Recommendations for Future Basic Research on Metallic Alloys and Composites in the 6th EU Framework Program

Metals and composites: basis for growth, safety, and ecology

Authors

Dierk Raabe, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Yves Bréchet, LTPCM, BP75, Domaine Universitaire de Grenoble, Saint Martin d'Heres, France

Günther Gottstein, Institut für Metallkunde und Metallphysik, RWTH Aachen, Aachen, Germany

Jeff De Hosson, Deptartment Applied Physics, University of Groningen, Groningen, The Netherlands

Paul Van Houtte, Department MTM, Katholieke Universiteit Leuven, Leuven, Belgien

Vasek Vitek, Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, USA

Max-Planck-Institut für Eisenforschung
Max-Planck-Str. 1
40237 Düsseldorf
Germany

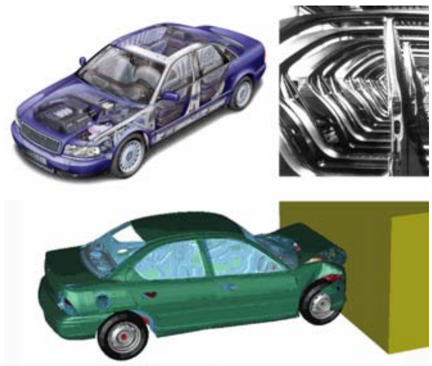
www.mpie.de

The place of metals in the world of materials

Metallic alloys and composites represent the dominant group of structural and functional materials worldwide and within the EU. This applies for their technological impact on society as well as for the scientific challenges associated with further discoveries and developments in this field. Fundamental and long-term oriented research on metals and composites leads to the development of well-tailored technological solutions which serve society with respect to sustainable progress, ecological benefits, advanced safety demands, and economic success. Prominent challenges along these lines lie in understanding and developing the fundamentals of lightweight structural materials and design solutions, self-organising microstructures, failure-tolerant materials systems, smart materials, and materials for ground and aerospace transportation.

This report gives an overview of the most important future research topics in the field of metals and composites research as collected and discussed within a group of about 100 leading experts from the EU, Asia, and the US. It gives corresponding recommendations for future basic research initiatives on metallic alloys and composites in the 6th EU Framework Program.

Space vehicles which are at the cutting edge of high technology are built of structural elements of steels, aluminium, magnesium and beryllium alloys and metal-matrix composites.



Modern automotive technology relies on safety equipment made of advanced steels, aluminium, and magnesium alloys.

State of the art and expected trends

The state of the art in the field of metals and composites research is characterized by a mature level of property optimisation and characterisation particularly as far as bulk mechanical aspects of conventional structural metallic materials are concerned.

Basic principles behind bulk materials kinetics and thermodynamics in such alloys are understood to an extent that they can be used for the further gradual optimisation of existing alloy concepts with respect to structural and/or functional properties. Recent European programs have focussed on improving and tailoring existing material concepts for matching technological and commercial boundary conditions and on designing new materials concepts beyond conventional R&D lines.

This research concept of the past decade has for many aspects matured to a level where future activities, when designed and pursued along the same lines as before, will lead to a more and more asymptotic research progress. Future long term research programs must therefore formulate concepts to achieve distinct progress steps leading EU projects beyond existing research plateaus.

This approach would maintain and strengthen the position of metals and composite research as a key science and technology providing progress-critical input to other key areas of science and high technology. It should thus be the aim of future research in this field that coming technology applications are being pushed forward by materials rather then vice versa.

Some key rules can be formulated to unleash unused potential of metallic and composite materials through a new European framework research initiative with the aim of entailing fundamental progress steps pushing this discipline beyond existing R&D asymptotes.

- **First, EU projects should make extensive use of <u>novel experimental and theoretical tools</u> as well as advanced combinations of them. Although further improvement and application of well developed "workhorse" methods is essential to provide serious and systematic data for novel materials concepts, it is less likely that they play a bottleneck role in future metals research such as the use of novel methods which will allow new observations, which have not been made so far (some of the new research tools will be specified below).**

