4.1 Final publishable summary report

Executive summary

In the NanoInterface project a multi-scale modelling approach has been developed to describe the failure behaviour of metal-oxide-polymer materials systems which cover approximately 95% of all interfaces in microelectronic components. To achieve this, dedicated models at atomic, mesoscopic, microscopic, and macroscopic scale have been developed. In addition, micro- and nano-scale characterization techniques have been developed and applied. The developments in the project have been focussed on the simple and complex carrier systems, defined and processed by the industrial partners. The project team was comprised by industrial partners, research institutes, universities and a commercial software developer.

More specifically, first, the materials, parameters, tests, test conditions, two simple and two complex industrial carriers have been fully specified. Following these choices, the multi-scale framework has been established, based on a sequential approach. For this framework, a new cross-linking procedure for simulating the polymer network formation with MD has been developed. As a result, material properties of the epoxy moulding compound and interfacial interaction energy levels of EMC/copper and EMC/cuprous oxide have been calculated. Tools and scripts have been developed to model the following materials and interfaces at atomic and meso-scopic scale: Cu, CuO, Cu₂O, cross-linked EMC, EMC/SiO₂, EMC/Cu, and Cu(111)/Cu₂O(111). To this end, a new interatomic potential for Cu₂O has been developed. Furthermore, a traction-separation law for EMC/Cu at the micro-scale has been created. Also, meso-scale models have been developed which include the use of a bead bond failure criterion allowing more realistic simulations of the adhesive interface and generation of the full stress-strain curve to complete failure. A coarse-grained MD environment, called Mesocite, has been developed and is a state-of-the-art coarse-grained simulation module for the study of materials at length scales ranging from nanometers to micrometers and time scales from nanoseconds to microseconds, which is required for the project. A micro-scale model based on numerical fracture mechanics has been established including adhesive and cohesive failure at a roughened polymermetal interface. Dielectric properties of a composite containing longitudinal cracks have been determined. Additionally, a correlation between the temperature dependency of bulk modulus and the dielectric permittivity of the EMC material has been formulated.

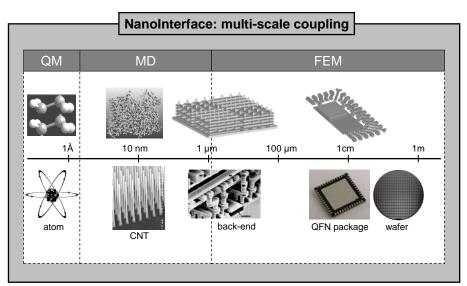
Experimental characterisation methods to measure the bulk and interface properties have been established. Consequently, the thermo-mechanical properties of the materials and interfaces have been determined, dependent on processing conditions. Surface and structure analysis on the micro-and nano-scale has been performed on the moulding compound, copper and its oxides, and the interfaces by means of SEM, FIB, EDX, AFM, AES, EBSD, FIBDAC and RAMAN. The thus developed experience of the applied characterisation methods is used to formulate guidelines and good practices which can be passed on to avoid repetition of mistakes or retrying dead-ends.

Two technological test carriers have been produced and modelled with 3D finite element simulations. From these models, design and reliability guidelines have been formulated with respect to delamination risk

A summary description of project context and objectives

Micro- and nano-electronic components are multi-scale in nature, caused by the huge scale differences of the individual materials and components in these products. This is driven by the ongoing miniaturization down to nano-scale (known as the "More Moore" principle) and the increasing functionality diversification (known as the "More than Moore" principle). Consequently, product behaviour is becoming strongly dependent on material behaviour and phenomena at the atomic scale. To prevent extensive trial-and-error based testing efforts for these new technology developments, new powerful quantitative knowledge-based modelling techniques are required. Despite the fact that current continuum-based finite element models ('FEM' in Figure 1) have become powerful engineering tools at scales larger than 1 μm, these phenomenological models still rely intrinsically on extensive characterisation efforts to quantify the parameters present in these models ('top-down' approach). On the other hand, state-of-the-art models at atomic scale, such as Quantum Mechanics ('QM' in Figure 1) and Molecular Dynamics ('MD' in Figure 1) are, to a certain degree, able to describe the material behaviour at molecular level, but predictions at product scale are not feasible yet.

