



Project no. 013862

Project acronym: INCEMS

Project title: Interfacial Materials – Computational and Experimental Multi-Scale Studies

Instrument: Specific Targeted Research Project

Thematic Priority: NMP-2003-3.4.2.1-2 Modelling and design of multi-functional materials

## **Publishable Final Activity Report**

Period covered: from 01/07/2008 to 30/06/2009

Date of preparation: 10/08/2009

Start date of project: 01/07/2005

Duration: 48 months

Project coordinator name: Peter Gumbsch

Project coordinator organisation name

Universität Karlsruhe (TH)

Kaiserstraße 12

76131 Karlsruhe

Germany

Revision 0

## Publishable final activity report

### INCEMS: Interfacial Materials – Computational and Experimental Multi-Scale Studies

INCEMS was a multidisciplinary team of leading EU experts in modelling and experiment of materials who joined their efforts for four years. It intended to predict the complex properties of industrially relevant multifunctional ceramics with interfaces like crystalline grain boundaries or nanometer-scaled intergranular films (IGF) by investigating and tailoring the materials phenomena governing the complex behaviour resulting from electric fields, and from interactions with different chemical environments. By using computational modelling at different length scales, from *ab-initio* quantum-theory to macroscopic continuum-theory approaches, we analyzed the stability, structure and composition of interfaces including the effect of chemical doping to identify conditions under which transient IGFs are formed at will during processing, and we explored strategies by which IGFs could be formed, modified or eliminated by an appropriate processing treatment to provide optimal properties for devices performance and durability. Scientific ideas for a new type of phase diagrams, an interfacial phase diagram, that includes the equilibrium properties of defects, such as the thickness of interfacial films, were explored in order to prepare a future general tool for designers of materials and processes. Based on the predictive models developed by the INCEMS consortium it will become possible in future to efficiently optimize existing ceramic-based devices and to develop completely new ones with higher functional density and new device application.

- project objectives:

INCEMS effectively studied ceramic interfaces by combining computational modelling across all length scales, from atomic structures to real-life devices, with a strong and critical validation by experiments. The target material for INCEMS was polycrystalline SrTiO<sub>3</sub> (STO) with varying microstructures, species and concentrations of defects and dopants.

This has been realised by:

1. Developing a next generation of theoretical models that will treat complex but technologically relevant impacts of multi-component chemistry, space charges and dispersion forces on the thermodynamic stability of interfaces. Modelling tools vary from *ab-initio* to continuum and are able to describe electronic and atomic structure (*ab-initio* theory, atomistic simulation), composition and stability of grain boundaries (phase field theory, self-consistent classical density functional theory - SCCDFT) as well as microstructural evolution (vertex dynamics).
2. Integrating the individual models to validate and inform companion methods, and to derive self-consistent descriptions of the material behaviour across all length scales.
3. Preparing materials with technologically relevant fabrication methods having decisively controlled compositions, grain boundaries and grain sizes. These materials are the basis for the characterization work as well as for the measurement of macroscopic properties for correlations with model predictions.
4. Experimental characterization of complex interfaces that typify those in real materials
5. Iterative validation of the models by experiments
6. Delivering predictive tools for the design of materials and processes that will promote a technological paradigm shift in materials design for microstructure.

## Participant organisations and principal investigators (with acronyms)

- University of Karlsruhe, Germany (UniKarl)
  - Peter Gumbsch and Michael Hoffmann (PG, MH)
- University of Oxford, United Kingdom (UOXF)
  - David Cockayne (DC)
- Imperial College, London, United Kingdom (Imperial)
  - Adrian Sutton and Michael Finnis (AS, MF)
- Max-Planck Institute for Metals Research, Stuttgart (MPG)
  - Manfred Rühle (MR)
- University of Ljubljana, Slovenia (UL)
  - Rudolf Podgornik (RP)
- Commissariat à l'Énergie Atomique, Paris, France (CEA)
  - Martine Gautier-Soyer (MG)

## Project coordinator:

Prof. Dr. Peter Gumbsch  
Universität Karlsruhe (TH)  
Kaiserstraße 12,  
76131 Karlsruhe  
Germany

## Project logo:



Project website: <http://www.mf.mpg.de/INCEMS/>

## Final project status after four year:

### Experimental investigations:

- Further sets of polycrystalline SrTiO<sub>3</sub> materials with varying microstructures, defect and dopant compositions were synthesized in Karlsruhe (MH) by sintering of powders under carefully controlled conditions. The microstructures and interfaces of these materials were characterized in Paris (MG) by photoelectron spectroscopy (XPS, UPS) and by reflection electron energy-loss spectroscopy (REELS), in Oxford (DC) by high-resolution transmission electron microscopy (HRTEM), by electron back-scattering diffraction (EBSD), and by high-angle annular-dark-field scanning transmission electron microscopy (HAADF-STEM), and in Stuttgart (MR) by HRTEM, and by transmission electron energy-loss spectroscopy (TEELS).

The most important and unexpected outcome from these experimental investigations in the first two years was that no evidence had been found for the existence of IGFs in these polycrystalline SrTiO<sub>3</sub> materials, which were highly pure or doped in well controlled manner, and that many analyzed grain boundaries were rather sharp and well ordered on the atomic scale. The major subsequent experimental effort was to vary the materials synthesis systematically and even better controllably, in order to determine processing conditions for a formation and, subsequently, a suppression of IGFs at will. The experimental challenge for the last two years was to augment interfaces in polycrystalline ceramic materials by interfaces in bicrystals. These extended the possibilities for controlled variations of interface structure

and composition in the search for the formation conditions of IGFs, which still remained absent although, and for atomic-scale characterisations by microscopy, spectroscopy, and theory, which developed indeed to a very productive and insightful line of activities.

Modelling and simulation:

- Computational methods and material models for all length scales were running productively: On the atomic scale, ab-initio electronic-structure calculations for stoichiometric  $\Sigma 3$  symmetrical tilt grain boundaries (twin interfaces), (111) stacking faults and (110) antiphase boundaries in pure SrTiO<sub>3</sub>, and for SrTiO<sub>3</sub>/Pt, BaTiO<sub>3</sub>/Pt and various other perovskite/metal interfaces were done in Karlsruhe (PG), ab-initio calculations for non-stoichiometric  $\Sigma 3$  twin interfaces, as interface models with less structural order, were pursued in London (MF). Also in London (AS) the degrees of structural order at a variety of atomic-scale models for asymmetric  $\Sigma 3$  grain boundaries,  $\Sigma 5$  twist and tilt grain boundaries were explored by empirical atomistic simulations. The self-consistent classical density functional theory (SCC-DFT) approach for thermodynamic modelling had been completed successfully for the one-component system silicon. The extension to the multi-component system SrTiO<sub>3</sub> had turned out to be conceptually too problematic and therefore no longer pursued. Thermodynamic phase-field modelling with meso-scale incorporation of interface properties was continued in Oxford (DC), microstructural vertex-dynamics modelling and simulation made strong progress in Karlsruhe (PG), and calculations of IGF properties by dispersion-force theory were continued in Ljubljana (RP).

The important output of the theoretical activities was that the needed theoretical and computational approaches on all relevant length scales got set up and operating for INCEMS. The decision to abandon SCC-DFT after the first two years and to concentrate on atomistic simulations with empirical potentials in the last two years has turned out to be very fruitful. By linking to first-principles calculations and to bicrystal experiments, the atomistic simulations enabled us to obtain a clear understanding of strengths and weaknesses of empirical interatomic potentials that had been originally developed for bulk SrTiO<sub>3</sub>, when applying them to SrTiO<sub>3</sub> interfaces. The major subsequent theoretical efforts used the atomistic simulation methods for supporting the search for criteria why no IGFs were detected so far in the experimentally investigated SrTiO<sub>3</sub> ceramics, and for elucidating thermodynamic and kinetic mechanisms at the sub-nanometre scale which could lead to the formation or suppression of IGFs at the sub-micrometre scale.

In addition to this summarized research work, continuous efforts were carried on in the last two years for the dissemination of knowledge, namely numerous invited and contributed presentations by INCEMS participants were given on international scientific conferences, and numerous papers were published or accepted for publication in refereed international journals. The board of five industrial advisors from five large European companies who are themselves experts in functional ceramics for industrial applications, continuously supported INCEMS by giving guidance to the scientific research work through their thoughtful advises.

The intensive and constructive scientific interaction of the eight groups of experimentalists and theoreticians at the six European locations, through the semi-annual project meetings, mutual discussion visits, semi-automated data-exchange procedures, during the four project years was working so well and synergistically that the final goal of INCEMS, a predictive multi-scale modelling of interface-controlled functional ceramic materials was achieved in by far most of the addressed aspects.