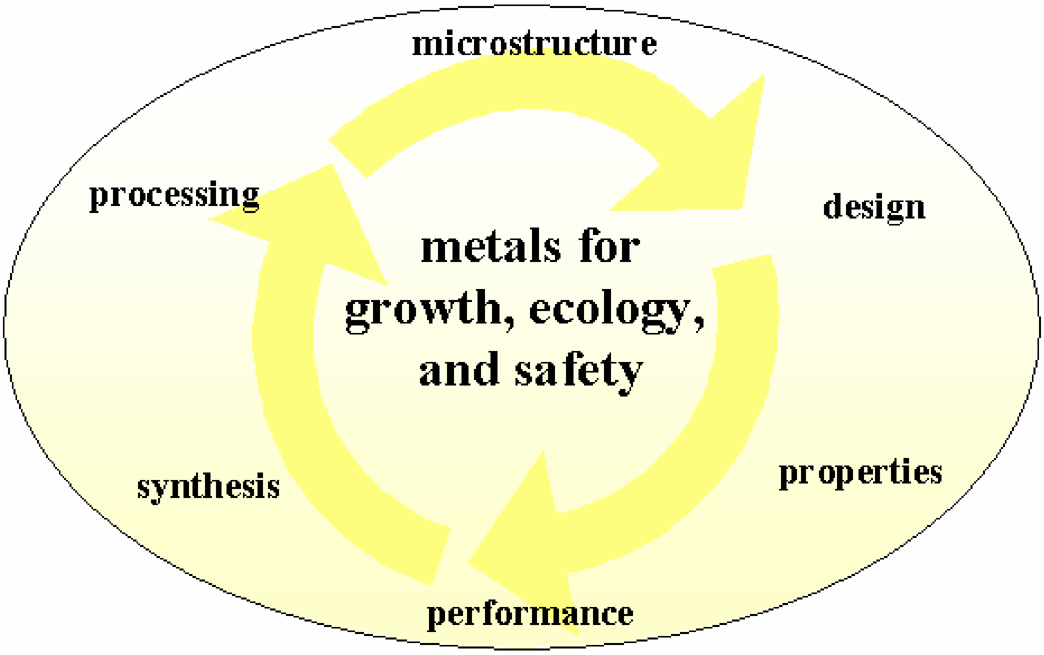
- **Second, EU projects should address fundamental long-term problems of existing and cutting-edge structural and functional metallic materials concepts which are the basis of our economy but are not covered by applied or industry research. In this context it is important to note that industry pushes materials developments only to a level of immediate commercial output and leaves behind numerous unanswered questions which often affect ecological, economic, performance, and safety aspects. Such concepts deserve in part more attention from the fundamental side in order to avoid long-term misconceptions and exploit and development better the potential of existing materials.**

- **Third, EU projects should create materials concepts far beyond conventional approaches, focussing particularly on so far less exploited combinations of different material classes, property-structure integrations, and property profiles. In this context it is important that new materials development should from the beginning be accompanied by fundamental research since material development is nowadays an integrated and interdisciplinary task.**

- **Fourth, future research initiatives should give very high priority to projects with highly interdisciplinary character closely integrating concepts and approaches from areas such as materials physics, materials engineering, information technology, materials chemistry, mathematics, and/or biology.**

Outline and principles of future research strategy

The basic research strategy required in this field can be classified into two major disciplines. The first one comprises **experiments on model systems**. The second one comprises **modelling and computer simulation**. As far as metals and composites are concerned the latter branch particularly concentrates on macro- and mesoscale simulation issues.



Essential elements of advanced metals and composites research.

Experiments on model systems should map essential ingredients of composition, synthesis, processing, and microstructure design which are not well understood but have key functions in novel material design as well as advanced conventional materials concepts. The following key points might characterise projects in this field:

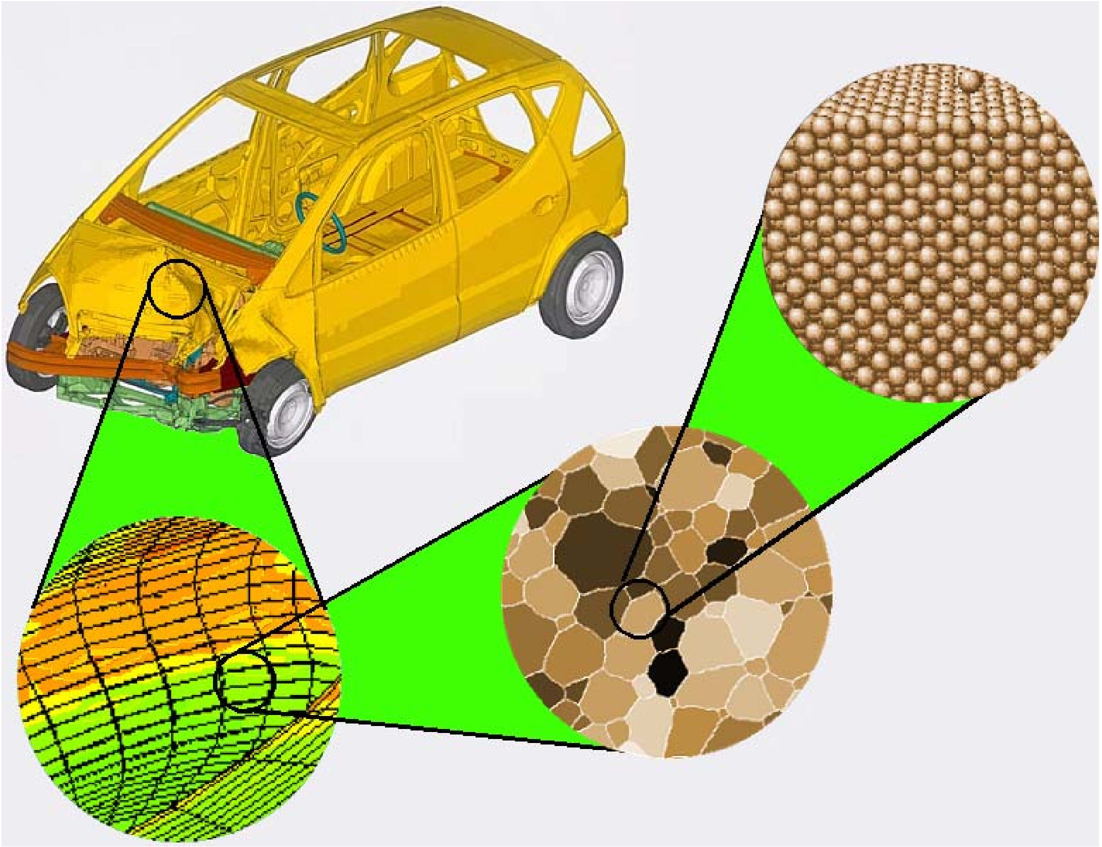
- First, projects should make use of novel experimental tools and/or advanced combinations of experimental tools exploiting observation methods that have not yet matured to their full potential. Examples[1] are nano-mechanical property characterization in conjunction with nanoscopic analytical and orientation characterisation; 3D atom probe methods; high resolution analytical microscopy in conjunction with automated high resolution orientation imaging microscopy; 3D synchrotron x-ray microscopy; field ion beam microscopy in conjunction with high resolution orientation imaging microscopy in FEG scanning electron microscopy; advanced neutron scattering methods; in-situ experimentation combining sample observation with heating or mechanical loading. Consideration must also be placed on fast and appropriate analysis tools which are capable of extracting and visualizing relevant information from the ever increasing experimental data sets.
- Second, projects should address fundamental long-term problems of existing structural and functional metallic materials concepts by use of model experiments which are the basis of our economy but are not covered by applied or industry research. Examples are integrated model design solutions exploiting materials as well as constructional aspects; metal-metal interfaces and grain boundary triple-points in the form of well-defined model bi- and tricrystals; metal-metal joins; advanced structural-functional as well as smart compounds.
- Third, projects should create experimental model systems heading beyond conventional approaches, focussing particularly on so far less investigated combinations of different material classes, microstructures and property profiles. Examples are entangled, cellular and porous metallic microstructures; nanoscale metal-polymer compounds; ultra thin layered metal-ceramic-polymer structures; nanostructured functional-structural composites; woven metallic systems; nanoscale integration of metals, polymers, and ceramics; self organising metal-polymer interfaces; composite foams; and metal-semiconductor-polymer sheet compounds.
- Fourth, design of model systems should be particularly pursued in projects with highly interdisciplinary character closely integrating concepts and approaches from materials physics, materials engineering, materials chemistry, mathematics, information technology, and/or biology. Examples are the application of nanoscale materials mechanics tests to large sets of material samples or graded samples using variational alloy chemistry methods in conjunction with nano-indentation; the design and investigation of metal-polymer interfaces with high resolution

[1] A more detailed and ranked overview of possible subjects is given in the ensuing chapter.

analytical experimental tools as projects between metal physics, physical chemistry, and process engineering; determination of elastic and plastic response of ultra thin layered structures under thermal, electromagnetic, mechanical loadings, or environmental loadings as projects between metal physics, physical chemistry; process engineering; design and investigation of self organisation effects in metal-polymer and metal-ceramic interfaces as projects between ceramics, metal physics, physical chemistry, and biology; and closer cooperation between experts from theory and experimentation.