NANOINTERFACE addresses this pressing need by developing a unique experimentally validated general multi-scale and multi-physics modelling approach in which models at atomic level will be explicitly coupled to models at macroscopic scale (see Figure 1). In this 'bottom-up' approach, a user-friendly software tool will be realised which incorporates chemical (van der Waals, hydrogen bonds, and Coulomb forces), physical (covalent, metallic, and ionic bonds) and mechanical (mechanical interlocking) information from the atomic level directly into the macroscopic models thereby enabling computational design towards highly reliable metal-oxide-polymer systems for so-called SiP (System in Package) products: complex micro- and nanoelectronic systems. In addition, new and efficient micro- and nano-scale measurement techniques are developed for a) obtaining detailed information about the most important phenomena at micro- and nano-scale and b) fast characterisation and qualification of SiPs in an industrial environment.



www.nanointerface.eu

Figure 1 Illustration of the proposed physically based multi-scale coupling framework of NANOINTERFACE: the theories and models valid at their typical length scales (QM = Quantum Mechanics, MD = Molecular Dynamics, FEM = Finite Element Method) are explicitly coupled. At the top, numerical models are shown of typical examples depicted below.

The focus is on metal-oxide-polymer material systems which cover approximately 95% of all interfaces, critical for reliability issues, in both current and future electronic devices. It should, however, be emphasised that the developed methods and concepts within this project could also be extended to other material systems in a rather straightforward manner.

A most distinguishing part of the project is that, due to the composition of the consortium, the whole industrial development chain is covered: from materials development, multi-scale models and experimental methods towards a fully functional commercial software package, ready to be used within an industrial environment. The project results are validated by comparison of the numerical results obtained from the multi-scale software tool with experimental testing of industrial technology carriers.

The success of this project is provided by the unique agglomeration of the consortium participants with world's leading expertise in atomic and macroscopic modelling (physics, materials science, electronics and engineering), micro- and nano-characterisation methods (physics and materials science), materials synthesis (chemistry), industrial electronics applications (engineering) and integrated software implementation. Hence, the key of this project lies in the combined presence of industrial partners, research institutes and the commercial software developer which results in the direct industrial valorisation of the project results.

S&T Objectives

To prevent extensive trial-and-error based testing efforts for new technology developments, a knowledge-based approach is pursued within this project, facilitated by the development and experimental validation of multi-scale modelling methods. Despite the fact that current continuum-based finite element models have become powerful engineering tools, these models lack true predictive power due to the absence of phenomena at the atomic scale. Consequently, these phenomenological models still rely on extensive characterisation efforts to quantify the parameters present in these models. On the other hand, models at atomic scale are able to describe the material behaviour at molecular level, but predictions at product scale are not feasible due to the infancy of these models and current hardware limitations. The overall technological objective is to facilitate knowledge-based material and interface engineering in an industrial environment by applying a user-friendly and experimentally validated multi-scale software tool towards highly reliable micro- and nano-electronic components (SiPs) such that all qualification tests are passed and reliability issues are prevented. To achieve this technological objective, the overall scientific objective is to establish an experimentally validated general multi-scale framework to explicitly couple the multi-physics phenomena at molecular and device level of metal-oxide-polymer systems.

To accomplish these challenging overall objectives, the following technological (T) and scientific (S) project objectives have been formulated:

- T1 Deployment of a multi-scale software platform in an industrial environment meeting the following demands: user-friendly, flexible, robust, and workflow based.
- T2 Knowledge-based integration of a decision support framework for the development of new materials and interfaces, including the multi-scale framework, experimental data and database systems within the software tool.
- T3 Industrial verification of the accuracy and assessment of the developed multi-scale method with respect to the given demands in T1.
- T4 Standardised experimental characterisation methods for micro- and nano-scale bulk and surface analysis.
- T5 Develop design and reliability guidelines for SiPs.

To achieve these technological objectives, the following scientific objectives should be realised:

- S1 The key challenge is to couple the atomic and continuum scales in an accurate and efficient way which will provide predictive macroscopic reliability models that take into account the details of the atomic models.
- S2 To enhance fundamental multi-physics knowledge of material properties and adhesion mechanisms at the atomic scale (chemical, physical and mechanical), including the influence of high temperature, moisture environments and pressure.
- S3 Multi-scale modelling of non-crystalline materials (such as interlinked epoxy resins).
- S4 Develop accurate inter-atomic potentials for metal-oxide-polymer material systems.
- S5 Develop standardised experimental surface and bulk characterisation method at micro- and nano-scale for reproducible and efficient analysis of micro- and nanoelectronic products.

