EUROPEAN CONCERTED ACTION
ON
"Advanced Solder Materials for High Temperature Application – HISOLD"

COST MP0602

Group Project:

1. INFORMATION EXPECTED FOR A GROUP PROPOSAL

1.1 Title of project
Modelling of the microstructural changes in the interdiffusion zone for Ag-Cu-Sn and Cu-Ni-Sn leadfree solder joints

Coordinator (full name and address)

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1.2 Information on participating members

Sections 1.2.x have to be filled in for each participating member!

1.2.1 **Participant 1**: (should not exceed ½ page)

1.2.1.1 **Dr. Nele Moelans**
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1.2.1.2 **A. Serbruyns**
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1.2.1.3 Expected effort in man/years per annum of research students, post doctoral researchers, scientists and technicians.

2 person / years PhD student

1.2.1.4 Expected cost of project, including: amount requested (or already awarded) from National resources; funding required for project per annum; total required for duration of the project. (*It is acknowledged that any sums entered here may only be approximate or estimated*).

Funding for 4 years: 265000 euro (Flamish government)
Salary + working budget for 1 PhD student for 4 years: +/- 250000 euro (Imec)

1.2.2 **Participant 2**: (should not exceed ½ page)

1.2.1.1 **Dr. Suzana Gomes Fries**
SGF Scientific Consultancy
Arndtstr 9, D-52064 Aachen
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1.2.1.2 Scientist responsible for the project (if different from the applicant)

Full name, title, office, complete address

Telephone fax and e-mail

1.2.1.3 Expected effort in man/years per annum of research students, post doctoral researchers, scientists and technicians.

1.2.1.4 Expected cost of project, including: amount requested (or already awarded) from National resources; funding required for project per annum; total required for duration of the project. (*It is acknowledged that any sums entered here may only be approximate or estimated*).

1.2.1 **Participant 3:** (should not exceed ½ page)

1.2.1.1 **Dr. Ingo Steinbach**

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1.2.1.2 Scientist responsible for the project (if different from the applicant) n.a.

1.2.1.3 Expected effort in man/years per annum of research students, post doctoral researchers, scientists and technicians.

1 persons for 3 years, PhD student

1.2.1.4 Expected cost of project, including: amount requested (or already awarded) from National resources; funding required for project per annum; total required for duration of the project. (*It is acknowledged that any sums entered here may only be approximate or estimated*).

65,000,- per year, total 195.000,- Euro (German science foundation DFG, pending)

1.2.1 **Participant 4:** (should not exceed ½ page)

1.2.1.1 **Dr. Alexander Kodentsov (in co-operation with Dr. M. Biglari, Mat Tech BV)**

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1.2.1.2 The same as above

1.2.1.3 Expected effort in man/years per annum of research students, post doctoral researchers, scientists and technicians.

1 person/year PhD student

1.2.1.4 Expected cost of project, including: amount requested (or already awarded) from National resources; funding required for project per annum; total required for duration of the project. (*It is acknowledged that any sums entered here may only be approximate or estimated*).

~ 300 000 €

1.2.1 **Participant 8:** (should not exceed ½ page)

1.2.1.1 **Dr Rada Novakovic**

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1.2.1.2 The same as above

1.2.1.3 Expected effort in man/years per annum of research students, post doctoral researchers, scientists and technicians.

1 person / years 1 PhD student

1.2.1.4 Expected cost of project, including: amount requested (or already awarded) from National resources; funding required for project per annum; total required for duration of the project. (*It is acknowledged that any sums entered here may only be approximate or estimated*).

Salary (Italian government) + 1 fellowship for 1 PhD student (≈ 160 000 euro)

1.2.1 **Participant 9:** (should not exceed ½ page)

1.2.1.1 **Dr. Natalia Sobczak**
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1.2.1.2 Scientist responsible for the project (if different from the applicant)

Full name, title, office, complete address

Telephone fax and e-mail

1.2.1.3 Expected effort in man/years per annum of research students, post doctoral researchers, scientists and technicians.

1.2.1.4 Expected cost of project, including: amount requested (or already awarded) from National resources; funding required for project per annum; total required for duration of the project. (*It is acknowledged that any sums entered here may only be approximate or estimated*).

1.2.1 **Participant 10:** (should not exceed ½ page)

1.2.1.1 **Prof. Jean-Georges Gasser**
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1.2.1.2 Scientist responsible for the project (if different from the applicant)

Full name, title, office, complete address

Telephone fax and e-mail

1.2.1.3 Expected effort in man/years per annum of research students, post doctoral researchers, scientists and technicians.

1.2.1.4 Expected cost of project, including: amount requested (or already awarded) from National resources; funding required for project per annum; total required for duration of the project. (*It is acknowledged that any sums entered here may only be approximate or estimated*).

1.2.1 **Participant 11:** (should not exceed ½ page)

1.2.1.1 **Prof. J.C. Tedenac**
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1.2.1.2 Scientist responsible for the project (if different from the applicant)

Full name, title, office, complete address

Telephone fax and e-mail

1.2.1.5 Expected effort in man/years per annum of research students, post doctoral researchers, scientists and technicians.

1.2.1.6 Expected cost of project, including: amount requested (or already awarded) from National resources; funding required for project per annum; total required for duration of the project. (*It is acknowledged that any sums entered here may only be approximate or estimated*).

1.2.1 1.2.1 **Participant 12:** (should not exceed ½ page)

1.2.1.1 **Prof. Jaromír Drápala**
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1.2.1.2 Scientist responsible for the project (if different from the applicant)
The same as above

1.2.1.3 Expected effort in man/years per annum of research students, post doctoral researchers, scientists and technicians.

Our working group has 10 members and other co-workers: **Prof. Ing. M. Kursa, CSc.** (metallurgy of non-ferrous metals), **Doc. Dr.Ing. M. Losertová** (microstructural analysis), **Ing. J. Malcharcziková** (chemical analysis OES), **Ing. R. Burkovič, CSc.** (preparation and melting of samples), **Prof. Ing. V. Vodárek, CSc.** (analyses EDX, WDX), **Doc. Ing. S. Lasek, PhD.** (corrosion behaviour), **Doc. RNDr. L. Čížek, CSc.** (mechanical properties), **Ing. B. Smetana** (DTA, DSC, TG analyses), **Ing. R. Dudek, Ph.D.** (surface tension, density, viscosity measurements), **Mgr. Z. Morávková, PhD.** (programming in Matlab), **Doc. Ing. T. Kozubek, PhD.** (calculation of diffusion processes MatLab, FemLab), external co-worker **Prof. Ing. P. Kubíček, DrSc.** (theory of diffusion), doctor student **Ing. R. Kozelková**, one student per year – graduant.

1.2.1.4 Expected cost of project, including: amount requested (or already awarded) from National resources; funding required for project per annum; total required for duration of the project. (*It is acknowledged that any sums entered here may only be approximate or estimated*).

Funding for 4 years: 90000 euro (Czech government – 65000 euro, own financial resources – 25000 euro), i.e. 26000 euro per annum (2008, 2009, 2010), 12000 euro in 2011 year.

1.2.1.7

1.2.1 **Participant 13:** (should not exceed ½ page)

1.2.1.1 **Prof. John Botsis**
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1.2.1.2 Scientist responsible for the project:

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1.2.1.8 Expected effort in man/years per annum of research students, post doctoral researchers, scientists and technicians.