Modelling and computer simulation projects should aim at fundamental understanding as well as process- and performance prediction of novel and advanced conventional structural and functional materials. The recognition of these basic needs from the theoretical side, along with the ever increasing computing power, has established computer modelling approaches as one of the major areas in materials research.

In this approach one formulates model descriptions based on fundamental principles and investigates their properties and behaviour by numerical simulations. Modelling and computer simulation will play a key role in understanding, tailoring, and predicting materials synthesis, processing, microstructures and properties. While modelling can produce realistic results for very complex situations, underlying theories, based on results of modelling, must be built as history–dependent and multi–scale concepts, integrating electronic and atomic level as well as continuum scale information whenever relevant. These allow generalization and deep physical understanding of phenomena studied. Modelling and simulation tools have in recent years matured to a state where available software is increasingly well designed and maintained and built on robust theoretical and mathematical grounds.



Important hierarchical scales of computer simulation methods in the field of metals and composites reserach. Future developments must integrate macroscopic finite element predictions, mesoscale methods, and atomic scale simulations for the design and optimization of new advanced products.

Distinct progress steps pushing this field of computer simulation forward can only be expected when the three above mentioned key points are considered. This means that

- first, projects should make use of and better <u>integrate novel tools from theory, mathematics, and information technology</u>. Examples are better exploitation of parallel algorithms and parallel computing power; application of distributed computing based on high speed network connections; development of robust and fast parallel non-linear variational methods for tackling large quantities of coupled differential equations; critical reliability investigations of numerical methods and existing codes; standardisation and sharing of computer codes and resources; closer integration of electronic ground state and atomic scale calculations into continuum concepts; improvement of physically motivated strain gradient and crystal plasticity continuum theory; better integration of and comparison with experimental data in case of non ab-initio methods; development of fast though robust simulation algorithms for the electronic, atomic, and continuum scale; and direct coupling of electronic and atomic dynamics simulations beyond the Born-Oppenheimer approximation. Furthermore, particularly large scale simulation efforts require closer integration of materials and constructional / design issues. For instance, aspects such as the overall part stiffness results from ingredients of both areas. Such projects should introduce design-oriented database-related approaches exploiting artificial intelligence methods. Another important point of integration are joint simulations of functional - constructional devices. Also, one should draw more attention to novel information treatment methods such as the neural net and fuzzy logic approaches.

- Second, simulations should aim at structure- and property predictions of model systems pertaining to existing structural and functional metallic materials. Focus should be placed on the mesoscopic and macroscopic scale. Examples are anisotropic continuum scale CPFE-based[2] simulations of elastic-plastic co-deformation of metallic systems as well as corresponding simulations considering metal-polymer, and metal-ceramic compounds; micromechanics predictions of polycrystalline matter under mechanical loads; micromechanics predictions of woven and foam composites; joint microstructure simulations integrating casting, thermomechanical and cold forming issues; and GL-based[3] simulations of structure- and concentration-dependent topological mesoscale aspects.
- Third, simulations should aim at designing and predicting structure- and properties of novel material concepts at the electronic-, atomic-, meso-, and macroscale. Examples are LDF-type[4] electronic scale predictions of the influence of foreign atoms on metal-metal interfaces; MD-based[5] simulation of interfaces and crack tips under loads; CPFE-based continuum scale simulations of behaviour under elastic-plastic loads; GL-based simulations of metal-polymer, metal-semiconductor, and metal-ceramic compounds; mesoscale joint GL- and CPFE-based predictions of self organisation kinetics at metal-polymer interfaces; micromechanics predictions for woven and foam composites; atomic scale process design simulations for micro- and nanoscale compound tailoring using hyperdynamics concepts.
- Fourth, simulations projects should be particularly pursued in projects with highly interdisciplinary character closely integrating concepts and approaches from materials physics, materials engineering, materials

[2] CPFE = crystal plasticity finite element methods
[3] GL = Ginzburg - Landau - type phase field methods
[4] LDF = local density functional theory
[5] MD = Molecular dynamics

chemistry, mathematics, information technology, and/or biology. Examples are the integration of electronic ground state simulation into continuum models as projects between physics and materials science; integration of polymer mechanics and metal mechanics into predictions of layered structures as projects between materials mechanics and physical chemistry; development of faster simulation methods and algorithms as projects between mathematics, information technology, metal physics, and chemistry; the development of parallel and distributed methods as projects between mathematics, information technology, metal physics, and chemistry; and closer cooperation between experts from theory and experimentation.