The following technological and scientific work packages have been defined (Figure 2):

- WP1: Technology carriers specification
- WP2: Multi-scale and multi-physics modelling framework
- WP3: Micro- and nano-scale characterisation
- WP4: Software integration of multi-scale framework
- WP5: Industrial validation on technology carriers

The technological objectives, as formulated above, will be addressed in WP4 and WP5, whereas the scientific objectives will be achieved in WP2 and WP3. Of course, several iterations will be performed between those work packages to achieve to final projects deliverables. In WP1, two industrial carriers (one simple and one complex carrier) will be defined to focus, test and validate the developed multi-scale and experimental characterisation methods from WP2 and WP3 and used as test vehicles in WP5. The objectives of WP4 are to bring together the knowledge gained from other work packages as well as the multi-scale modelling software developed in WP2 in such a way as to support the workflow of end users in an optimal way. End user requirements, experimental insights and the software will be brought together to integrate tools in a way which impacts the development of new materials and devices. In WP5, the developed software tool and characterisation methods from WP2 & WP3 & WP4 will be applied on the technology carriers from WP1. Upon testing of carrier 1 in WP5, several iterations will be performed in WP2 and WP3 in the case of discrepancies between modelling and experimental results. Subsequently, the more complex carrier, carrier 2, will be used in WP5 to really assess the predictive capabilities of the developed multi-scale modelling framework by the end-users.

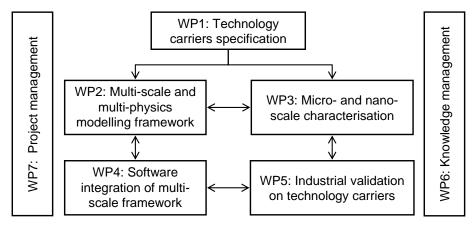


Figure 2 Pert diagram of the work packages

A description of the main S&T results/foregrounds

At the start of the project, the material systems, tests and testing conditions were defined thereby taking into account the industrial challenges and interests. Consequently, it was decided that the technological test carrier is a bi-material strip consisting of either Epoxy Moulding Compound (EMC) on copper based lead-frame material. The adhesion properties of this interface are highly interesting for the industrial partners and samples can be provided using commercial EMC types. The composition of commercial EMC is usually unknown with ingredients not disclosed by the suppliers. Alternatively, an EMC with known recipe and ingredients is used which is an essential requirement for the atomistic simulations that are carried out in the project. This EMC is specifically designed and processed for usage within this project. Next to this technological test carrier, a complex carrier has been defined: a QFN-type package defined and produced by the industrial partners Infineon and NXP. Clearly, surfaces and materials used in the complex carrier variants are as similar as possible to those of the simple bi-material carriers. In addition, tests and test conditions were defined.

Concerning the multi-scale modelling of the considered materials, first a validated tool has been developed to build crosslinked models of epoxy networks on nanoscale (atomistic models) as well as on mesoscale (coarse grained models). Subsequent molecular dynamics/molecular statics simulation predicts well material properties, including densities, glass transition temperature, volumetric coefficient of thermal expansion and isotropic mechanical properties, indicating the validity of the adopted polymer network formation methodology. A coarse-grained molecular dynamics environment (Mesocite) has been developed and is a state-of-the-art coarse-grained simulation module for the study of materials at length scales ranging from nanometers to micrometers and time scales from nanoseconds to microseconds, which is required for the project. Furthermore, large scale molecular statics and dynamics simulations were conducted on Cu-Cu tilt grain boundary interface and on Cu/Cu₂O interfaces, results of which are used as input to develop interfacial constitutive laws at larger scale. Such models are paramount in developing predictive capabilities related to reliability and failure of microelectronic components. Molecular simulations were conducted on various Cu-Cu tilt grain boundary structures using EAM potential. An intergranular crack is introduced and local traction and crack opening displacement data is extracted from the simulation results. To bridge length scales between atomistics and continuum, the data obtained from MD simulations is re-cast within the framework of the continuum cohesive zone model (CZM) to quantify the cohesive zone law. Atomistic simulations were also used to construct a large-scale Cu(111)/Cu₂O(111) optimized structure which was subjected to external loading to obtain the interface excess energy, stress-strain, and interfacial delamination and failure of the structure.