1 person / years PhD student

1.2.1.9 Expected cost of project:

1.2.1.10 Budget for 4 years (1 PhD salary + working budget) : ~150'000 euros (financial requested to Swiss Secretariat for Teaching and Research)

Expected cost of project, including: amount requested (or already awarded) from National resources; funding required for project per annum; total required for duration of the project. (*It is acknowledged that any sums entered here may only be approximate or estimated*).

1.2.1 **Participant 15:** (should not exceed ½ page)

1.2.1.1 Mauro Palumbo

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1.2.1.2 Scientist responsible for the project (if different from the applicant)

Full name, title, office, complete address

Telephone fax and e-mail

1.2.1.11 Expected effort in man/years per annum of research students, post doctoral researchers, scientists and technicians.

Expected cost of project, including: amount requested (or already awarded) from National resources; funding required for project per annum; total required for duration of the project. (*It is acknowledged that any sums entered here may only be approximate or estimated*).

1.2.1 **Participant 16**

1.2.1.1 **Prof. Jozef Janovec and Prof. Milan Ožvold**

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1.2.1.2 The same as above

1.2.1.3 Expected effort in man/years per annum of research students, post doctoral researchers, scientists and technicians.

4 person / years 1 PhD student

1.2.2.4 Expected cost of project, including: amount requested (or already awarded) from National resources; funding required for project per annum; total required for duration of the project. (*It is acknowledged that any sums entered here may only be approximate or estimated*).

Funding for 4 years: 80 000 EUR (national scientific grants)

1.2.1 **Participant 17**

1.2.1.1 **Prof. Jolanta Janczak-Rusch**

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1.2.1.2 n.N. Post-doc

Swiss Federal Lab. for Materials Testing and Research (EMPA)

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Switzerland

1.2.1.3 Expected effort in man/years per annum of research students, post doctoral researchers, scientists and technicians.

1 person / years Post-doc

1.2.1.4 Expected cost of project, including: amount requested (or already awarded) from National resources; funding required for project per annum; total required for duration of the project. (*It is* *acknowledged that any sums entered here may only be approximate or estimated*).

Budget for 4 years (1 Post doc salary + working budget):

~100'000 euros (founded by Swiss State Secretariat for Education and Research)

1.2.1 Other participants of COST MP0602 with who we will exchange information

Flandorfer,

Ab initio data

Hotas,

Alan Dinsdale

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Phase diagram assessment, calculation of phase diagram information and Gibbs free energies

Jürgen Villain, Ioan Plotog

Effect of cooling rate (experimental)
EBSD for grain orientations
Determination of mechanical properties (Young's modulus, yield strength, micro/nano hardness)

Prof. Dr. Jürgen Villain
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1.2

1.3 Probable duration of project.

4 years

1.4

1.5 Probable duration of project.

4 years

1.4 Start date

October 2007

1.5 International co-operation with other Signatory States of the Memorandum of Understanding (if not mentioned above)

... partners from .... countries

1. ABSTRACT **(maximum 200 words please)**

The main purpose of this group project is the development of theoretical models and simulation techniques that predict the microstructural changes in the interdiffusion zone in lead-free solder joints. Different modeling techniques such as the phase field method, finite element modeling, the CALPHAD-method and ab-initio calculations, will be combined to describe processes at different length scales. The modeling will be supported by experimental studies (diffusion couple experiments, annealing, surface tension and contact angle measurements) to obtain the necessary information for the input parameters, information on the sequence of phase formation, and for validation of the modelling approaches. Different phenomena important in the life cycle of a solder joint will be considered, such as nucleation, solidification of the solder, growth of the intermetallic layer and precipitates, Kirkendal voiding, and crack formation. Also the effect of oxygen on the morphological evolution will be studied. The work will focus on the systems Ag-Cu-Sn and Ni-Cu-Sn for which the thermodynamic properties have been studied extensively, amongst others in COST 531.

2. INFORMATION EXPECTED IN EACH PROPOSAL **(recommended maximum 5 pages)**

3.1 **Aim of the study** (approx. ½ page)

In this group project the morphological changes and stress distribution in lead-free solder systems due to diffusion and reaction at the solder/substrate interface will be modelled. For this purpose the phase field technique will be combined with

- finite element an other mesoscale models for elastic and plastic deformation, crack formation, heat and mass diffusion and convection,
- thermodynamic and kinetic databases developed according to the CALPHAD-approach (cooperation with WG1),
- models for surface tension,

- ab initio calculations, and
- experiments.

The complete description must treat the effect of phase transformations, diffusion, curvature driven interface motion, externally applied load, volume effects and anisotropy, on the morphological evolution in lead-free solder joints, and the complex interaction between them. Different modeling approache will be compared. Diffusion couple and annealing experiments in combination with different characterization techniques (SEM, EPMA, EDS, WDS, OLM,…) will be performed to obtain information on the diffusion behavior and interfacial reactions, on the one hand, and for validation of the modeling techniques, on the other hand. Furthermore, surface tension, contact angle and ultra-short contact measurements will be performed to obtain information on the surface properties and the sequence of phase nucleation during formation of the joint.

Due to the complexity of the processes and to enhance the exchange of information between different participants, the study will be limited to the ternary Ag-Sn-Cu and Ni-Sn-Cu systems, for which there is already a lot of information available on thermodynamic, kinetic and physical properties. The effect of oxygen on the properties of the solder joint and the different processes will be studied experimentally and by comparison of simulations with experiments. These are no typical high temperature solder alloys. However the approaches developed in this GP can be applied to high temperature solders afterwards.

The group project consists of 3 subprojects, each focusing on a different aspect of the main goal

- Processing -- experimental characterization -- Transient Liquid Phase bonding -- Cu-Ni-Ag-Sn(-Bi)
    - Participants: Ozvold, Janovec, Dràpala, **Kodentsov**[1]+Mattech, Villain, Janczak-Rusch,, Tedenac, Hotas, Plotog, Sobczak
- Kinetic modeling (stresses, voids, diffusion, phase transformations, intermetallics, heat and mass transport, …), coupling of different modeling approaches (phase field – finite elements – CALPHAD – ab initio) and multi-scale
    - Coupling of phase field with ab inito/CALPHAD/crystallography; participants: Gasser, **Steinbach**, Fries, Flandorfer
    - Microstructure simulation with the phase field method; participants: Steinbach, Serbruyns, Moelans
    - Finite element modeling; participants: Cugnoni, Botsis, Barrico, Palumbo
- Surface tension modeling -- effect of oxygen -- segregation -- size dependence -- nanosystems -- coupling Cahn-Hilliard equation/surface tension models
    - Participants: Moelans, **Novakovic**, Fries

There will be a large interaction between the 3 subprojects as well as with group projects in WG1 and WG2.

[1] For each subproject a coordinator is indicated in bold.

Ag-Cu-Sn and Ni-Cu-Sn alloys are typically not applicable for high temperature soldering. However, the main goal of the project is to develop models for microstructure evolution. Moreover, the simulations require information on amongst others phase stabilities and diffusion coefficients. Therefore, it is most appropriate to apply and validate the models for well-known systems first. For Ag-Cu-Sn and Ni-Cu-Sn numerous experimental investigations have been performed to study the phase stabilities and the formation and growth of the intermetallic layer. There are also several thermodynamic (according to the CALPHAD method) optimizations and phase diagrams available in the literature. The systems were also studied extensively in COST-531. The knowledge and databases obtained in this action will be very useful for the development of the models. Nevertheless the proposed modelling approaches are generally applicable and therefore, in a later stage of COST MP0602, they might be applied to study the behavior of typical high-temperature solder alloys (using information on phase stabilities and physical properties obtained in WG1 and WG2 during the course of the action).