Final project status concerning the five research work packages in more detail

### **WP1: Cooperative knowledge exchange (MR)**

The objective of this workpackage 1 was to promote the most distinguishing feature of the INCEMS project: the close linkage of modelling across different length scales as well as between theoretical modelling and actual experiments (see Figure 1 for an illustration of the cooperative structure of the INCEMS consortium). Both sides (i.e. modelling and experiments) have attacked the same systems as closely as possible, and have benefitted from the other by the insight and information that is not accessible using any single approach: i.e., accessing relevant knowledge that can only be reached through extensive knowledge exchange between groups. Within INCEMS this knowledge exchange has been facilitated in the following ways:

- Exchange of data sets among the modelling groups and between modelling groups and experimentalists.
- Definition of common data formats, protocols for the exchange of experimental data and theoretical atomic positions, and design of suitable data reduction methods.
- Round robin tests: Relaxation of atomic structure models by a genetic algorithm (GA) developed within INCEMS and density functional theory (DFT) methods and simulation of high-resolution transmission electron microscope (HRTEM) images from atomistic models predicted by these theories and their comparison with experimental images (see the WP2 and WP3 reports for details).
- Allowing a direct comparison between theory and experiment by properly choosing the right sample geometry for each one of the methods, i.e. bicrystals for comparing atomistic simulations with HRTEM, electron holography, and spectroscopy and polycrystalline ceramics for comparing vertex dynamics simulations with grain growth studies, grain orientation and local work function mapping as well as holography (see the WP2, WP3 and WP4 reports for details).
- A website [www.mf.mpg.de/INCEMS](http://www.mf.mpg.de/INCEMS) has been created very early in the project to facilitate the exchange of information and data. This site hosts, for example, talks presented by the different INCEMS partners at the our semi-annual meetings and protocols thereof, all publications that have come out of this work, as well as a number of experimental and theoretical data sets to be exchanged between the groups.

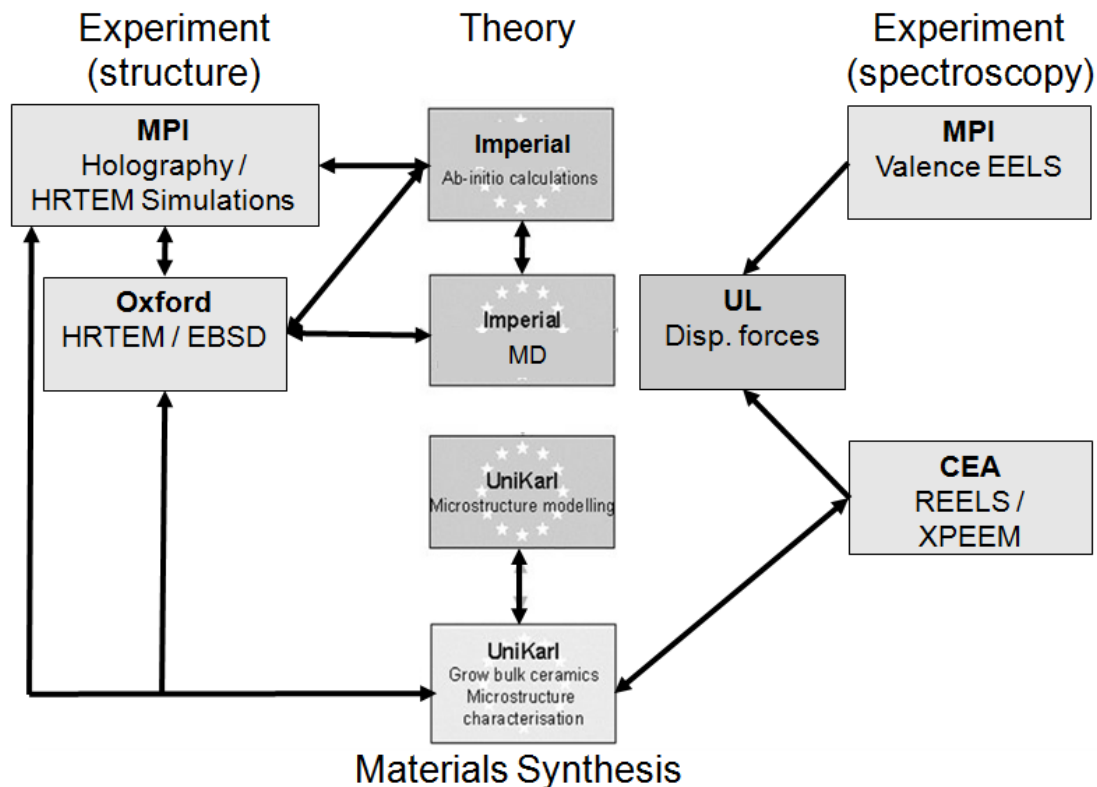


Figure 1: Diagram illustrating the exchange of theoretical modelling data, experimental data and samples between the different INCEMS members.

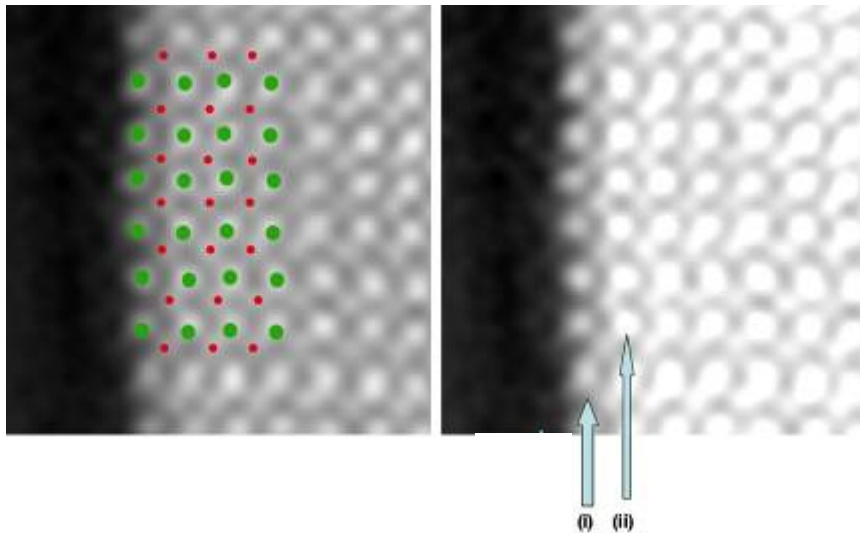
## **WP2: Atomic and electronic level (MF,DC)**

The objectives of this WP2 have been to obtain, by correlation of theoretical calculations with experimental observations, a description of atomistic and electronic structures of interfaces with special emphasis on the role of defects. The tasks to reach these objectives have been the following:

- Calculation of relaxed atomic coordinates and electronic structure for interfaces using ab-initio methods
- Calculation of formation and segregation energies of oxygen vacancies at interfaces using ab-initio methods
- Scale-bridging Modelling of defect distributions and electrostatic potentials at interfaces
- Experimental atomic-scale measurement of optical properties and electronic structures of interfaces with high spatial and/or energetic resolution (XPS, REELS, TEELS)
- Quantitative comparison of modelling and simulation results with experimental data in order to achieve reliable and predictive interpretations of experimental observations down to the atomic level.

One illustrative case for this is the structure determination for an atomically flat asymmetric GBs with one grain terminating in a  $\{100\}$  plane (termed GB $\{100\}$ ) in undoped SrTiO<sub>3</sub>. This system has been investigated in detail by (i) comparing high resolution transmission electron microscopy (HRTEM) image simulations with experimental HRTEM images taken at varied focal values, and (ii) high angle annular dark field scanning transmission electron microscopy (HAADF STEM) imaging, to discriminate possible from impossible atomic models for the GB $\{100\}$  boundaries. The results confirm that the GB $\{100\}$  surfaces are most likely SrO terminated with a further incomplete TiO plane..

Fig. 1 shows HAADF STEM images of the GB{100}, with the final SrO layers indicated by (i) and (ii). Four possible defect models based on SrO termination of the GB{100} have been proposed and investigated. Two further atomic models from the literature [1] [2] were examined.

