for piezoelectric materials, and the group at BAM developed a staircase-like structure that enables different surface finishes and thickness within one lamella sample to be explored. In addition, preparation techniques were optimised to minimise surface layer amorphisation. In collaboration with NPL, the group investigated the effect of a gallium Focused Ion Beam on the electrical properties of the piezoelectric and the results were presented at an international conference. The CNRS group used these defect free lamella and carried out the very first strain measurement in PZT (lead zirconate titanate perovskite, a piezoelectric material) and piezoelectric single crystal thin films by dark-field electron holography. Initially nanoindentation was used to image in-situ material's response as function of applied stress, but subsequently the nanoindentor was used to apply an electric field to a lamella, and the resultant strain imaged in situ.

This objective was fully completed. TEM was used to measure strain in piezoelectric materials at the nanoscale. While the TEM method has a much better spatial resolution than for X-ray diffraction, the sample preparation is more complex and testing more time consuming.

Develop multiphysics materials modelling

This objective was to provide a theoretical insight into the origin and control of strain in nano-scaled piezo- and ferroelectric materials, both to support the experimental work in this project and to provide tools for future device development. Most of the modelling work related to piezoelectric materials is currently at the mesoscale, using Finite Element Analysis (FEA) or analytical methods. The focus here was to develop atomistic models, using first principles i.e. ab initio simulation methods that would enable the exploration of different material architectures and structures. A simple nanocapacitor was modelled and the properties of the metal/piezoelectric interface was investigated as a function of the crystallography of the boundary. The issue of scalability was also investigated; looking at how small the device is before the piezoelectric effect is lost. The nanocapacitor (a Pt/PZT/Pt system) was shown to have stable ferroelectric states at all thicknesses and terminations, an important discovery for the future miniaturisation of devices.

The theoretical work complemented experiments. The temperature dependence of polarization switching in PZT was investigated with molecular dynamics simulations. The polarisation switching mechanism was found to be fundamentally different at low temperatures, where switching occurs via polarisation rotation, than at high temperatures, where domain nucleation dominates. The results showed that the apparent loss of ferroelectricity at low temperatures was due to insufficient applied magnetic field during experiments, and repeat experiments using higher fields confirmed the findings.

Extend the use of Digital Image Correlation processing to nano-scale functional atomic force microscopy, SEM and other strain mapping images.

Within this objective the use of Digital Image Correlation was extended to nanoscale functional AFM and SEM to characterise piezoelectric strains. Optical imaging DIC was successfully demonstrated, including measuring shear strain, however the SEM based imaging DIC revealed technique limiting artifacts. In fact these artifacts had been noted in other studies outside this project, however the work here concentrated on successfully identifying the cause of these artifacts and developed ways to minimise them.

The modelling part of this objective was completed, generating a suite of atomistic modeling routines that were proven by simulating piezoelectric materials. The visualisation using DIC was also completed, however the use in AFM methods was limited by the inherent noise of functional AFM imaging. In addition NPL developed methods to extend DIC to the measurement of piezoelectric strains.

Actual and potential impact

Dissemination of results

16 scientific papers were published in peer reviewed journals. There were several high profile articles in the trade press, initially to promote the beginning of the project, and towards the end to coincide with recent interest in energy consumption of server farms, (www.computerweekly.com/opinion/Reinstating-Moores-Law-a-next-gen-transistor-for-mobile-technology). The project website was hosted on the piezo institute website. Seven newsletters, 4 webinars and over 50 presentations/ tutorials were given by consortium members. Good practice guides, hosted on the XMaS beamline site, gave practical information about the equipment and how to operate it.
(http://www2.warwick.ac.uk/fac/cross_fac/xmas/other_projects/nanostrainproject/ and http://www2.warwick.ac.uk/fac/cross_fac/xmas/xmas_offline/electrical_measurements/)

Impact on standards

Although the Nanostrain activity was largely pre standards, the results on evaluating measurement best practice were fed into VAMAS, who develop the standards for advanced materials. Participation in this group led to the development and publication of the ISO TC206 standard (NP1013) on high strain measurements of piezoelectrics.

Actual impact

The outcomes of the project have led to the development of some unique and world leading facilities to characterise piezoelectric devices, which are now available for use by researchers worldwide.

- The in-situ facilities at XMaS have been in high demand and resulted in many new collaborations with high profile research groups at the University of Wisconsin, and Penn State

- A new analytical capability, synchrotron-based nano-FTIR spectroscopy was established at the PTB low-energy storage ring, the MLS and is available for users.
- The DIC expertise developed during the project is now freely available for users of the open source AFM analysis package Gwyddion.
- The development of ab initio modelling capabilities the origin and control of strain in nano-scaled piezo- and ferroelectric materials, mostly at NPL, resulted in requests to access the expertise in modelling oxide films from a company developing dielectric coatings.

The project also helped to train young scientists working in this field, both within and beyond the consortium. The establishment of these new capabilities were the scientific and technical objective of the project and will support industry to develop the next generation of processors.

Potential impact

The partners involved in the Nanostrain project will continue their collaboration, and further develop the expertise and capabilities started in Nanostrain in two related follow on European projects. The first of these is the European Horizon 2020 project PETMEM (Piezoelectronic Transduction Memory Device). This is a European partnership of Universities, Research Institutions, SMEs and businesses including IBM, SolMateS and aixACCT that aims to build a proof of concept prototype PET memory device and to develop the tools and processes to allow other people to design with and make piezoelectric transistor technology. Alongside PETMEM is the EMPIR project, “Metrology for advanced energy-saving technology in next-generation electronics applications”. A consortium has been established, which includes some of the Nanostrain partners such as NPL and PTB, with the PETMEM project included as a supplier of materials and devices. The ADVENT project will look at low-powered high efficiency microelectronics, with the aim of developing the suite of metrology needed for industry to develop and to use low powered materials, electronics, components and systems.

In the longer term the development of the new technologies from this project will help stimulate innovation in the microelectronics industry, with consequential economic benefits in ensuring strong European participation in the growth of the nanotechnology market. Additional environmental benefits arise from the reduced energy requirements of electronic devices utilising this technology, and therefore increased battery life of devices. Better sensing and electronic technologies will also increase the speed of computers.

List of publications

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