3.2 **Background to the study** (suggested 1-2 pages)

The morphology of the intermetallic compound (IMC) layer and the intermetallic precipitates in the interdiffusion zone between solder and substrate strongly affect the mechanical and physical properties of the joint. Due to diffusion, the IMC layer and intermetallic precipitates in the solder alloy continue to grow and voids (Kirkendal voiding) may form during device use. Moreover, stress fields develop near the intermetallic layer, precipitates and voids, especially under thermal and mechanical loading. This may lead to crack formation and enhance corrosion. Since the growth of the intermetallic layer and coarsening of the microstructure are much faster for lead-free solders as they were for the classical Pb-Sn alloys, these are two main issues in current reliability studies.

Phase field models have proven to be able to predict the evolution of complex morphologies, as those observed for solder joints, during solidification, phase transformations and coarsening. Various thermodynamic driving forces (such as those related to phase stabilities, interfacial energy and elastic strain energy) and various transport processes (such as heat and mass diffusion) can be considered in phase field simulations. They allow therefore the study of the role of diffusion, anisotropy and transformation strains on the growth of the interfacial reaction zone. The effect of temperature and external load during the operation of the soldered assembly can be simulated as well.

The phase field model, in combination with mechanical mesoscale models, requires as input

- CALPHAD-expressions for the Gibbs free energy,
- diffusion mobilities,
- crystallographic data (lattice parameters) and thermal expansion coefficients,
- interfacial energies as a function of orientation,
- elastic constants, yield strength, creep data,…
- data on interfacial and grain boundary diffusion,

- sequence of formation of the intermetallic phases at the interface,
- ...

For Ag-Sn-Cu and Ni-Sn-Cu, the Calphad expressions are mostly available in the thermodynamic database developed in COST 531 and will be improved during COST MP0602 (WG1). Information on mobilities (or diffusion coefficients), crystal structure (symmetry + lattice parameters), thermal expansion coefficients, elastic constants, yield strengths and surface tension will be taken from the property database developed in COST 531, experimental information obtained by participants in the group project and from the literature (interaction with WG2). Furthermore, elastic constants, lattice spacings and diffusion coefficients can be calculated using an ab inito approach. Information on anisotropy and grain boundary and surface diffusion will be estimated from diffusion couple and annealing experiments. The sequence of formation of the intermetallic phases will also be investigated experimentally.

As output the phase field simulations give information on

- the spatial distribution and shape of the different phases, for example the shape and distribution of the intermetallic precipitates, the morphology of the interfacial layer, the grain size,...
- the stress distribution in the solder joint, which allows to identify localized stress peaks,
- crack formation.

This information can be used as input for macroscopic models that predict the properties and reliability of a solder joint as a function of microstructural characteristics and the magnitude and distribution of residual stresses.

Experiments (diffusion couples, annealing, surface tension, contact angle, ultra-short contact experiments) will be designed specifically to support the modeling. It is for example important that they are performed using very pure and well-characterized samples, under highly controlled conditions (temperature, atmosphere, …) and for simple geometries. In this way, the experiments can provide fundamental material properties that can be used as input for the simulations and for validation of the newly developed modeling approaches.

Furthermore, the effect of oxygen on the above mentioned processes will be studied experimentally for the ternary systems Ag-Cu-Sn and Ni-Cu-Sn in combination with oxygen. The experimental microstructures, affected by the presence of different amounts of oxygen, will be compared with the experimental and calculated microstructures for pure systems in order to characterize and quantify the effect of oxygen on the properties and behavior of a Pb-free solder joint. If possible, the effect of oxygen will also be considered with simulations.

3.3 **Practical value of the project** (approx. ½ page)

Practical problems which the study will address

The models and simulations in combination with experimental characterization will help to understand the complex processes that govern the growth of the intermetallic phases and the evolution of stresses at the Pb-free solder – substrate interface. Aspects that will be studied are

- Solidification of the solder alloy, effect of cooling rate
- Formation of intermetallic layers, for example during transient liquid phase bonding
- Coarsing of the intermetallic layer and intermetallic precipitates during thermal annealing
- Effect of the microstructure/grain structure on diffusion
- Kirkendal voiding
- Effect of stresses due to diffusion, transformation strains
- Effect of thermal and mechanical loading
- Plastic deformation/crack formation near the intermetallic layer and intermetallic precipitates
- Effect of oxygen
- Transient Liquid Phase (TLP) bonding
- ....

Major strength of the phase field method is that it allows to consider several concurrent microstructural processes (phase transformations, coarsening, elastic stress-strain interaction) at the same time and complex grain shapes and distributions, without a considerable increase of the mathematical complexity. The effect of different parameters (composition, external conditions, geometry, …) on the morphological evolution will be studied systematically using simulations.

The models and simulation results will give a better insight in the physical processes that control the morphological evolutions in lead-free solder joints and can help to interpret experimental results.

Economic benefit expected from the research

Mesoscale simulations can reduce the number of expensive and time-consuming experiments in the development of new solder alloys and soldering techniques. They indicate which alloy compositions and processing parameters may result in the desirable microstructural features for a particular application. Moreover, the output on the evolution of the stress distribution may give an idea on the life time, and hence reliability, of the soldered assembly.

Sections 3.4.x - 3.5.x have to be filled in for each participating member!

3.4 Plan of research (approx. 1 page)

Participant 1 (Nele Moelans)

Phase field modelling

Coarsening, diffusion, stress/strain

3.4.1 Our contribution consists of a study of the effect of diffusion, transformation strains, thermal expansion and external loading, on the growth and coarsening of the intermetallic layer and precipitates in the solder, by means of phase field simulations. A systematic study of the role of different material and process parameters will be performed. The modelling technique will be validated by comparing experimentally obtained micrographs of annealed diffusion couples with simulated microstructures.

3.4.2 Year 1 + 2:

- Model formulation and implementation
- Collection of input parameters for the Cu-Sn system
- Simulations, analysis of model parameters and validation with experimental micrographs for the Cu-Sn system

Year 3 + 4:

- Extension of the model and implementation towards ternary systems
- Collection of input parameters for the Ag-Cu-Sn and Ni-Cu-Sn system
- Simulations for solder joints based on the Ag-Cu-Sn and Ni-Cu-Sn systems
- Comparison with experimental micrographs for Ag-Cu-Sn and Ni-Cu-Sn diffusion couples

3.4.3 Staff required

Participant 2 (Suzana Gomes Fries)
Relations with WG1 and WG2 and ab initio

3.4.4 Description of the approach applied in the study
3.4.5 Outline of work plan and time schedule (in form of a diagram if so convenient)
3.4.6 Staff required (graduates and technicians only)

Participant 3 (Ingo Steinbach)
Phase field modelling
Coupling with Thermo-Calc
Solidification, stress/strain, cracks

3.4.7 Phase-field modeling of strong thermodynamic non-equilibrium immediately after the contact of two bulk phases, Transient to quasi-equilibrium, formation of intermetallic phases, interdiffusion.
3.4.8 Year 1: Model formulation, collection of themodynamic- and interdiffusion data, model implementation
Year 2: Simulation 1-D, Model verification
Year 3: Simulation 2D and 3D, investigation of different models of diffusion in intermetallic phases, comarison to experiments
3.4.9 Staff required 1 PhD student for 3 years
3.4.10