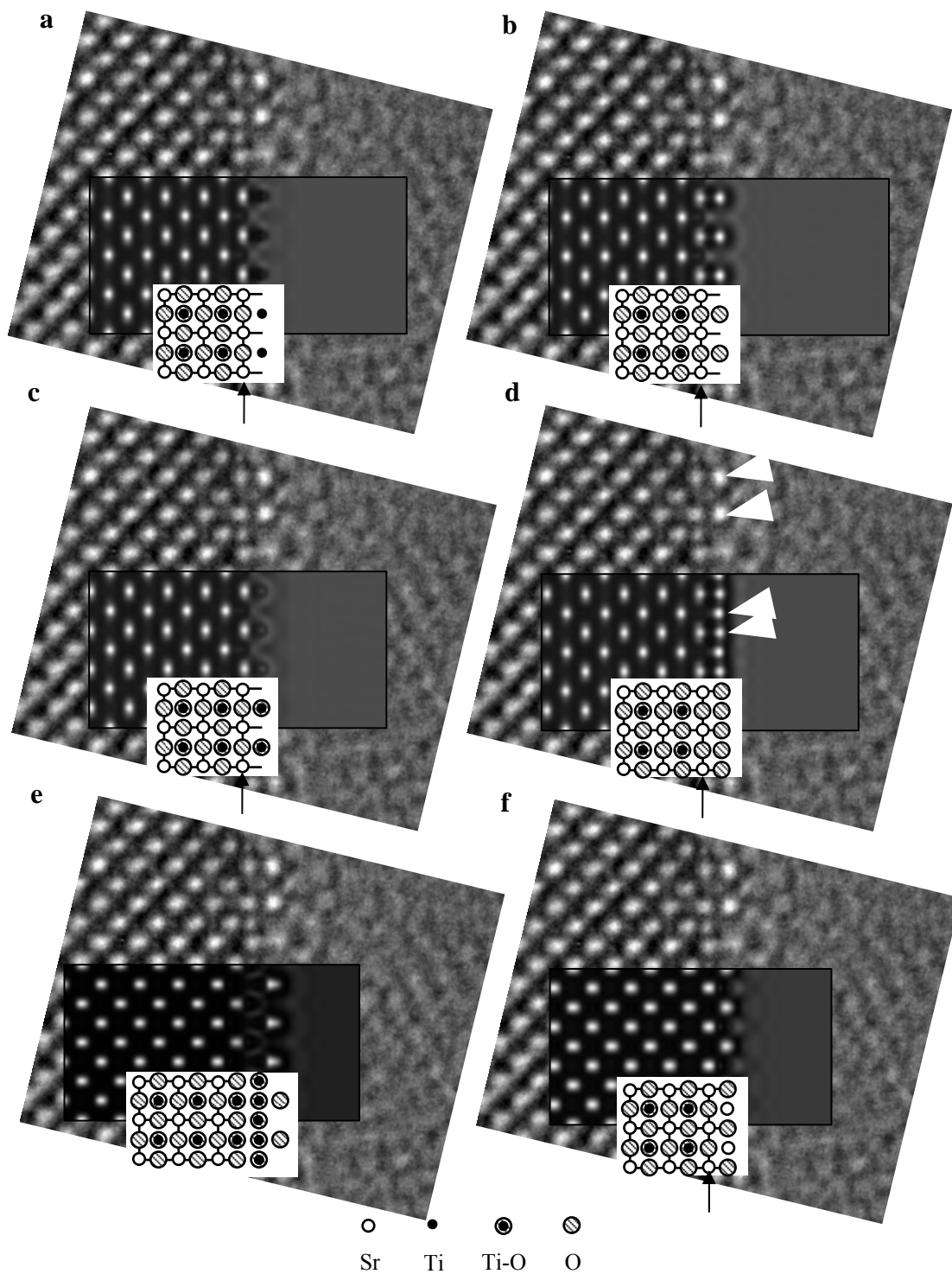


**Figure 1** HAADF-STEM imaging of a straight GB{100} in undoped SrTiO<sub>3</sub>. Left: Image at optimum contrast for viewing bulk structure; both Sr (green) and Ti-O (red) columns are imaged. Right: Increasing the contrast shows that the terminal layer (i) consists of Sr and is of reduced intensity compared to the adjacent layer (ii), and indeed to all other nearby layers.

The comparisons of the experimental and simulated HRTEM images generated from four possible defect models and two atomic models are shown in Fig. 2. For the four defect models, the first model (Sr-I) has only Ti atoms on the Ti-O columns; the second model (Sr-II) has only O atoms on the Ti-O columns; the third model (Sr-III) has O atoms on both the O and the Ti-O columns, and no Ti atoms on the Ti-O columns; the fourth model (Sr-IV) has the Ti-O columns fully occupied, and the O columns unoccupied. It should be noted that only O columns show up in the bulk SrTiO<sub>3</sub> crystal for the experimental parameters chosen. The Sr-II model, containing one oxygen vacancy and one titanium vacancy (shown in Fig. 2b), shows the best fit of the periodic spots (indicated using white triangles) near the SrO interface in the experimental image of the GB{100} boundaries. Energy dispersive X-ray (EDX) results measured with a STEM show Sr enrichment at the GB, supporting the existence of Ti vacancies at the GB. The fifth model was constructed based on the TiO<sub>2</sub>-rich surface on SrTiO<sub>3</sub> free surfaces reported by Erdman et al. [1] (Fig. 2e), while the sixth model was based on a GB with an SrO-rich Ruddlesden-Popper-type interlayer [2] (Fig. 2f). Simulated HRTEM images from these models showed no agreement with the experimental images (e.g. Figs 2e and 2f). Neither the TiO<sub>2</sub>-rich surface nor the GB with Ruddlesden and Popper phase were consistent with the HAADF STEM results.

[1] N. Erdman, K. R. Poeppelmeier, M. Asta, O. Warschkow, D. E. Ellis and L. D. Marks, *Nature* 419 (2002) 55.

[2] S. N. Ruddlesden and P. Popper, *Acta Crystallographica* 11 (1958) 54.



**Figure 2 Comparison of experimental HREM image with six possible models.** Experimental image at thickness of  $\sim 20$  nm compared with the simulated images (on the bottom) generated from four possible defect models and the two atomic models at the  $\{100\}$  interface: (a)  $\text{SrO} + \text{Ti}_{\text{Ti}} + 2\text{V}_{\text{O}}$ , (b)  $\text{SrO} + \text{O}_{\text{O}} + \text{V}_{\text{O}} + \text{V}_{\text{Ti}}$ , (c)  $\text{SrO} + \text{Ti}_{\text{Ti}} + \text{O}_{\text{O}} + \text{V}_{\text{O}}$  and (d)  $\text{SrO} + 2\text{O}_{\text{O}} + \text{V}_{\text{Ti}}$  (e)  $\text{SrO} + \text{TiO}_2 + \text{TiO}_2$  ( i.e. a  $\text{TiO}_2$ -rich GB)[1] and (f)  $\text{SrO} + \text{SrO}$  (Ruddlesden-Popper phase[2]). The black arrow indicates the SrO termination, and the white triangles indicate the bright spots.



### **WP3: Meso level (MS,AS)**

The original objectives of WP3 were to describe the effects of temperature, pressure, and chemistry on structural and compositional features of intergranular films (IGFs) in SrTiO<sub>3</sub> with a continuum modelling approach, using a phase-field model tuned with experimentally determined data and the self-consistent classical density functional theory (SCC-DFT), and to characterize experimentally and calculate theoretically dispersion forces for systems with a gradient in the dielectric response.

These objectives had to be revised during the project, because no IGF's were observed experimentally, and the focus was put on carefully selected grain boundaries and pure STO bicrystals. The original objectives of understanding and predicting how thermodynamic variables such as temperature, pressure and chemical potentials influence the structure and chemistry of the interfaces were retained.

Major theoretical achievements were obtained in this workpackage, such as the development of a completely new approach to describe SrTiO<sub>3</sub> interfaces, based on the combination of a genetic algorithm using empirical potentials, and the development of a theory for a continuous dielectric profile across boundaries taking into account dispersion as well as electrostatic interactions.

On the experimental side, a powerful method was developed to obtain potential maps at grain boundaries from tomographic inline holography experiments in the transmission electron microscope. And the combination of X-PEEM measurements (X-ray photoemission electron microscopy) and EBSD (Electron Backscattering Diffraction) allowed to show a clear correlation between work function and grain crystallographic orientation.

As concerns the theoretical part:

1) Some of the foreseen theoretical approaches turned out to be too difficult to manage with interfaces of multicomponent systems such as SrTiO<sub>3</sub>: the phase field modelling from ab initio approach was abandoned, the SCC-DFT as well, and a completely new approach was developed to describe SrTiO<sub>3</sub> interfaces, based on the combination of a genetic algorithm, using empirical potentials, with first principles electronic density functional theory. A crucial point is that a proper description of such interfaces requires the removal of atoms from grain boundaries, which had been only very rarely carried out before. This implies taking into account the chemical potentials of all species. A genetic algorithm was necessary because of the huge number of configurations of the boundaries. Detailed predictions of the structures and compositions of the (111) and (112) twins in SrTiO<sub>3</sub> throughout the full range of chemical potentials of TiO<sub>2</sub> and SrO could be obtained, as well as detailed comparisons with high resolution microscopy.

2) Another project objective was to create a theory to describe the influence of dispersion interactions on the grain boundary properties. This required also new techniques that describe the dispersion interactions in smoothly varying media, and a way to include these interactions into self-consistent models that describe the grain boundary. A theory for a continuous dielectric profile across boundaries was developed, involving a minimization of a density functional taking into account dispersion as well as electrostatic interactions. The results of these calculations were the self consistent density profiles. The results of dispersion interactions and the electrostatics were observed to be largely independent, with the dispersion interactions affecting more the near wall, atom size regions, whereas the electrostatic interactions changed the overall density profile more.

Another goal was to use the actual dielectric density profiles from the VEELS measurements in order to estimate the dispersion interactions in the grain boundary.

A dielectric response model was derived from the VEELS experimental data recorded from different SrTiO<sub>3</sub> interfaces, from which it was possible to estimate the Hamaker coefficients of the various types of grain boundaries by applying a suitably formulated Lifshitz theory of dispersion interactions. In fact, the calculation of Hamaker coefficients only make sense for well separated boundaries, as expected initially in IGF's, unexpectedly not observed. In the case of the abrupt crystalline studied grain boundaries, only a few atoms thick, the delocalization of the dielectric response, which is not accessible from experiment, is a significant effect yielding large variations in the free energy results. Then it remains not entirely clear whether the gradients in the dielectric response in the VEELS data are due to the actual response gradients or rather due to the fact that the electrons passing through the material excite a significant region of the material rather than just the point directly at the electron beam position.

As concerns the experimental part :

Main effort was focused on the determination of potential maps at grain boundaries from in-line holography experiments in the transmission electron microscope, and on using XPEEM and EBSD on SrTiO<sub>3</sub> polycrystalline ceramics to get spatial information on grain orientation, surface termination and work function.

3) A method has been developed and refined to reconstruct potential maps from Fresnel focal series, for several grain boundaries in SrTiO<sub>3</sub> ceramics and bicrystals. Tomographic in-line holography experiments have been performed on polycrystalline SrTiO<sub>3</sub> and, at the atomic resolution, on  $\Sigma 17$ , the  $\Sigma 13$ , and the  $\Sigma 3$  bicrystal samples. The reconstruction algorithm has been extended to allow the reconstruction of very low spatial frequency information in the potential maps. Within the phase object approximation the phase shift is proportional to variations in the mean inner potential. This experimental work is a major achievement of the INCEMS project.