Additionally, a novel interatomic potential for Cu_2O has also been developed which was used to conduct the analysis of $Cu(111)/Cu_2O(111)$ interfacial failure by using specifically developed scripting tools. The obtained results for copper oxide systems are of paramount importance in addressing the failure behaviour of the copper/polymer interface which encompasses a thin layer of copper oxide (both, CuO and Cu_2O) and invariably influences its failure characteristics.

Both semi-analytical and transient finite element (FE) models at the meso-scale on Cu/polymer roughened interface have also been developed to establish cohesive or adhesive interfacial delamination criteria under external loading. In this way, the effect of microscopic surface roughening on macroscopic adhesion properties can be established.

Atomistic simulations on the epoxy resin were conducted to compute its material properties and interfacial interaction energy on its interfaces with Cu and Cu₂O. Using the developed crosslinking approach, models for interfaces between a 2D polymer network and copper as well as Cu₂O were constructed and subjected to energy minimization. The interfacial interaction energy for both systems was extracted while results related to the interfacial debonding strength were also reported. An MD model was developed to calculate the traction-displacement function of a separation process between

an epoxy-copper interface. Both the impact of time scale and model size on the traction-displacement relations was studied. Migration processes under the influence of a high current density and mechanical strains were described, as well as the effects of structure defects in the degradation process. A correlation between the temperature dependency of the bulk modulus and the dielectric permittivity of the EMC material has been found.

Experimental methods to characterize bulk properties (e.g., viscoelasticity, elastoplasticity, hygroscopic and dielectric properties, fracture toughness) and interface properties (e.g., interface toughness as function of mode angle) have been designed, developed and validated. As a result, material and interface properties for the manufactured test specimens have been obtained, several of which as function of processing (e.g., curing, moisture). Surface and structure analysis on the microand nano-scale has been performed by means of e.g., SEM, FIB, EDX, AFM, AES, EBSD, FIBDAC and RAMAN, to analyse the respective materials and (delaminated) interfaces and to calculate residual stresses. To a greater or lesser extent, the results of these methods depend on careful preparation of specimens and samples as well as on usage of the available equipment. The obtained results were used for the development of realistic models of the bulk material as well as the interface area and for the validation of the results of the multi-scale modelling. The thus developed experience of the applied micro- and nano-scale characterization methods was used to formulate guidelines and good practices in order to avoid repetition of mistakes or retrying dead-ends.

A system has been developed which enables access to some of the complex atomistic modelling and simulation calculations with a simple web-based interface. Although the focus was on the prediction of the glass transition temperature and mechanical properties, the framework itself will easily allow the addition of new property calculators.

For the complex carrier system, two- and three-dimensional FE models have been established which describe interface delamination. These models originate from the multi-scale modelling framework as well as from the results of the experimental methods. Results of these parameterized models have been summarized in the form of design and reliability guidelines for the considered package family.

The potential impact (including the socio-economic impact and the wider societal implications of the project so far)

European dimension

The achievement of the challenging project objectives and a significant impact is only feasible through the agglomeration of industrial expertise and requirements, and world leading expertise in modelling, characterisation, materials synthesis and software implementation, clearly represented by the project consortium. This requires knowledge and expertise that is not available on national level only.

Economical impact

The current economic trend in microelectronics industry shows that packaging will become more important. Packaging revenues increased from 5% in 2001 to 14% in 2006. Innovations in new package technologies, like system in package (SiP), are inevitable. Moreover, improved reliability of SiP structures opens new opportunities for new applications. Especially for automotive applications, where Europe is very strong, improved SiP reliability can lead to new applications. Semiconductors industry and its suppliers, as the cornerstone of today's high-tech economy and modern society, represented a worldwide sales value of \in 250 billion in 2005, supported a global market of more than \in 1 trillion in terms of electronic systems and an estimated value of \in 4.5 trillion in services, with

applications covering virtually all aspects of human life (telecommunications, automotive, environment, healthcare, security and energy efficiency). Direct service costs (field call rates) amounted to approximately \in 2 billion of which roughly \in 600 million could be attributed to interface reliability issues. Moreover, costs of the indirect consequences of these reliability issues, such as extended maintenance and training, could surpass \in 10 billion. Furthermore, material costs are a major determining factor in this industry which could be reduced significantly through the development of material design by applying the developed knowledge-based multi-scale software tool. Finally, legal costs as a result of accidents occurring by non-reliable electronics could also easily exceed \in 5 billion.