Participant 4+5 (Alexander Kodentsov + Mat-tech)
Diffusion couple experiments, annealing + characterization
Reactive diffusion, Kirkendall voiding

3.4.10

It is our intention to explore a possibility of employing a Transient Liquid Phase (TLP) joining process for the fabrication of high-temperature Pb-free interconnections. In the proposed work, we seek to exploit knowledge gained from our previous activities on Pb-free soldering. In the course of study about the influence of nickel on the interaction of copper with tin it was observed that small additions (a few percents) of Ni in Cu significantly alter the course of the interfacial reactions. No ε-Cu_3Sn-phase is formed at the substrate/solder interface, and the Cu_6Sn_5-based reaction product was found to grow almost an order of magnitude faster compared to that in the Cu/Sn binary diffusion couple. Therefore, through the judicious selection of Sn-based interlayer between Cu-Ni metallization and substrate pad, the Sn-based liquid phase can be completely eliminated by the interfacial reactions already at ~240 °C, and the transient liquid-phase bonding can be achieved within a processing time of a few seconds resulting in joints capable of service at elevated temperatures. This part of the programme will address thermodynamics and kinetics of the interfacial reactions in the Cu-Ni/Sn-Ag system, phenomenological description of the Kirkendall-effect manifestations accompanying the interaction, texture development in the reaction layer and defect structure generated in the reaction zone. Based on the analysis of the results, both the design of the Cu-Ni/Sn-Ag/Cu-Ni (interlayer) system and processing conditions required for fabricating high-temperature interconnects will be defined.

3.4.11
Year 1+2

- Experimental investigation of the intermetallic formation at the Cu-Ni/Sn-Ag interfaces and evaluation of the reaction kinetics in the temperature range 200-270 °C. Various diffusion couple techniques will be employed.

Year 3+4

- Phenomenological description of the Kirkendall effect manifestations (pore formation) accompanying reactive diffusion within the interconnects.
- Development of the concept of "Local Nominal Composition of the Effective Joint Area" for optimisation of the interlayer design for TLP bonding.

3.4.11

Participant 8 (Rada Novakovic)
Effect of oxidation

Development of theoretical models describing the phenomena of oxygen transport at the interface of 1) molten metallic material / atmosphere and 2) molten metallic material / solid metal substrate. The theoretical results will be compared with experiments.

1) The first part of this work will be to describe the oxygen transport in the liquid phase and to analyse a tensio-active effect of oxygen on the surface tension and wetting characteristics of solder alloys in contact with metallic substrates.

The modelling of 2) will be to describe separately the growth of all single transformation products, by using a simple one-mechanism diffusion model. Once all reaction products are individually analysed, they will be coupled obeying the equilibrium and conservation conditions. If possible, we will try to contribute to develop a model based on the Cahn-Hilliard equations to describe the kinetic evolution of a heterogeneous system with diffuse interface.

- Theoretical and experimental study on the effects of oxygen on the surface tension of liquid metals and alloys. The oxygen transport will be consider taking account the adsorption and surface segregation phenomena.

- The study of the effects of oxygen on wetting characteristics of molten metallic material / solid metal substrate.

- The experimental work on wetting will be done in collaboration with other groups.

- By a simple one-mechanism diffusion model the growth of all single reaction products will be described. Once all reaction products are individually analysed, they will be coupled obeying the equilibrium and conservation conditions. If possible, we will try to contribute to develop a model based on the Cahn-Hilliard equations to describe the kinetic evolution of a heterogeneous system with diffuse interface.

3.4.12 Outline of work plan and time schedule (in form of a diagram if so convenient)

Year 1+2

- Development of a model for oxygen transport in liquid phase (model for pure metals and its extension to the binary alloys)
- Test of a model
- Comparison with experimetal work

Year 3+4

- Development of a model to analyse the effects of oxygen on wetting characteristics of molten metallic material / solid metal substrate.
- Test of a model
- Comparison with experimetal work

3.4.13 Staff required (graduates and technicians only)

1 PhD student

3.4.14

Participant 9 (Natalia Sobczak)

Effect of oxidation

Ultra-Short contact experiments, reactions at the interface

3.4.15 Description of the approach applied in the study

3.4.16 Outline of work plan and time schedule (in form of a diagram if so convenient)

3.4.17 Staff required (graduates and technicians only)

Participant 10 (Jean-Georges Gasser)

Calculation of diffusion coefficients for the liquid using ab initio (pseudo-potential approximation) with molecular dynamics simulations

3.4.18 Description of the approach applied in the study

3.4.19 Outline of work plan and time schedule (in form of a diagram if so convenient)
3.4.20 Staff required (graduates and technicians only)

Participant 11 (J.C. Tedenac)
Microstructure formation and interfacial diffusion studies
3.4.21 Description of the approach applied in the study
3.4.22 Outline of work plan and time schedule (in form of a diagram if so convenient)
3.4.23 Staff required (graduates and technicians only)

Participant 12 (Jaromír Drápala)

Experimental investigation of reactive diffusion in diffusion joints Cu/solder, or Ni/solder in order to obtain interaction and diffusion coefficients and to determine phase equilibria.

3.4.28 Description of the approach applied in the study

Mechanical, physical and chemical properties of joints involving high-temperature solders will be studied. It is important to characterize the associated reactive diffusion processes in binary, ternary and in particular in quaternary alloy solder joints and their subsequent effect on the long-term mechanical properties of the joint. Reactive diffusion as well as interdiffusion owing to selective and concurrent oxidation of the solder joint will be computed on both the meso- and macro-scale. The following mechanisms will be numerically addressed: interdiffusion of elements owing to compositional differences, stress generation/relaxation during interdiffusion and variable temperature excursions, structural transformations owing to interdiffusion (e.g. precipitation of new phases), displacement and degradation of selected elements.

We have moreover experience also in the field of diffusion, which could contribute to solution of mutual behaviour of solders with Ni and Cu based substrates. We have developed procedures for preparation of layers on the samples, methodology for obtaining of experimental results and physical-mathematical procedure for their evaluation.

3.4.29 Outline of work plan and time schedule (in form of a diagram if so convenient)

Application of reactive diffusion will provide important information about behaviour of diffusion joints of functionally gradient materials. At solution we will deal with cases of interaction solidus/solidus and solidus/liquidus, when conventional behaviours enter into these processes. All experimental works will be oriented in such a manner that they complete the necessary data about investigated binary and ternary systems, so that the results could be actively used at creation of a database of thermo-dynamic characteristics of selected systems. The experiments will be focused on study of reactive diffusion in the joints Cu/solder or Ni/solder in order to investigate formation of inter-metallic phases after long-term heat treatment.

2007 – 2008 Three variants of arrangement will be applied: cylindrical dissolving, planar dissolving and capillary tests. Optimum temperature modes for diffusion annealing will be proposed, which will have the best information capability. At these experiments reactive diffusion occurs between the solder melt and compact Cu (Ni) block, when it is possible to observe at the same time also considerable dissolving of copper (nickel) by solder and formation of local compact formations of some phases in the melt at proximity of the phase interface Cu(Ni)/solder. The samples processed under certain temperature modes will be then quenched for preservation of thermodynamically equilibrium state of samples for obtaining of information about behaviour of individual phases. It will be necessary to make detailed structural and chemical micro-analysis with use of methods WDX and SEM for obtaining of necessary information.