4) An in-depth X-ray photoelectron emission microscopy (XPEEM) was performed on SrTiO<sub>3</sub> polycrystalline ceramics, coupled to an Electron Backscattering Diffraction (EBSD) study of the same samples. At the beginning of the INCEMS project, there was only one paper in the literature reporting XPEEM experiments on SrTiO<sub>3</sub>, so our contribution to XPEEM on SrTiO<sub>3</sub> appears to be significant.

Stereographic plots have been used to show the correlation between surface composition and orientation for several grains, and predominant surface terminations had been assigned to major orientations. Moreover, a correlation between work function (XPEEM) and grain orientation (EBSD) was clearly evidenced.

#### **WP4: Device level (MH,PG)**

The main objective of WP4 was the investigation of the influence of structural changes at the grain boundaries on the macroscopic behaviour e.g. coarsening dynamics of the microstructure and the electrical properties of the boundary regions. The objectives were divided into two major parts. First, the preparation of samples for the TEM and spectroscopy investigation performed at the partner groups and second, the simulation of the collective behaviour of the grain structure during heat treatment by a three dimensional vertex dynamics model. Experimental results as starting point and validation for the simulations have been produced in WP4. The simulation activity started from an existing three dimensional simulation tool, which has been adapted for the description of ceramic materials.

Contrary to the initial assumption of the project no IGFs have been found in the high purity STO specimens, chosen as model material to be able to link to the computational modelling chain from DFT, atomistic, phase field and vertex dynamics model. To ensure the observation of the absence of IGFs in the prepared samples multiple processing parameters were varied systematically: Sintering temperature, perovskite A/B ratio, oxygen partial pressure during sintering, pressure and dopant levels. From a literature study a critical point seemed to be the cooling rate after the last heat treatment and the sintering atmosphere. For this reason a new furnace setup was installed to allow quenching samples in a defined atmosphere to freeze a high temperature state.

On the experimental side grain growth data has been linked to composition profiles around GBs from EDS measurements in a HRTEM. A correlation between abnormal grain growth and Ti-excess at grain boundaries was found. Ti-excess at the grain boundaries reduces the apparent grain boundary mobility. A contribution of special grain boundaries with low misorientation has not been found by orientation imaging via EBSD.

A mesoscopic model for treating the motion of a three dimensional grain structure has been adapted to handle also anisotropic grain boundary properties, e.g. inclination dependent GB energy and mobility. The three dimensional vertex dynamics model has reached a state of maturity which allowed first simulations for exploring the occurrence of abnormal grain growth (Fig. 1) and the effect of faceting. These studies suggest that a de/faceting transition may be a possible explanation for the experimentally observed grain growth behaviour, which shows abrupt changes in the apparent GB mobility with temperature, as shown in Fig. 2.

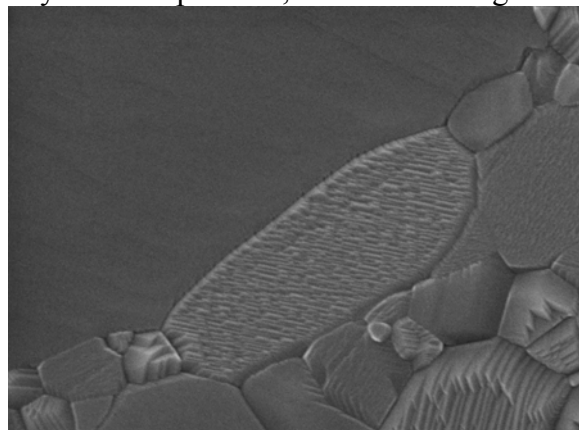
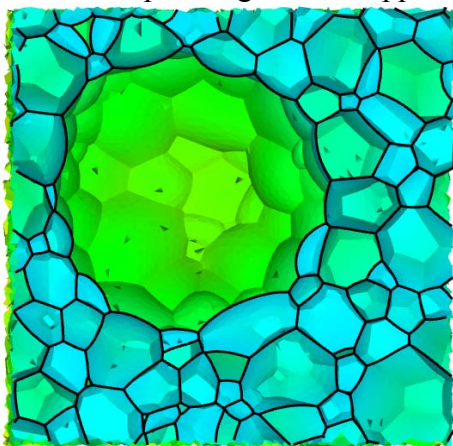


Fig. 1: comparison between simulated and experimental microstructure (a) abnormally growing grain with an GB energy advantage of 20% with respect to the other grains; (b) border between abnormal and matrix grains in experiments.

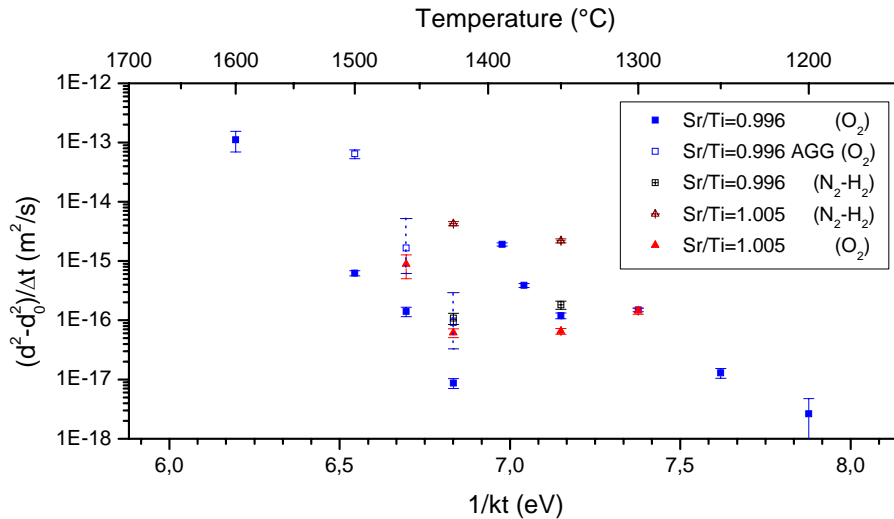


Fig. 2: Arrhenius plot of apparent grain boundary mobility in undoped SrTiO<sub>3</sub> for different sintering atmospheres.

The simulated GB structures, shown in Fig. 3, show the different GB shapes for isotropic and an inclination dependent GB energy. In the latter case, the GBs are less curved due to torque contributions, which reorient the GB along the direction with lowest GB energy.

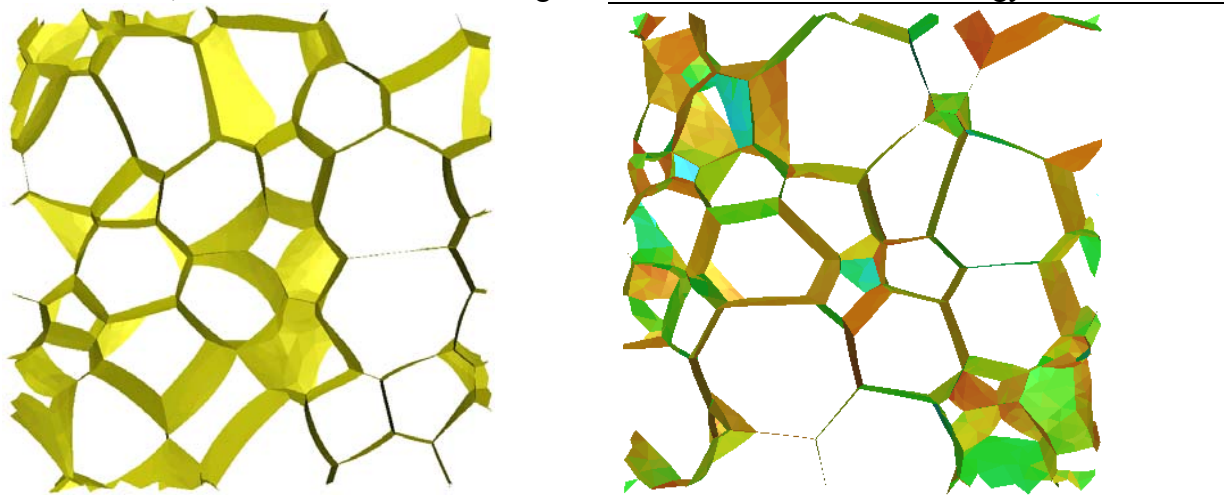


Fig. 3: 3D slice of same start configuration treated isotropically (left) respectively anisotropically (right), regarded after the loss of about the same amount of grains.

### **Work Package 5: Exploitation of new materials phenomena (AS)**

At the start of INCEMS it was assumed that intergranular films (IGFs) would be found in strontium titanate. Despite many attempts to produce samples under carefully controlled growth conditions no IGFs were observed by electron microscopy techniques. Thus, the original goal of exploring the thermodynamic conditions, under which IGFs may be induced or eliminated from grain boundaries in strontium titanate, turned out to be without any basis in experimental reality. The focus of the INCEMS consortium turned to the development of new theoretical, computational and experimental techniques to analyse grain boundaries in strontium titanate that do in fact exist. This work is described in the previous work packages. Here we provide a brief summary of some of the main outcomes.

One of the most striking results of our work is the apparently strong influence of anisotropy of the grain boundary energy on grain growth. This suggests that segregation of dopants, which alter the anisotropy of grain boundary energy, may influence grain shapes, such as aspect ratios, which are known to influence the toughness by making the paths of intergranular cracks more convoluted.