Direct and indirect economic benefits:

- a. High competitive advantage for the European industry (automotive, semiconductor, telecommunication, healthcare, consumer electronics, security) due to improved reliability and production time with respect to USA and Asia. As a result, new business can be created.
- b. Cost- and time-efficient material design and extended lifetime of electronics systems.
- c. Energy saving due to decreased number of redesigns and time-to-market.
- d. Accurate reliability prediction allows rapid prototyping that can open new business opportunities.
- e. The envisioned application area covers nearly all aspects of human life, such as telecommunication, automotive, environment, healthcare, security, energy efficiency.
- f. A common language between material suppliers and end-users: material synthesis efforts will be reduced ('first-time-right' production).

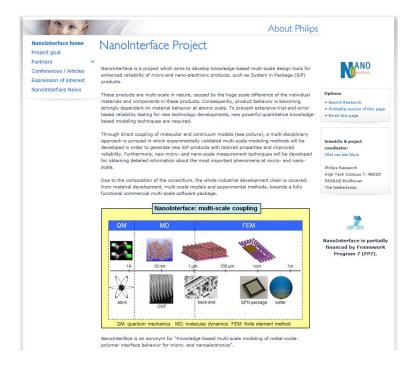
Societal impact

- Quality of life: Citizens expect from everyday life microelectronic products that they last long and require little maintenance during their lifetime. To meet these expectations and address citizens' needs, high reliability is required. The NANOINTERFACE project will significantly contribute to maintaining and increasing citizens' confidence in European micro-electronic products in all kinds of activities (e.g., transport, telecommunication, information systems) while introducing miniaturised products, enhancing thus the quality of life at European and international levels.
- *Health and safety*: the stringent requirements of microelectronics in automotive, rail transport and aeronautic industry contribute to the public opinion demand for a minimum, if not zero, transport accidents. An increased level of safety will be requested to overcome the increase of risks linked to traffic growth. The current proposal aims to improve the general lifetime of microelectronics components and the thermo-mechanical reliability thereof, one of the sources of damage risk, thus increasing the safety margins of transports and ensuring safety of European citizens. This will help the EU to develop and implement safety transportation policies.
- Employment: increased reliability of microelectronic materials in high added value applications will allow developing European consumer electronics industry, thus increasing job opportunities in sectors like telecommunications, automotive and aeronautic industry for technicians, engineers and researchers. The R&D institutes and universities benefit from the project results to strengthen their leading position as competence centres and to extend their research position in the multi-scale modelling field, respectively. The close contact between industry, institutes and academia will facilitate industrial recruitment. Furthermore, future cooperation of the partners with SMEs could increase the competitiveness of these SMEs through indirect application of these project results in future projects.

• Environment: material design will decrease the amount of toxic contents (e.g., microelectronic materials towards halogen free/dark-green materials). Furthermore, the amount of energy used during the product creation process will be decreased by 30%, due to the decreased time-to-market. Less physical prototyping will be needed and consequently, less waste materials will be produced due to the fact that specific material systems are developed by knowledge-based predictive models.

The main dissemination activities and exploitation of results

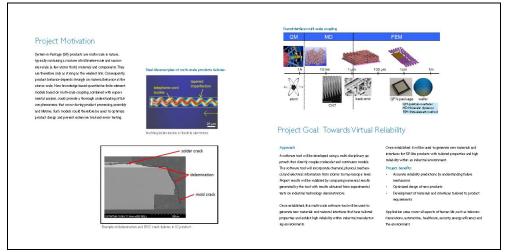
The project website can be found at www.nanointerface.eu which is part of the external dissemination activities, where the focus lies on offering a description of project objectives, partners, technologies, applications and results in a professional manner, but without putting constraints on accessibility or limit the audience by using heavy graphics material (see figure below).