2009 – 2010 Determination of diffusion characteristics under the condition of movable inter-phase interface by using our own computing program (MatLab) for the binary systems,. For the ternary systems, where the situation is much more complicated, in the first stage the relevant diffusion and interaction coefficients will be estimated in a qualified manner and we will attempt to develop our own theory of reactive diffusion at presence of dissolving of the substrate by a solder, i.e. under conditions of convection in the melt (theory and its verification is required by an external collaborator).

3.4.30 Staff required (graduates and technicians only)

3.4.24 See point 1.2.1.7

Participant 13 (Joël Curgnoni)

Link between microscopic & macroscopic mechanical behaviour: Identification & homogenization of visco-plastic constitutive models by direct & inverse finite element methods

3.4.25 Description of the approach applied in the study:

Our contribution will focus on establishing a link between the microstructural properties of the alloy and its macroscopic mechanical properties. More specifically, our work will concentrate on the modelling of the visco-plastic properties of the solder at different temperatures with respect to its microstructural morphology and its characteristic size. Direct and inverse homogenization methods based on 3D finite element models will be developped to represent the interactions of the visco-plastic deformations at the microstructural level with the characteristic size of a macroscopic joint. Appropriate visco-plastic constitutive models will also be developped and characterized based on macroscopic mechanical tests of alloys with different microscrutures and compositions. Finally, the effect of imperfect interfaces (IMC layer and/or grain boundaries) will be studied numerically and compared with experiments.

3.4.26 Outline of work plan

Year 1+2:

- Development of a tool to generate FE models of the microstructure
- Development & validation of an homogenization procedure to predict the macroscopic visco-plastic behaviour of the solder

Year 3+4:

- Characterization of the visco-plastic properties of selected solder alloys at the macroscopic level
- Identification of constitutive properties at the micro-structural level
- Investigations on the effects of imperfect interfaces

3.4.27 Staff required (graduates and technicians only)

3.4.28

Participant 15 (Mauro Palumbo)

Nucleation, Calphad, Finite elements

3.4.29 Description of the approach applied in the study

Our company will contribute to the project mainly in the implementation of models based on the classical nucleation and growth theory in order to study the formation of intermetallic precipitates in the solder. An interface with current thermodynamic and kinetic databases will be developed in order to obtain input parameters for nucleation models. Finite elements simulations will also be performed to study mass and heat diffuson and thermofluidodynamics phenomena in the solder. A model for phase selection during the solidification process could also be implemented.

3.4.30 Outline of work plan and time schedule (in form of a diagram if so convenient)

Year 1+2:

- Definition of modelling approach and input parameters necessary to simulations
- Collection of input parameters (interfacial energy, thermodynamic driving force, diffusion coefficients,...)
- Implementation of the nucleation and growth model and interfacing with thermodynamic and kinetic databases

Year 3+4:

- Comparison of simulation results with experimental findings
- Corrections and extension of the model
- Implementation of the solidification model (phase selection)

3.4.31 Staff required (graduates and technicians only)

Participant 16 (Jozef Janovec and Milan Ožvold)
Processing of solders, characterisation of solders and solder/substrate interfaces, thermodynamic calculations

1. Processing of solders based on Sn-Zn, Sn-Ag-Cu, and Sn-Co-Cu systems and their chemical analysis (resistive and induction heating, WDX, EDX). Investigation of thermal properties of the solders (TA, DSC).
2. Development of solders containing rare earth elements. Studies to wetting, spreading, and surface tension of the solders (in vacuum or various controlled atmospheres).
3. Investigation of the intermetallic phase formation at the solder/substrate interfaces during soldering and subsequent aging. Characterization of the interfaces with light microscopy, scanning and transmission electron microscopy, x-ray diffraction and measurement of microhardness.
4. Calculation of phase equilibria and specifying phase diagrams by Thermocalc software.

All activities are planed for 4 years

Participant 17 (Jolanta Janczak-Rusch)
Experimental: processing of solders and solder joints, microstructural characterisations, diffussion multiples

3.4.32 Description of the approach applied in the study

Our contribution will focus on the development of a low temperature, short duration bonding method for the fabrication of high-temperature (260-320°C), high-performance joints. Two main approaches are be studied during the course of the project

– the use of Transient liquid phase (TLP) bonding with sacrificially passivated melting point depressant layers,

– the development of nanostructured lead free solders enabling a decrease in processing temperature and time.

The numerical approaches developed in the frame of the group project (e.g. microstructural models) should help to reach the goal, while the experimental results worked out by the Participant will allow verifying the models developed by Group Partners.

3.4.33 Outline of work plan and time schedule (in form of a diagram if so convenient)

<u>Year 1+2:</u>

- <u>Development and Optimisation of Transient Liquid Phase (TLP) bonding technique</u>
- <u>Development and characterisation of nanostructured solders</u>

The focus of development and initial optimisation of Transient Liquid Phase (TLP) bonding technique will aim at decreasing process temperature. To obtain this, encapsulated nanoparticles will be used in the bond formation experiments and simulations. This work will involve close co-cooperation with Dr. Kodentsov (Department of Chemical Engineering and Chemistry, Eindhoven University of

Technology, The Netherlands) and consideration of suggestions/input from the industrial partners.
The microstructure of nanoparticles and nanostructured solders will be characterised by means of qualitative and quantitative image analysis coupled with detailed phase and chemistry characterisation using Scanning Electron Microscopy (SEM) with Energy-dispersive X-ray spectroscopy (EDS) as well as electron microprobe analysis (EPMA). For detailed analysis of chosen specimen the Transmission Electron Microscopy (TEM) will be used.

<u>Year 2+3:</u>
<u>- Manufacturing of the solder joints</u>
<u>- Microstructural and mechanical characterisation of joints</u>
<u>- Theory-Model Comparison, Analysis of the microstructure-property relationship</u>

<u>Year 3+4</u>
<u>- Verification of models</u>
<u>- Analysis of the microstructure-property relationship</u>

The joints will be produced via optimised Transient Liquid Phase (TLP) bonding technique on substrate material (predominantly Cu) under controlled conditions. The intension is to create the processing condition for the industrial practise and simplify future scaling up manufacture. The repeatability of soldering conditions will be established and checked by means of temperature recording devices and metallographic controls.

The microstructure of the joints will be investigated using optical microscopy, Scanning Electron Microscopy (SEM) with Energy-dispersive X-ray spectroscopy (EDS), Transmission Electron Microscopy (TEM), electron microprobe analysis (EPMA). The solder-substrate interface will be studied in details. The interdiffusion processes will be analysed by Auger Spectroscopy.
The mechanical properties will be evaluated in tensile, shear and creep tests. This work will be carried out in close cooperation with LMAF-EPFL (Prof. Botsis), which will investigate the joint performance. The expertise of this group on the thermo-mechanical behaviour of the joints is crucial for the establishment study of the correlation between microstructure refinement and diffusion bond formation.

The effect of processing parameters on the thermo-mechanical behaviour and reliability of the joints will be determined in order to develop practical recommendations for high-temperature, high reliability solders by means of microstructure modification combined with Transient Liquid Phase (TLP) bonding. This work will be carried out in close cooperation with LMAF-EPFL (Prof. Botsis). The results of the microstructural characterisation will be used for verification of models developed at LMAF-EPFL.