Our discovery that the rate of grain growth *decreases* above a certain temperature is significant commercially. For example materials displaying this behaviour can be densified at high temperatures *without* significant coarsening of the microstructure. The resulting ceramic has improved mechanical properties as a result of the absence of pores and a relatively fine grain structure. In addition it is translucent without the additional expensive processing step of hot isostatic pressing to reduce porosity.

Another exciting outcome of our research is the development of a new approach to model grain boundaries in multi-component systems using a combination of a novel genetic algorithm and thermodynamics based on first principles density functional theory. Our approach enables the configurational complexity of these interfaces to be considered more fully than before, while treating the *free* energy of the interface with first principles accuracy. Clearly the approach we have developed is applicable to other alloy systems. It is also clear how it may be developed further to address charged interfaces with adjoining space-charge layers.

Much of WP5 was centred on dissemination of the work of the consortium, and all members of the consortium have worked hard to inform colleagues in academe and industry about our work. The directions of our research were significantly influenced by the constructive discussions we had with the industrial advisors who joined our management committee. Their comments were particularly helpful at the M18 meeting when we realized we had to rethink the original goals of the programme, and at the M45 meeting when we discussed the powerpoint presentation for industry.

- In 2007 we organized an international workshop: Symposium J of the E-MRS meeting in Strasbourg, entitled *Interfacial nanostructures in ceramics: a multiscale approach*. The Proceedings were published by the Institute of Physics. They comprise 15 papers, 7 from the INCEMS consortium.
- Three meetings with industry companies took place. Furthermore, we have created a powerpoint presentation for future meetings with industry companies to give them a digest of the work that has been carried out within the INCEMS consortium.
- More than 60 invited talks have been given by members of the consortium on INCEMS-related work..
- At least 25 contributed talks and posters have been given by members of the consortium on INCEMS-related work.
- More than 50 papers based on INCEMS-related work have been published or are being submitted for publication
- 5 PhD theses and 4 undergraduate projects have been carried out based on INCEMS research. An extended visit by an overseas PhD student to carry out work related to INCEMS has also taken place.

A list of publications is posted on the INCEMS website. The listings for the meetings with industry, invited talks, contributed talks or posters, published or submitted papers, PhD theses and other student projects are given in the appendices WP5:1-5.

## Appendix WP5:1

### Meetings with industry

Sept. 19, 2007 meeting at Robert Bosch GmbH, Stuttgart, Germany, discussing application of inline electron holography to study grain boundary potentials in applied ceramics.

Participants: P. van Aken (MPI), C. Koch (MPI), S. Hinderberger (Bosch), U. Eisele (Bosch), R. Satet (Bosch), K. Bindler (Bosch)

Dresden, June 17/18, 2009: meeting for German BMBF project "RealMak" on perovskite based lead free piezoelectrics; participants from the industry companies Siemens, Robert Bosch and PI Ceramics; invited talk of M Bäurer on defect chemistry in BTO; discussion about grain growth.

Stuttgart, June 15, 2009: Materials Science Colloquium of the industry company Robert Bosch; invited lecture of C. Elsässer on "First-principles modelling of interfaces in metal-oxide devices; discussion about multi-scale modelling of (multi-)functional materials.

## Appendix WP5:2

### Invited talks

#### 2006

C. Elsässer, Electroceramic perovskite-type thin-film heterostructures – ab-initio theory of interfacial atomistic structures, electronic states, and mechanical stabilities, Materials Science Colloquium, Technical University Darmstadt, May 2006, Darmstadt, Germany

C. Elsässer, Electroceramic perovskite-type thin-film hetero-structures, EPSRC Workshop on “Multiscale modelling approach to engineering functional coatings”, July 2006, Loughborough University, UK

M W Finnis, Bear Creek, International Workshop on Interfaces in Functional Materials, “First-Principles Calculations”.

A P Sutton, “Twist boundaries in silicon: a new look at an old problem”, PSI-K/COST workshop on "Multiscale modeling of extended defects and phase transformations at materials interfaces", September 24-26, Wroclaw Poland

#### 2007

Nick Barrett: X-ray photoelectron emission microscopy (SR-XPEEM) with aberration corrected energy filtering Politecnico di Milano 19th December 2007

D. J. H. Cockayne, **Plenary lecture**, “High Resolution Studies of the Nanoworld,” Inter American Society of Electron Microscopy, Cusco Peru. September 2007

C. Elsässer, First-principles theory of interfacial electronic structures, mechanical and ferroelectric stabilities of electroceramic thin-film heterostructures, The Materials Research Society's Spring Meeting 2007, April 2007, San Francisco, California, USA

C. Elsässer, First-principles theory of extended structural defects in electroceramic oxides, Center of Nanoelectronic Systems for Information Technology at the Research Center Jülich, September 2007, Jülich, Germany

M W Finnis, ““Strontium titanate grain boundaries, successes and failures of theory and simulation”, **Plenary lecture** at MMM2007, Melbourne.

M W Finnis, Carnegie Mellon, International Workshop in honour of Paul Wynblatt, “Another application of quaternions”.

M W Finnis, OXMOS/MULTIMAT Workshop on Microstructure, “Grain boundaries at the atomic scale, theory, mathematics and simulation”.

C T Koch et al., Microscopy Conference, MC 2007, "Mapping Grain Bondary Potentials by Inline Electron Holography”

C T Koch, Seminar at Ernst-Ruska-Center (Nov. 28, 2007), Forschungszentrum Jülich 2007: "Nonlinear Inline Electron Holography"

C.T. Koch, "Nonlinear Inline Electron Holography", Frontiers of Electron Microscopy in Materials Science, FEMMS, San Francisco, CA, USA, 2007.

C.T. Koch, "Mapping grain boundary potentials using inline electron holography", E-MRS Spring Meeting, Strasbourg 2007.

C T Koch, Nov 28, 2007 at the Ernst-Ruska-Center, Forschungszentrum Julich, "Nonlinear Inline Electron Holography"

C T Koch, Sept. 21, 2007 at the Department of Chemistry, LMU Munich, Germany, "Doing Materials Science with Interfering ElectronWaves"

C T Koch, Nov. 8, 2007 at the FakultÄat fÄur Mathematik und Naturwissenschaften of the Technical University Dresden, Germany: "Solving Materials Science Problems by Interfering Electron Waves"

C T Koch, Winter HAADF and EELS Workshop (WHEW), Dec. 10 - 12, 2007 at Orsay, France, "Simulating HAADF-STEM images"

A P Sutton, **Hume-Rothery Memorial Lecture**, "Orderly and disorderly behaviour at interfaces", Oxford University, October 2007

A P Sutton, "New explorations of the configurational phase space of interfaces", iib07 Barcelona.

## 2008

Bäurer, M. & Hoffmann, M.J., 'Grain growth in Strontium Titanate', Seminar, Massachusetts Institute of Technology, 11.04.2008.

Nicole Benedek, "Classical Simulations of Grain Boundaries in SrTiO<sub>3</sub>" Department of Chemistry, University of Pennsylvania, November 25th 2008.

Catherine M. Bishop "A Phase-Field Model for Grain Boundaries in Ceramics: Strontium Titanate" International Workshop on Interfaces: New Materials via Interfacial Control, Santiago de Compostela, June 2008.

D J H Cockayne April 2008 TMS Hume-Rothery Symposium, New Orleans, USA "The structure of amorphous Nanovolumes"

D J H Cockayne February 2008 **Plenary Lecture** - ACMM20, Perth, Australia "The Nanoworld explored with electron Microscopy"



D J H Cockayne February 2008 ACMM20, Perth, Australia "Studies of amorphous materials using electron RDF analysis and model refinement"

D.J.H. Cockayne, S-J. Shih, K.J. Dudeck, N.P. Young, "Grain boundary interfaces in ceramics", European Microscopy Congress, 1st – 5th September 2008, Aachen, Germany

C. Elsässer, Modeling of structural and functional ceramics at the atomic scale by ab-initio electron theory, DGM-Symposium "High-performance Ceramics", University of Hamburg-Harburg, March 2008, Hamburg, Germany

C. Elsässer, First-principles modeling and simulation of structure and function of metals and ceramics with defects and dopants, International Symposium on "Structure-Property Relationships in Solid State Materials", Université de Nantes, June 2008, Nantes, France

M W Finnis, OxMOS/Multimat workshop in Oxford "Grain Boundaries at the Atomic Scale; Theory, Mathematics and Simulation"

M W Finnis, MML Seminar in Oxford "Grain boundaries and quaternions in strontium titanate"

M W Finnis, Bernkastel-Kues, Germany, Workshop on Limits to characterization and modeling of atomic scale processes and defects, "Some current limitations on simulation of interfaces".

M W Finnis, AFRL, Dayton, Ohio, seminar "Theory and simulation of materials at the atomic scale".

M W Finnis, Institute of Physics, London, UK, Workshop on Modelling and Characterisation of Interfaces, "Progress and Challenges in the Atomistic Simulation of Interfaces in Strontium Titanate".

P Gumbsch: "Modelling grain growth in STO ceramics: linking physical properties to measurable statistical quantities", International Workshop on Interfaces: New Materials via Interfacial Control, Santiago de Compostela, June 2008.

P. Gumbsch, L. Yue, D. Weygand: "Simulation of grain growth with a 3D vertex dynamics model", 7th International Workshop on Interfaces New Materials via Interfacial Control Santiago de Compostela, Spain 22 – 26.06.2008.

C.T. Koch, "Mapping grain boundary potentials and space charge in ceramics", Interfaces in Ceramics, Santiago de Compostella, 2008.