The content of the external website has been generated with text material from partners and with help from graphical experts. The website consists of a public section, for which Philips is responsible. In order to be realized in a short time span and with minimal efforts related to graphical layout, the content of the website has been located within the Philips website structure, while access is arranged via an external web address. The website has been updated including all project-related publications.

The project folder has been developed for promotion of project goals, partners and potential customers. The flyer has already been distributed at conferences and other events (see figures below).





Additionally, a press release was issued by the consortium to technical trades and magazines and announcements about NanoInterface project on websites of partners (see figures below)







As illustrated, some of the project partners (PHI, ACC, GTL, ETU) have announced the project by means of releases through their press contacts and announcements on their websites, which have been picked-up and further published by printed and online media (for example, see below excerpts from UK's IET – the Institution of Engineering and Technology – article entitled "Simulation and the art of making nanotechnology work" and from System-Level Design Community – article entitled "Progress Report: Nanoelectronics").

"...Philips Applied Technologies is leading a similar collaborative effort to develop a multi-scale modelling approach to understand the behaviour of metal oxide polymer interface materials in system-in-package (SiP) products. SiPs contain many components interfaced with very thin layers of metal oxide polymers, whose job is to stick the whole lot together while also handling high thermal stresses and environmental hazards like the ingress of water. Increasing component miniaturisation is in turn increasing the influence of the atomistic structure of the materials. As a result, product behaviour is becoming strongly dependent on material behaviour at this atomistic scale.

The goal of the NanoInterface consortium is to try to predict with simulation where failures might occur and then make design or material changes in advance to improve reliability, according to Philips Applied Technologies.

The NanoInterface partners are particularly keen to understand the processes that lead to delamination between the moulding compound and the lead-frame. Automotive customers, for instance, have become fussy in this respect.

'This de-lamination is caused at the molecular level but at this stage all we know is that if we clean the lead frame, we have fewer problems, but we don't understand why,' explains NXP Semiconductors, one of the partners in the NanoInterface project...."

Article available at http://kn.theiet.org/magazine/issues/1002/nanoelectronics-1002.cfm

"(...) Nanoelectronics around the world

Additionally, a European initiative aimed at improving engineering efficiency at the nanoscale just recently won funding under the European Union's Seventh Framework Program. The initiative is being led by a consortium of microelectronics companies like Philips Applied Technologies, Fraunhofer IZM, Infineon, and NXP, as well as research institutions like the Georgia Institute of Technology Lorraine. The project, NanoInterface, hopes to realize a number of scientific, technological and societal advances, including the development of a multiscale design approach for microelectronic materials, a contribution towards the industry's 'zero defect' objectives and the implementation of environmentally-friendly materials. As part of the project, partners will develop a software tool that incorporates chemical, physical and mechanical information from the atomic level directly into macroscopic models. It will be used to enable highly-reliable metal oxide-polymer systems for System in Package (SiP) products and complex micro- and nanoelectronic systems. (...)."

Article available online at http://chipdesignmag.com/sld/blog/2009/09/24/progress-report-nanoelectronics/

The partners have contributed to 52 papers (journal publications and conference proceedings) as well as 20 presentations (additional to the conference presentations). These can be found on the project internet website (www.nanointerface.eu).

The following project results are suited for exploitation:

- The developed design and reliability guidelines for the considered package family;
- The development of the coarse-graining MD environment Mesocite;
- The guidelines for micro- and nano-scale characterisation methods.

The list of all beneficiaries with the corresponding contact names

Beneficiary Number *	Beneficiary name	Contact	Country
Number '	Dhiling Eleganoning Nederland	Olof wan dan Claria	NII
	Philips Electronics Nederland	Olaf van der Sluis	NL
(coordinator)			
2	NXP Semiconductors	John Janssen	NL
3	Infineon Technologies AG	Heinz Pape	DE
4	Fraunhofer IZM	Bernhard Wunderle	DE
5	Centre National de la Recherche Scientifique	Mohammed	FR
		Cherkaoui	
6	Delft University of Technology	Kaspar Jansen	NL
7	Accelrys	Stephen Todd	GB
8	AMIC GmbH	Jürgen Keller	DE
9	St. Petersburg Electrotechnical University	Irina Vendik	RUS
10	Honeywell	Nancy Iwamoto	USA
11	Georgia Tech Lorraine	Mohammed	FR
		Cherkaoui	