In cooperation with other COST MP0602 partners, phenomena on the nanostructured solder/substrate interface during low temperature processing and relationship between interface structure and bond formation and strength will be studied. Optimal parameters will be verified and confirmed on the real joints. Whenever possible, the results will be compared with data obtained for the standard procedure.

3.5 Experience and Resources of the Institutions (approx. 1 page)

3.5.1 Participant 1 (Nele Moelans)

Previous and current research:
Critical assessment and CALPHAD-optimization (Bi-In-Sn-Zn, Ga-In-Si), phase field simulations for grain growth and coarsening

Publications in the last two years.
N. Moelans, B. Blanpain, P. Wollants, A phase field model for the simulation of grain growth in materials containing finely dispersed incoherent second-phase particles, Acta Mater. 53(6), 1771-1781, 2005.
N. Moelans, B. Blanpain, P. Wollants, Phase field simulations of grain growth in systems containing second-phase particles, TMS Letters, 2(2), 59-60, 2005.
N. Moelans, B. Blanpain, P. Wollants, Phase field simulations of grain growth in two-dimensional systems containing finely dispersed second-phase particles. Acta Mater., 54(4), 1175-1184, 2006.
N. Moelans, B. Blanpain, P. Wollants, A phase field model for grain growth and thermal grooving, Solid State Phenomena, 129, 89-94, 2007.
N. Moelans, B. Blanpain, P. Wollants, Pinning effect of second-phase particles on grain growth in thin films studied by 3D phase field simulations, Acta Mater., 55, 2173-2182, 2007.
L. Vanherpe, N. Moelans, B. Blanpain, S. Vandewalle, Bounding box algorithm for three-dimensional phase field simulations of microstructural evolution in polycrystalline materials, Phys. Rev. E, Submitted.
N. Moelans, B. Blanpain, P. Wollants, An introduction to phase-field modeling of microstructurev evolution. CALPHAD, Submitted.

Staff and equipment available at the laboratory:
.High performance computer, classical microscopic techniques (SEM,EPMA, microprobe,...) and furnaces for sample preparation

3.5.2 Participant 2 (Suzana Gomes Fries)

Brief summary of previous or current work in similar or related fields. Publications in the last two years. Staff and equipment available at the laboratory for the efficient execution of the proposed research work.

3.5.3 Participant 3 (Ingo Steinbach)

Previous and current research:
Phase-field modelling of structure formation during solidification and solid state transformation coupled to CALPHAD thermodynamics

Publications in the last two years.

I. Steinbach, M. Apel: "The Influence of Lattice Strain on Pearlite Formation in Fe-C "; Acta Materialia 55 (2007), pp. 4817-4822
J. Eiken, B. Böttger, I.Steinbach: "Simulation of Microstructure Evolution During Solidification of Magnesium-Based Alloys"; Trans. Indian Inst. Met 60 (2007) pp.178-184
I. Steinbach, B. Böttger, J. Eiken, N. Warnken, S. G. Fries: "CalPhaD and PhaseField Modeling: A Successful Liaison"; Journal of Phase Equilibria and Diffusion 28 (2007), pp. 101-106
I. Steinbach, M. Apel: "Phase-field simulation of rapid crystallization of silicon on substrate"; Materials Science and Engineering A (2007) pp. 95-98
J. Eiken, B. Böttger, I. Steinbach: "The role of solute in grain refinement of magnesium-based castings investigated by phase-field simulations". Proceedings of the 5th decennial international conference on solidification processing, edit. H. Jones, Sheffield 2007, pp. 148-152
N. Warnken, D. Ma, A. Drevermann, S.G. Fries, I.Steinbach: "Phase-field simulations of microstructural evolution in Ni-base superalloys". Proceedings of the 5th decennial international conference on solidification processing, edit. H. Jones, Sheffield 2007, pp. 109-112
I. Steinbach, M. Apel: "Multi phase field model for solid state transformation with elastic strain"; Physica D 217 (2006) 2, pp. 153-160
J. Eiken, B. Böttger, I. Steinbach: "Multiphase-field approach for multicomponent alloys with extrapolation scheme for numerical application"; Physical Review E 73 (2006), 066122
B. Böttger, J. Eiken, I. Steinbach: "Phase field simulation of equiaxed solidification in technical alloys"; Acta Materialia 54 (2006), pp. 2697-2704
B. Böttger, J. Eiken, M. Ohno, G. Klaus, M. Fehlbier, R. Schmid-Fetzer, I. Steinbach, A. Bührig-Polaczek: "Controlling microstructure in magnesium alloys: a combined thermodynamic, experimental and simulation approach"; Advanced Engineering Materials 8 (2006) 4, pp. 241-247
K. Nakajima, M. Apel, I. Steinbach: "The role of carbon diffusion in ferrite on the kinetics of cooperative growth of pearlite: a multi-phase field study"; Acta Materialia 54 (2006) 3665-3672
J. Eiken, B. Böttger, I. Steinbach: "Phase field simulations of microstructure evolution during solidification of magnesium-based alloys". Modeling of Casting, Welding and Advanced Solidification Processes XI. Ed. by C.-A. Gandin (et. al.), TMS: Warrendale, 2006, pp. 489-496.
M. Apel, H.J.-Diepers, I. Steinbach: "On the effect of interdendritic flow on primary dendrite spacing: A phase-field study and analytical scaling relations". Modeling of Casting, Welding and Advanced Solidification Processes XI. Ed. by C.-A. Gandin (et. al.), TMS: Warrendale, 2006, pp. 505-512

3.5.4 Participant 4 + 5(Alexander Kodentsov + Mat-tech)

Brief summary of previous or current work in similar or related fields. Publications in the last two years. Staff and equipment available at the laboratory for the efficient execution of the proposed research work.

3.5.5 Participant 8 (Rada Novakovic)

Brief summary of previous or current work in similar or related fields. Publications in the last two years. Staff and equipment available at the laboratory for the efficient execution of the proposed research work.

Modelling of thermophysical properties of molten metallic materials, Surface and wetting properties of molten metals and alloys