C.T. Koch, "Electron Inline Holography of interfaces", International Workshop on Functionality of Interfaces, Shanghai, China, 2008

C.T. Koch, "Electron inline holography and its application to grain boundaries", Seminar at Hahn Meitner Institute in Berlin, 2008

C.T. Koch, "Various alternatives to off-axis electron holography", ESTEEM Holography Workshop at the Technical University Dresden, 2008

C.T. Koch, "Quantitative TEM and STEM Simulations", European Microscopy Congress, Aachen 2008.

C T Koch, Nov. 25, 2008 at the Electron Microscopy Center of the Materials Science Department of the Technion, Haifa, Israel: "3-dimensional atomic structures from dynamically diffracted electrons"

C T Koch, May 20, 2008 at the Hahn-Meitner-Institut, Berlin, Germany: "Electron Inline Holography and its Application to Grain Boundaries"

C.T. Koch, ESTEEM Holography Workshop, May 12 - 15, 2008 at the Technical University Dresden, Germany: "Various alternatives to off-axis electron holography"

C.T. Koch, "Mapping potentials at grain boundaries in ceramics by nonlinear in-line electron holography", Gordon Conference on High Temperature Materials, Processing and Diagnostics, Waterville, ME, USA, 2008

Podgornik, Rudolf. Fluctuation forces between carbon nanotubes : [lecture given at Kavli Institute for Theoretical Physics, University of California, Santa Barbara]. 2008. [COBISS.SI-ID 2120548]

Podgornik, Rudolf. van der Waals interactions between carbon nanotubes : [lecture given at Universität Stuttgart, 17. 11. 2008]. 2008. [COBISS.SI-ID 2136420]

Podgornik, Rudolf. Molecular attractions : van der Waals, electrostatic correlations and polyelectrolyte bridging interactions : [invited talk at an International School of Viomembrane Physics, Indian Institute of Technology Madras, Chennai, India, 7-18 January 2008]. 2008. [COBISS.SI-ID 2041188]

M. Rühle, Seminar at International Center for Young Scientists at NIMS, March 7, 2008 "Structure, Composition and Bonding of Grain Boundaries in Functional Ceramics"

M. Rühle, Internal Seminar on Developments in Ceramic Science and Engineering: The last 50 years (A meeting in celebration of Professor Sir Richard Brook's 70th Birthday), City College London, April 11-12, 2008 "Microstructure of Defects in Ceramics at the Atomic Level"

M. Rühle, Gordon Research Conference in Solid State Studies in Ceramics Proctor Academy, Andover /NH, August 10-15, 2008 "Do Ceramists Need to Know the Atomic Structure of Grain Boundaries in Ceramics?"

M. Rühle, The University of Sydney- Electron Microscope Unit, Golden Jubilee 2008, Commemorative Symposium, December 3-5, 2008 "Structure and Composition of Internal Interfaces in Materials"

M. Rühle, Workshop on Ultra-High Resolution TEM: Imaging and Diffraction, Monash Centre for Electron Microscopy, Dec 9, 2008: "Challenges of Microscopy in Materials Science"

A P Sutton, "Orderly and disorderly behaviour at interfaces", ACerS meeting, Daytona Beach January 2008.

A P Sutton, "Orderly and disorderly behaviour at interfaces", Institute of Physics meeting on "Modelling and characterisation of interfaces", London June 2008.

A P Sutton, "Orderly and disorderly behaviour at interfaces", Department of Mechanical Engineering, Imperial College London, April 2008.

A P Sutton, "Orderly and disorderly behaviour at interfaces", **Opening lecture** International workshop on "Mathematical challenges of molecular dynamics", Warwick 14-16 July 2008.

A P Sutton, "Order and disorder at interfaces", CCP5 Annual meeting on "Surfaces and Interfaces", London, September 2008.

D. Weygand: Erich Schmid Colloquium, Leoben, Austria, Modellierung des Kornwachstums von zwei- und dreidimensionalen Gefügen: Abnormales Kornwachstum und Kornvergrößerung in STO Keramiken. 10.09.2008.

L. Yue, D. Weygand, P. Gumbsch, "Grain growth modelling by a three dimensional vertex dynamics simulation". 4<sup>th</sup> International Conference on Multiscale Materials Modelling (MMM2008) Oct 27 – Oct 31 2008 Tallahassee, Florida United States.

## 2009

Nicole Benedek, "Complexity at Interfaces: Grain Boundaries in SrTiO<sub>3</sub>", Computational Materials Science Seminar, Cornell University, February 3rd 2009.

C. Elsässer, Electronic-structure theory of structure-property relationships for functional materials with dopants and interfaces, CAMM Workshop "Possibilities and Limitations of Characterization and Modeling of Solid/Solid Interfaces, May 2009, Bernkastel-Kues, Germany

C. Elsässer, First-principles modelling of interfaces in functional metal-oxide devices, Materials Science Colloquium of the Robert Bosch GmbH, June 2009, Stuttgart, Germany

C. Elsässer, First-principles modelling of interfaces in functional metal-oxide devices, Physics Colloquium of the Technical University of Freiberg, July 2009, Freiberg, Germany

C. Elsässer, Atomic-scale modeling of interfaces in functional metal-oxide devices, CECAM Workshop "Reflections on Metal/Ceramic Design" at the ETH Zürich, July 2009, Zürich, Switzerland

C T Koch, *Understanding Materials through Electron Microscopes: Realising the Potential*, April 22 - 24, 2009 at Imperial College, London: C.T. Koch, "Mapping grain boundary potentials by inline electron holography"

C T Koch, *TEM Workshop*, May 7 - 8, 2009 at University of Oslo, Norway, "Various kinds of electron holography and what holography can tell us about charges at grain boundaries"

M. Rühle, University of Tokyo, March 27, 2009: "Segregation of Impurities to Grain Boundaries in Ceramics"

M. Rühle, **Plenary Lecture**, Japan Institute of Metals, Spring Meeting 2009, March 28 -30, 2009, Tokyo Institute of Technology "TEM Investigations of Segregation of Impurities to Grain Boundaries: A few atoms may change the properties of a material"

A P Sutton, *Symposium in honour of Professors D J Bacon, P J Goodhew and R C Pond* at the University of Liverpool, January 23 "Interfaces, radiation damage and postgraduate education"

A P Sutton: "Theory and simulation of materials at Imperial College London", Hokkaido University Simulation Salon, Japan, February 24th 2009.

#### INCEMS-related, invited talks to be given after June 30, 2009

*Merging Atomistic and Continuum Analysis of Nanometer Length-Scale Metal-Oxide Systems for Energy and Catalysis Applications*, Nov. 14 - 17, 2009 in Berlin, Germany: C.T. Koch, "What can inline holography tell us about charges at grain boundaries in ceramics?"

*Frontiers of Electron Microscopy in Materials Science (FEMMS)*, Sept. 27 - Oct. 2, 2009 in Nagasaki, Japan: C.T. Koch, "What can inline holography tell us about charges at grain boundaries in ceramics?"

*International Workshop on Interfaces in Functional Materials*, October 19 - 24, 2009 at the Bear Creek Inn, Macungie, PA USA: C.T. Koch, "Interface potentials in ceramics"

C. Elsässer, ITF-Seminar, First-principles modelling of interfaces in functional metal-oxide devices, Leibniz Institute for Solid-state and Materials Research (IFW), September 2009, Dresden, Germany

C. Elsässer, Atomic-level theory of structure and function of interfaces, 1<sup>st</sup> Conference of EU-FP7-CSA MACAN on "Bridging the gap between atomistic and continuum approaches to the science of interfaces", November 2009, Berlin, Germany

C. Elsässer, Ab-initio DFT modelling of interface adhesion in metal/ceramic systems, 12<sup>th</sup> International Conference on "Modern Materials and Technologies" (CIMTEC), June 2010, Montecatini Terme, Italy

## Appendix WP5:3

### Contributed talks and posters

Acker, J., Kungl, H., Bäurer, M., Picht, G., Hoffmann, M.J., "Role of stoichiometry on powder characteristics, sintering behaviour and microstructure of KNN ceramics", contributed poster, *Electroceramics XI, Manchester, UK, 31.08.2008-04.09.2008*

Bäurer, M., Harmer, M.P. & Hoffmann, M.J., 'Grain growth and microstructure control in undoped strontium titanate', contributed talk, International Conference on Sintering, La Jolla, USA, 16.11.-20.11.2008

Bäurer, M. & Hoffmann, M.J., 'Korngrenzphasen in Strontiumtitanat', contributed poster, *Symposium Hochleistungskeramik, Stuttgart, 05.04.-06.04.2006*

Bäurer, M. & Hoffmann, M.J., 'Intergranular Films in Strontium Titanate', contributed poster, *Junior Euromat, Lausanne, Switzerland, 04.09.-08.09.2006*

Bäurer, M., Zagonel, L.F., Barrett, N. & Hoffmann, M.J., 'Changes in macroscopic behaviour through segregation in Niobium doped Strontium Titanate', contributed talk, *EMRS Spring Meeting, Strasbourg, Frankreich, 28.05.-01.06.2007*

Bäurer, M., Zagonel, L.F., Barrett, N. & Hoffmann, M.J., 'Changes in Macroscopic Behaviour through Segregation in Niobium Doped Strontium Titanate', contributed talk, *Euromat, Nürnberg, 10.09.-13.09.2007*

Bäurer, M., Harmer, M.P. & Hoffmann, M.J., 'Grain growth in undoped strontium titanate', Posterbeitrag, *International Workshop on Interfaces, Santiago de Compostela, Spanien, 22.06.-26.06.2008*