1. I. Egry, R. Brooks, D. Holland-Moritz, R. Novakovic, T. Matsushita, E. Ricci, S. Seetharaman, R. Wunderlich, D. Jarvis, Thermophysical Properties of γ - Titanium Aluminide: The European IMPRESS Project, Int. J. Thermophys. **28** (2007) 1026-1036.
2. A. Passerone,, M.L. Muolo, R.Novakovic, D. Passerone, Liquid metal/ceramic interactions in the (Cu, Ag, Au)/ZrB_2 systems, Journal of the European Ceramic Society 27 (2007) 3277–3285.
3. F.Gnecco, E.Ricci, S.Amore, D.Giuranno, G.Borzone, G.Zanicchi, R.Novakovic, Wetting behaviour and reactivity of lead free Au-In-Sn and Bi-In-Sn alloys on Copper substrates, J. of Adhesion & Adhesives 27 (2007) 409-416.
4. R. Novakovic, E. Ricci, F. Gnecco, Surface and transport properties of Au-In liquid alloys, Surface Science, 600 (2006) 5051-5061.
5. R. Novakovic, M.L. Muolo, E.Ricci, E.Ferrera, D.Giuranno, F.Gnecco, A.Passerone, The Surface Properties of Ag-Cu-Zr liquid alloys in relation to the Wettability of Boride Ceramics, Materials Science Forum, Trans Tech Publ., vol. 512 (2006) 211-216.
6. R. Novakovic, E. Ricci, S. Amore, T. Lanata, Surface and transport properties of Cu-Sn-Ti liquid alloys, Rare Metals 25 [5] (2006) 1-12.
7. R. Novakovic, T. Tanaka, Bulk and surface properties of Al-Co and Co-Ni liquid alloys, Physica B 371 (2006) 223-231.
8. R. Aune, L. Battezzati, I. Egry, J. Etay, H.J. Fecht, D. Giuranno, R. Novakovic, A. Passerone, E. Ricci, F. Schmidt-Hohagen, S. Seetharaman, R. Wunderlich, Surface tension measurements of Al-Ni based alloys from ground-based and parabolic flight experiments: results from the ThermoLab project, Microgravity. Sci. Technol. XVIII-3/4 pp. 73-76. Z-Tec Publishing, Bremen, 2006.
9. R. Novakovic, E. Ricci, F. Gnecco, D. Giuranno, G. Borzone, Surface and transport properties of Au-Sn liquid alloys, Surface Science, 599 (2005) 230-247.
10. R. Novakovic, T. Tanaka, M.L. Muolo, J. Lee, A. Passerone, Bulk and surface properties of liquid Ag- X (X = Ti, Hf) compound forming alloys, Surface Science, 591 (2005) 56-69.
11. R. Novakovic, D. Zivkovic, Thermodynamics and surface properties of liquid Ga-X (X = Sn, Zn) alloys, J. of Materials Science, 40 (2005) 2251-2257.
12. R. Novakovic, E. Ricci, D. Giuranno, A. Passerone, Surface and transport properties of Ag-Cu liquid alloys, Surface Science, 576 [1-3] (2005) 175-187.

Theoretical part supported by MATLAB software

Experimental method

The surface tension and contact angle measurements will be performed by the sessile drop technique.

Equipment

The research activity in the CNR-IENI, Genoa are supported by the following facilities: 4 High vacuum furnaces (1 with Pt resistor for use also under oxidising atmospheres; 3 for controlled atmospheres) for the surface tension and the contact angle measurements, A.S.T.R.A. – real time acquisition software, SEM, EDS, ICP, XRD.

3.5.6 Participant 9 (Natalia Sobczak)

Brief summary of previous or current work in similar or related fields. Publications in the last two years. Staff and equipment available at the laboratory for the efficient execution of the proposed research work.

3.5.7 Participant 10 (Jean-Georges Gasser)

Brief summary of previous or current work in similar or related fields. Publications in the last two years. Staff and equipment available at the laboratory for the efficient execution of the proposed research work.

3.5.8 Participant 11 (J.C. Tedenac)

Brief summary of previous or current work in similar or related fields. Publications in the last two years. Staff and equipment available at the laboratory for the efficient execution of the proposed research work.

3.5.10 Participant 12 (Jaromír Drápala)

Brief summary of previous or current work in similar or related fields. Publications in the last two years. Staff and equipment available at the laboratory for the efficient execution of the proposed research work.

LOSERTOVÁ, M., BARABASZOVÁ, K., DRÁPALA, J. and KURSA, M. Study of Kirkendall Effect in Ni/Ni_3Al Welded Joint after the High Temperature Annealing. In „*Diffusion and Thermodynamics of Materials*“. *Defect and Diffusion Forum,* Trans Tech Publication, Switzerland. Vol. 263, 2007, pp. 213-218. ISSN 1012-0386, ISBN 3-908451-35-3.

DRÁPALA, J., KUBÍČEK, P., VŘEŠŤÁL, J.and LOSERTOVÁ, M. Study of Reaction Diffusivity in the Copper – Indium – Tin Ternary System. In „*Diffusion and Thermodynamics of Materials*“. *Defect and Diffusion Forum,* Trans Tech Publication, Switzerland. Vol. 263, 2007, pp. 231-236. ISSN 1012-0386, ISBN 3-908451-35-3.

DRÁPALA, J. and KUBÍČEK, P. Study of concentration-dependent diffusivity in the Ni-Al and Ni-Si binary systems with moving interface from experimental data. *Горный информационно-аналитический бюллетень. Отдельный выпуск No 2 „Функциональные металлические материалы“.* 2007, s. 177-190. ISBN 0236-1493, in English.

DRÁPALA, J. and KUBÍČEK, P. Diffusion with the noviny interface boundary – Analytical solving of the Stefan problem by means of the thermal potential of a double layer. In Abstracts of the *International Conference and Exhibition „Materials Science & Technology 2006 MS&T'06*”, Ohio, Cincinnati. 15.-19.10.2006, p. 157. Full text on CD ROM in Section „*Phase Stability, Diffusion, and their Application, Fundamentals and Characterization*”, Vol. 2, 2006, pp. 163-174.

DRÁPALA, J., KUBÍČEK, P. and VŘEŠŤÁL, J. Study of the reactive diffusion in the copper – indium – tin ternary system. In *Metal 2007*. 22.-24.5.2007, Hradec nad Moravicí, Ed. Tanger, spol. s r.o. Ostrava, Proceedings of the 16th International Metallurgical & Materials Conference, paper no. 42 p. 94 (Abstract) and CD ROM (10 pp.). ISBN 978-80-86840-33-8, in Czech.

DRÁPALA, J., KOZELKOVÁ, R., KUBÍČEK, P., VŘEŠŤÁL, J.and KROUPA, A. Interaction of elements in the copper / indium – tin diffusion joints at 400 and 600 °C. In „*The 12th International Conference on Problems of Material Engineering, Mechanics and Design*“, Jasná – Nízké Tatry, Slovakia, 29.-31.8.2007, book of abstracts, p. 45, full text 6 p. on CD ROM. ISBN 978-80-969728-0-7, EAN 9788096972807.

Equipment available at the laboratory for the efficient execution of the proposed research work - see point 1.2.1.7.

3.5.9 Participant 13 (John Botsis & Joël Cugnoni)

Previous & current research in this field:

identification of constitutive models of lead-free solder, study of size and constraining effects in solder joints, numerical homogenization methods used in the development of particle reinforced active-brazing fillers.

Selected Publications in the last two years:

Sorensen, L., et al., *Delamination detection and characterisation of bridging tractions using long FBG optical sensors.* Composites Part a-Applied Science and Manufacturing, 2007. **38**(10): p. 2087-2096.

Matter, M., et al., *Improved modal characterization of the constitutive parameters in multilayered plates.* Composites Science and Technology, 2007. **67**(6): p. 1121-1131.

Cugnoni, J., T. Gmur, and A. Schorderet, *Inverse method based on modal analysis for characterizing the constitutive properties of thick composite plates.* Computers & Structures, 2007. **85**(17-18): p. 1310-1320.

Cugnoni, J., et al., *Experimental and numerical studies on size and constraining effects in lead-free solder joints.* Fatigue & Fracture of Engineering Materials & Structures, 2007. **30**(5): p. 387-399.

Cugnoni, J., J. Botsis, and J. Janczak-Rusch, *Size and constraining effects in lead-free solder joints.* Advanced Engineering Materials, 2006. **8**(3): p. 184-191.

Galli, M., J. Botsis, and J. Janczak-Rusch, *Relief of the residual stresses in ceramic-metal joints by a layered braze structure.* Advanced Engineering Materials, 2006. **8**(3): p. 197-201.

Equipment:

static, high speed, vibration and fatigue testing facilities, optical strain measurements (ESPI, DIC, Laser vibrometer), high performance computing & FEA simulation codes

3.5.10 Participant 15 (Mauro Palumbo)

Brief summary of previous or current work in similar or related fields.

CALPHAD assessment of binary and ternary systems (Fe-B, Ce-Ni, Co-Cu, Co-Cu-Fe, Cu-Mg, Cu-Mg-Y, Al-H-Mg), simulation of diffusion, nucleation and growth processes (DICTRA)

Publications in the last two years.

- M. Palumbo, M. Baricco, *Modelling of bcc-Fe crystal primary growth in a $Fe_{85}B_{15}$ amorphous alloy*, Acta Materialia 53 (2005) pp. 2231-2239
- M. Palumbo, C. Papandrea, L. Battezzati, *Nucleation of crystals in deeply undercooled metals*, Journal of Materials Science 40 (2005) pp. 2431-2435
- M. Palumbo, S. Curiotto, L. Battezzati, *Thermodynamic analysis of the stable and metastable Co-Cu and Co-Cu-Fe phase diagrams*, CALPHAD 30 (2006) pp. 171-178
- M. Palumbo, M. Satta, G. Cacciamani, M. Baricco, *Thermodynamic Analysis of the Undercooled Liquid and Glass Transition in the Cu-Mg-Y System*, Materials Transations, Vol. 47, No. 12 (2006) pp. 2950 to 2955
- M. Baricco, M. Palumbo, *Phase diagrams and glass formation in metallic systems*, Advanced Engineering Materials 9, No. 6 (2007) pp. 454-467
- M. Satta, M. Palumbo, P. Rizzi, M. Baricco, *Ternary compounds and Glass Formation in the Cu-Mg-Y system,* Advanced Engineering Materials 9, No. 6 (2007) pp. 475-479
- M. Palumbo, F. J. Torres, J. R. Ares, C. Pisani, J. F. Fernandez, M. Baricco, *Thermodynamic and ab initio investigation of the Al-H-Mg system*, CALPHAD 31 (2007) pp. 457-467

Staff and equipment available at the laboratory for the efficient execution of the proposed research work.
High performance computers, software for thermodynamic and kinetic calculations, software for finite elements simulations

3.5.16 Participant 16 (Jozef Janovec and Milan Ožvold)

Jozef Janovec
Previous and current research:
Diffusion related phenomena at internal surfaces, prediction of phase equilibria
Milan Ožvold
Processing and characterisation of solders and solder/substrate interfaces

Publications in the last two years (2006-2007)
Ž. Bihar – A. Bilšić – J. Lukatela – A. Smontara – P. Jeglič – P. J. McGuiness – J. Dolinšek – Z. Jagličić – J. Janovec – V. Demange – J. M. Dubois: Magnetic, electrical and thermal transport properties of Al-Cr-Fe approximant phases, Journal of Alloys and Compounds, **407**, 2006, 65-73.

J. Janovec – B. Šuštaršič – M. Godec - M. Jenko – J. Medved: Characterisation of the phases in as-cast CF3M steel, Praktische Metallographie, **43**, 2006, 30-44.

J. Janovec – J. Pokluda – M. Jenko – P. Lejček – B. Vlach – J. Horníková: Influence of phosphorus enrichment at grain boundaries on energy of intergranular fracture in Fe-Si-P alloys, Surface and Interface Analysis, **38**, 2006, 401-405.

J. Janovec – P. Lejček – J. Pokluda – M. Jenko: Effects of grain size and grain boundary segregation on fracture behaviour of a polycrystalline Fe-2.65Si-0.028P alloy, Kovové Materiály, **44**, 2006, 81-87.

J. Janovec – M. Svoboda – A. Kroupa – A. Výrostková: Thermal-induced evolution of secondary phases in Cr-Mo-V low alloy stels, Journal of Materials Science, **41**, 2006, 3425-3433.

J. Janovec – M. Svoboda – J. Dolinšek – M. Godec – J. Buršík – J. Dusza: Microstructure characterisation of Al65Cr28Fe7 quasicrystalline approximant, Kovové Materiály, **44**, 2006, 313-320.

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J. Janovec – J. Pokluda – P. Lejček: Influence of phosphorus grain boundary segregation on fracture behaviour of iron-base alloys, Materials Science Forum, **567-568**, 2007, 33-38.

P. Lejček – R. Konečná – J. Janovec: Solute segregation to ferrite grain boundaries in nodular cast iron: experiment and prediction, Surface and Interface Analysis, **40**, 2008, 503-506.

The research team members at the Laboratory for Interface and Joining Technology (Section 124) of Swiss Federal Laboratories for Material Testing and Research (EMPA) in Dübendorf, ZH, have both theoretical and experimental background from materials science and engineering, mechanical engineering, physics and chemistry, to pertain the proposed scope of the study. The Research of the Group Advance is focused on soldering and brazing, application of composite concepts into soldering technology and the relation between processing, properties and microstructure, especially at the interfaces.

Available apparatus

- Vacuum furnace: Torvac 30 with automatic control system for brazing and heat treatment. Capacities: Temperatures up to 1400°C; Vacuum at 1000°C = min. $5x10^{-6}$ mbar; Chamber size: 200x210x450 mm.
- Two inert gas furnaces (Nabatherm, Solo)
- Several atmospheric furnaces.
- Soldering Apparatus
- Rapid Thermal Annealing (RTA) Furnace
- Software: Image Analysis System, ThermoCalc, DICTRA.

1. M. Galli, J. Cugnoni, J. Botsis, J. Janczak-Rusch, Identification of the matrix elastoplastic properties in reinforced active brazing alloys, *Composites Part A: Applied Science and Manufacturing*, *Volume 39, Issue 6*, *June 2008*, *Pages 972-978*
2. N.S. Bosco, B.A. Manhat and J. Janczak-Rusch, Sacrificial passivation of nanoscale silver particles, Scripta Materialia, Volume 58, Issue 10, May 2008, Pages 858-86
3. V.Sivasubramanian, N.Bosco, J.Janczak-Rusch, J. Botsis, Interfacial Intermetallic Growth and Strength of Composite Lead-free Solder Alloy through Isothermal Aging", accepted for Journal of Electronic Materials
4. M. Galli, J.Botsis, J.Janczak-Rusch, *An elastoplastic three-dimensional homogenization model for particle reinforced composites*, Computational Materials 4 1(2008) 312-321
5. J.Janczak-Rusch, *Design, brazing and characterization of metal-ceramic joints*, Inżynieria Materiałowa 157-158(2007)547-551.
6. V. Bissig, J. Janczak-Rusch, M. Galli, *Selection and Design of Brazing Fillers for Metal-Ceramic Joints*, Materials Science Forum, 539-543(2007)4008-4012.
7. G. Blugan, J. Kübler, V. Bissig, J. Janczak-Rusch, *Brazing of silicon nitride ceramic composite to steel using SiC-particle-reinforced active brazing alloy*, Ceramics International 33(2007)1033-1039.

3.6 Co-operation **(minimum of 3 partners in at least 2 countries,** approx. 1 page**)**

The proposal shall include a clear description of the co-operation agreed with partners from other countries. The minimum information expected includes:

- division of work among partners **(see 3.4)**
- which information they will exchange **(see 3.4)**

- confirmation of the partnership