Nicole Benedek: "First-Principles Studies of Polarisation at Interfaces in Strontium Titanate" MRS Fall Meeting 2008, Boston, USA

Nicole Benedek: "To What Extent Can Current Interatomic Potentials Accurately Describe Grain Boundaries in Strontium Titanate" MRS Fall Meeting 2008, Boston, USA

Nicole Benedek: "A Better Way to Calculate Grain Boundary Misorientation Relations from Electron Microscopy Data", Institute of Physics Modelling and Characterisation of Interfaces Meeting, London, June 2008

Nicole Benedek: "Dielectric Properties of Interfaces in Strontium Titanate", EMRS Spring Meeting, Strasbourg, France, June 2007

K. J. Dudeck, S. J. Shih, C.T. Koch, D. J. H. Cockayne, "High Resolution TEM Studies of Grain Boundaries in Si<sub>3</sub>N<sub>4</sub> and SrTiO<sub>3</sub>," Electron Microscopy and Analysis Group Conference, Glasgow, UK, 03-07 September 2007

K.J. Dudeck and D.J.H. Cockayne, "HREM study of the SrTiO<sub>3</sub> sigma-3(112) grain boundary", ,European Microscopy Congress, 1st – 5th September 2008, Aachen, Germany

K. J. Dudeck and D. J. H. Cockayne, "Quantitative high resolution electron microscopy investigation of the SrTiO<sub>3</sub> S3(112)[-110] grain boundary", *EMAG 2009* Sheffield, September 2009.

K. J. Dudeck and D. J. H. Cockayne, "HREM study of the SrTiO<sub>3</sub> S3(112)[-110] grain boundary", *7<sup>th</sup> International Workshop on Interfaces: New Materials via Interfacial Control*, Santiago de Compostela, June 2008

C.T. Koch, B. Rahmati, W. Sigle, M. Shirpour, R. Merkle, J. Maier, and P.A. van Aken, "Mapping Grain Boundary Potentials in Ceramics by Nonlinear Inline Electron Holography and Impedance Spectroscopy" Microscopy Conference 2009, August 30 - September 4 (2009), Graz, Austria

S. J. Shih, N. A. Benedek, M. W. Finnis, A. P. Sutton, M. Bäurer, M. Hoffmann and D. J. H. Cockayne, "Measurement of Grain Boundary Orientations in Polycrystalline Materials," Electron Microscopy and Analysis Group Conference, Glasgow, UK, 03-07 September 2007

Shao-Ju Shih, Neil Young, Karleen Dudeck, Si-Young Choi, Michael Bäurer, Michael Hoffmann, David Cockayne, "Structural and orientation investigations of planar grain boundaries in polycrystalline SrTiO<sub>3</sub>", *Electroceramics XI*, 31st August - 4th September 2008, Manchester, UK

M. Syha , L. Yue , D. Weygand , and P. Gumbsch, "3D Vertex Dynamics Simulation of Grain Growth in Ceramics Including the Anisotropy of Grain Boundary Energy". DPG Tagung Dresden 25.3.2009

L. Yue, D. Weygand, P. Gumbsch, "Grain growth modelling by a three dimensional vertex dynamics simulation". 4th International Conference on Multiscale Materials Modelling (MMM2008) Oct 27 – Oct 31 2008 Tallahassee, Florida United States.

D. Weygand: Erich Schmid Colloquium, Leoben, Austria, Modellierung des Kornwachstums von zwei- und dreidimensionalen Gefügen: Abnormales Kornwachstum und Kornvergöberung in STO Keramiken. 10.09.2008.

Luiz F. Zagonel, Nicholas Barrett, Olivier Renault, Aude Bailly, Michael Bäurer, Michael Hoffmann, Shao-Ju Shih, David Cockayne, "Strontium titanate grain boundaries", Orientation dependent surface terminations of *in situ* annealed polycrystalline SrTiO<sub>3</sub> determined by energy filtered XPEEM", *ECASIA-2007* Bruxelles, September 2007-12-18

L.-F. Zagonel, N. Barrett, O. Renault, A. Bailly, M. Bäurer, M. Hoffmann, S.-J. Shih, D. Cockayne, "Orientation dependent surface composition of in situ annealed strontium titanate", *ALC'07* Kanazawa October 2007.

N. Barrett, L. F. Zagonel, A. Bailly, O. Renault, J. Leroy, J. C. Cezar, N. Brookes Shao-Ju Shih, D. Cockayne, "Surface orientation dependent termination and work-function of in situ annealed strontium titanate", *European Microscopy Conference Aix la Chapelle (Germany)* September 2008.

L F Zagonel, M Bäurer, A Bailly, O Renault, M Hoffmann, S-J Shih, D Cockayne, N Barrett "Orientation dependent work function of in situ annealed strontium titanate", *LEEM-PEEM-6 Trieste (Italy)* September 2008

## Appendix WP5: 4

### Publications

D. Abou-Ras, C.T. Koch, V. Küstner, P.A. van Aken, R. Scheer, H.-W. Schock, "Mean inner-potential profiling at Cu(In,Ga)Se<sub>2</sub> grain boundaries from focus series using transmission electron microscopy" E-MRS 2008 Spring Meeting, Symposium L, in Strasbourg, France, 26 - 30 May 2008.

J.M. Albina, M. Mrovec, B. Meyer, C. Elsässer, [Proceedings of MMM 2006](#) *A study of the semi-coherent ceramic SrTiO<sub>3</sub>/SrZrO<sub>3</sub> interface by first principles DFT calculations*

J.M. Albina, M. Mrovec, B. Meyer and C. Elsässer, [Phys. Rev. B, 76 \(2007\) 165103](#) *Structure, stability, and electronic properties of SrTiO<sub>3</sub>/LaAlO<sub>3</sub> and SrTiO<sub>3</sub>/SrRuO<sub>3</sub> interfaces*

N. Barrett, O. Renault, « La spectromicroscopie XPEEM avec le rayonnement synchrotron » (XPEEM spectromicroscopy using synchrotron radiation) to be published (in french) *Matériaux et Techniques* (2009).

M. Bäurer, L. F. Zagonel, N. Barrett and M. J. Hoffmann, [Journal of Physics: Conference Series 94 \(2008\), 012015](#) *Changes in macroscopic behaviour through segregation in Niobium doped Strontium Titanate*

Michael Bäurer, Hans Kungl, Michael J. Hoffmann, [Journal of the American Ceramic Society 92, 601-606 \(2009\)](#) *Influence of Sr/Ti Stoichiometry on the Densification Behavior of Strontium Titanate*

M. Bäurer, D. Weygand, P. Gumbsch and M.J. Hoffmann, [Scripta Materialia \(2009\) 61 \(2009\) 584–587](#) *Grain growth anomaly in strontium titanate*

Bäurer, M.; Shih, S.-J., Bishop, C., Harmer, M., Cockayne, D., Hoffmann, M. (2009), 'Abnormal grain growth in Strontium Titanate', *in preparation*

N. Benedek, C. Elsässer and M. W. Finnis, [Journal of Physics: Conference Series 94 \(2008\), 012005](#) *First Principles Investigation of Polarisation at Interfaces in Multilayered Strontium Titanate*

Nicole A. Benedek, Alvin L.-S. Chua, Christian Elsässer, Adrian P. Sutton and Mike W. Finnis, [Phys. Rev. B 78, 064110 \(2008\)](#) *"Interatomic potentials for strontium titanate: An assessment of their transferability and comparison with density functional theory"*

S. Bhattacharyya, C.T. Koch, M. Rühle [Proceedings of IMC16 2006, Sapporo, Japan, p. 1138](#) *Measuring projected potential profiles across interfaces by reconstructing the exit face wave function from through focal series images*

S. Bhattachayya, C.T. Koch and M. Rühle, [Ultramicroscopy 106 \(2006\) 525-538](#) *Projected potential profiles across interfaces obtained by reconstructing the exit face wave function from through focal series*



S. Bhattacharyya, C.T. Koch and M. Rühle, "Determination of projected potential profiles across interfaces using through focal series reconstruction", *Microsc. Microanal.* 12, Suppl. 2: Proceedings (Cambridge University Press, Cambridge, UK, 2006) p. 1016-1017

A L-S Chua, C C Lin, N A Benedek, M W Finnis and A P Sutton, *A Genetic Algorithm to Predict the Structures of Interfaces in Multicomponent Systems*, Submitted to Nature Materials.

K. J. Dudeck, N. A. Benedek, M. W. Finnis and D. J. H. Cockayne, in preparation, *Three-dimensional atomic scale characterization of the SrTiO<sub>3</sub> S3(112) grain boundary*

K. J. Dudeck and D. J. H. Cockayne, in preparation of Journal of Physics: Conference Series, *Quantitative high resolution electron microscopy image matching applied to the strontium titanate S3(112) grain boundary*

M. Escher, K. Winkler, O. Renault, N. Barrett, "Applications of high lateral and energy resolution Imaging XPS with a double hemispherical analyser based microscope"  
J. Electr Spectr. Relat. Phenom. (2009) <http://dx.doi.org/10.1016/j.elspec.2009.06.001>

V. Fouquet-Parry, F. Paumier, M.J. Guittet and M. Gautier-Soyer, [Journal of Physics: Conference Series 94 \(2008\), 0120010](#) "Dielectric properties of pure and Nb-doped SrTiO<sub>3</sub> surfaces: a reflection electron energy loss spectroscopy study"

C.T. Koch and S. Garofalini, [Ultramicroscopy 106 \(2006\) 383-388](#)  
*Determining the radial pair-distribution function within intergranular amorphous Films by numerical nanodiffraction*

C.T. Koch [Ultramicroscopy \(2006\) submitted](#) *A flux-preserving inline electron holography reconstruction algorithm for illumination of partial spatial coherence*

C.T. Koch, B. Rahmati, P.A. van Aken, "Nonlinear Electron Inline Holography", 14th European Microscopy Congress (EMC) 2008, September 01 - 05 (2008), Aachen, Vol. 2: Materials Science (Springer, Berlin Heidelberg), pp. 236-237

C.T. Koch, B. Rahmati, P.A. van Aken, M. Bäurer, M. Hoffmann, "Mapping Grain Boundary Potentials by Inline Electron Holography", MC2007, Proc. 33<sup>rd</sup> Conference Deutsche Gesellschaft für Elektronenmikroskopie, Saarbrücken, Germany 2.-7.9.2007, Eds.: Th. Gemming, U. Hartmann, P. Mestres, P. Walther, *Microsc. Microanal.* 13 (Suppl. 3), 2007, 334-335

C.T. Koch, S. Bhattacharyya and M. Rühle, "Diffraction Tomography and its Application to Intergranular Glassy Films in Ceramics", Proceedings of the 16<sup>th</sup> International Microscopy Congress 2006, held Sept. 3-8 in Sapporo, Japan. (International Federation of Societies in Microscopy, 2006) p. 999-999

M. Mrovec, J.-M. Albina, B. Meyer, and C. Elsässer [Phys. Rev. B 79, 245121 \(2009\)](#) *Schottky barriers at transition-metal/SrTiO<sub>3</sub>(001) interfaces*

A. Pancotti, N. Barrett, L.F. Zagonel, G. M. Vanacore, *Multiple scattering X-ray photoelectron diffraction study of the SrTiO<sub>3</sub>(100) surface*, accepted for publication in J. Appl. Phys. (2009)

M.B. Park, S.J. Shih and D.J.H. Cockayne, [Journal of Microscopy 227 292-297 \(2007\)](#) *The preferred CSL misorientation distribution in polycrystalline SrTiO<sub>3</sub>*

R. Podgornik, R.H. French and V.A. Parsegian, [J. Chem. Phys. 124 \(2006\) 044709](#) *Nonadditivity in van der Waals interactions within multilayers*

G. Pruessner and A.P. Sutton, [Phys. Rev. B 77, 054101 \(2008\)](#) *Phase field model of interfaces in single-component systems derived from classical density functional theory*

G. Pruessner and A. P. Sutton, [Journal of Physics: Conference Series 94 \(2008\), 012002](#) *Phase field modeling of interfaces from first principles*

B. Rahmati, W. Sigle, J. Fleig, M. Konuma, U. Eigenthaler, C. T. Koch, P. A. van Aken, J. Maier and M. Rühle, [Journal of Physics: Conference Series 94 \(2008\), 012013](#) *Effect of surface orientation on intrinsic island formation on SrTiO<sub>3</sub> surfaces*

Rick F. Rajter, Rudi Podgornik, V. Adrian Parsegian, Roger H. French, and W. Y. Ching, [Phys. Rev. B 76 \(2007\), 045417](#) *van der Waals–London dispersion interactions for optically anisotropic cylinders: Metallic and semiconducting single-wall carbon nanotubes*

R. F. Rajter and R. H. French, [Journal of Physics: Conference Series 94 \(2008\), 012001](#) *New Perspectives on van der Waals - London Interactions teractions of Materials. From Planar Interfaces to Carbon Nanotubes*

H. Rösner, C.T. Koch, and G. Wilde [Acta Materialia \(2009\) submitted](#) *Strain Mapping along Al-Pb interfaces*

S.J. Shih, M.B. Park and D.J.H. Cockayne, [Journal of Microscopy 227 309-314 \(2007\)](#) *The interpretation of indexing of high Sigma CSL grain boundaries from ceramics*

S.-J. Shih, K. Dudeck, S.-Y. Choi, M. Bäurer, M. Hoffmann and D. Cockayne, [Journal of Physics: Conference Series 94 \(2008\), 012008](#) *Studies of grain orientations and grain boundaries in polycrystalline SrTiO<sub>3</sub>*

M. Syha, D. Weygand, P. Gumbsch, "A generalized vertex dynamics model for grain growth in three dimensions", submitted to MSMSE (2009).

Y. Umeno, B. Meyer, C. Elsässer, and P. Gumbsch [Phys Rev. B 74 \(2006\), 060101R](#) *Ab initio study of the critical thickness for ferroelectricity in ultrathin Pt/PbTiO<sub>3</sub>/Pt films*

Y. Umeno, T. Shimada, T. Kitamura, C. Elsässer [Phys. Rev. B 74 \(2006\), 174111](#) *Ab initio DFT study of strain effects on ferroelectricity at PbTiO<sub>3</sub> surfaces*

Y. Umeno, C. Elsässer, B. Meyer, P. Gumbsch, T. Shimada, T. Kitamura, [Proceedings of MMM 2006](#) *Ab initio DFT study on ferroelectricity on perovskite surfaces and in thin film capacitors*

G. M. Vanacore, L.-F. Zagonel, and N. Barrett, *Experimental investigation of surface enhanced covalency in Nb doped SrTiO<sub>3</sub> (100), (110) and (111)*, submitted to Phys. Rev. B (2009)

K. van Benthem, G. Tan, R.H. French, L.K. DeNoyer, R. Podgornik and V.A. Parsegian [Phys. Rev. B \*\*74\*\* \(2006\), 205110](#) *Graded interface models for more accurate determination of van der Waals-London dispersion interactions across grain boundaries*

G. Veble, R. Podgornik, [Phys. Rev. B \*\*75\*\*\(2007\), 155102](#) *Comparison of density functional theory and field approaches to van der Waals interactions in plan parallel geometry*

G. Veble and R. Podgornik, [Eur. Phys. J. E \*\*23\*\* \(2007\), 275-279](#) *The boundary element approach to Van der Waals interactions*

G. Veble and R. Podgornik, [Journal of Physics: Conference Series \*\*94\*\* \(2008\), 012003](#) *Self-consistent inhomogeneous dielectric response profiles from a nonlocal continuous Lifshitz formulation of van der Waals interactions*

S von Alfthan, P D Haynes, K Kaski and A P Sutton, Phys. Rev. Letts. **96**, 055505 (2006) *Are the structures of twist grain boundaries in silicon ordered at 0K?*

S. von Alfthan, K. Kaski, and A.P. Sutton, Phys. Rev. B. **76**, 245317 (2007), *Temperature-induced structural transitions at twist boundaries in silicon*

S. von Alfthan, K. Kaski, and A. P. Sutton [Phys. Rev. B \*\*74\*\* \(2006\), 134101](#) *Order and structural units in simulations of twist grain boundaries in silicon at absolute zero*

L. F. Zagonel, N. Barrett, O. Renault, A. Bailly, M. Bäurer, M. Hoffmann, S.-J. Shih and D. Cockayne, [Surface and Interface Analysis \(2008\), in print](#), *Orientation dependent surface composition of in situ annealed strontium titanate*

L F Zagonel, M Bäurer, A Bailly, O Renault, M Hoffmann, S-J Shih, D Cockayne , N Barrett *Orientation dependent work function of in situ annealed strontium titanate* to be published J. Phys. Condens. Matter (2009)

## Appendix WP5:5

### PhD theses and other student projects

#### PhD theses

Sebastian von Alfthan, "Computational Studies of Silicon Interfaces and Amorphous Silica", Helsinki University of Technology, December 2006.

<http://lib.tkk.fi/Diss/2006/isbn9512285401/isbn9512285401.pdf>

Jan-Michael Albina "Theoretical study of interfaces in electroceramic thin films - influence of the interface and planar defects on the electronic structure", University of Nantes, December 2007.

Michael Bäurer, "Kornwachstum in Strontiumtitanat", University of Karlsruhe (2008)

<http://digbib.ubka.uni-karlsruhe.de/volltexte/1000010124>

Shao-Ju Shih, "Nanometre-scaled structural studies of strontium titanate by electron microscopy and microanalysis" Oxford University, 2009

Karleen Dudeck, "Quantitative high resolution electron microscopy investigation of the strontium titanate S3(112) grain boundary" Oxford University, 2010

#### Other student projects

Giovanni VANACORE contributed while an undergraduate spending several months at Saclay in 2006-2007. He is a co-author of some papers related to INCEMS. Now he is a PhD student in Politecnico de Milano.

A. PANCOTTI completed a four-month visit during his PhD thesis (the PhD is registered at University of Campinas, Brazil) at the CEA-Saclay to undertake multiple scattering simulations optimized using a genetic algorithm to calculate surface rumpling of SrTiO<sub>3</sub> (100).

An undergraduate in the Department of Physics at Imperial College, C C LIN, carried out a 10-week summer project with AS, MF and Drs A Chua and N Benedek in 2008. The student made a seminal contribution to the development of the genetic algorithm for simulating grain boundary structures in strontium titanate.

Two 3-month undergraduate projects in the Department of Physics at Imperial College (at no cost to the project):

(a) Student: Philipp FLEIG:

Title: Calculation of space charge around a grain boundary.

Duration: October- December 2008

(b) Student: Binghao NG:

Title: Correlation energy of classical charges on a lattice.

Duration: October-December 2008.