Details of future research programme

Introduction

Based on the concept explained in chapter 2 this part gives a more detailed outline of recommendations for future research topics in the fields of metallic alloys and composites. The organisation of topics in this chapter follows in the first place the key subjects as agreed at the Ludwigsburg symposium but gives suggestions with relation to the above introduced organisation of projects into model system experimentation and computer simulation.

The key areas of future fundamental research in the field of metallic alloys and composites as agreed at the Ludwigsburg symposium are:

- Interface science and microstructure design
- Thermodynamics and kinetics
- Synthesis and processing
- Mechanical and functional properties

Interface science and microstructure design

Laws of interface motion and energy often follow strong dependencies on state variables. Metal and composite interfaces typically have bottleneck function in materials properties and design. It is likely that substantial new fundamental insights and outstanding progress in performance can be expected particularly from metallic alloys and composites with a high density of homophase and heterophase interfaces. Such concepts can be realized in the form of bulk

systems with intricate 3D interface percolation, layered systems, and bamboo-type structures.
The key focus in this area is a better understanding of nucleation events and the role of the mechanisms of interface formation as well as interface motion. Materials are getting increasingly dominated by interfaces. This includes metal / ceramic, metal / metal, metal / polymer etc. interfaces. Investigating such phenomena requires to focus on the electronic and atomic aspects as well as on macroscopic aspects.

Topics in this context with fundamental importance include

1. self-organising and self repairing surfaces and interfaces
2. generation, structure, and properties of interfaces with fractal dimension
3. nano- and microtribology
4. interface and surface systems under thermal, elasto-plastic, electromagnetic, environmental and coupled loadings
5. surface- and strain driven continuous and discontinuous subgrain coarsening
6. elastic-plastic and functional interaction across heterophase and homophase interfaces
7. nucleation phenomena
8. mechanics at interfaces
9. interfaces and surfaces turbine blade alloys under complex loadings
10. functional-structural optimisation of interfaces
11. interface phenomena in woven and foamed metals and composites including corrosion
12. role of interfaces in smart materials, particularly in nanoscale filter, electronic, and catalytic matter
13. interface mobility and effects of other lattice defects, triple junction effects
14. recrystallisation and grain growth phenomena
15. orientation and misorientation evolution at the nano- and microscale
16. grain cluster-mechanics
17. micromechanics of interfaces and surfaces
18. precipitation phenomena under complex loadings, in constrained and layered systems, and in multi-component systems
19. interface design and manipulation

Thermodynamics and kinetics

Thermodynamics and kinetics data are essential for tailoring and predicting novel materials. Particularly in interface dominated systems thermodynamics and kinetics are not well understood though they have key function in novel materials design. Topics in this context with fundamental importance include

1. thermodynamic and kinetic data of multi-component systems and interface-intensive systems
2. transformations under elasto-plastic and electromagnetic loads, effects of point and line defects on interface transformations
3. transformation in confined, low-dimensional, layered, and small scale structures
4. development, standardisation, and intercalibration in the field of experimental materials thermodynamics
5. Non isothermal and reversal problems in heat treatment
6. microstructures arising from competing kinetics

Synthesis and processing

Microstructure design will play a critical role in the synthesis of novel multi-layered and small scale structured materials. Key points to be addressed are the fundamentals of:

1. self-organisation and self-assembly of microstructures with desired properties
2. in situ processing of functional-structural materials
3. layered and graded structures
4. super strong metals composites, matter close to the limits of theoretical strength
5. ordering effects of magnetic particles and domains
6. metallic foams
7. casting defects
8. microstructures inheritance in materials processing
9. nanoscale particles: processing, self organisation, quantum dots
10. fabrication of bulk and thin film nanostructured metals
11. microstructure percolation effects
12. intermetallics and oxides: combination of high strength, ductility, and creep/fatigue resistance, internal oxidation
13. in-situ nanostructuring through deformation, metallurgical methods, deposition, and diffusion
14. solid state decomposition
15. field assisted annealing
16. high temperature alloys and compounds: turbine materials, aerospace composites, alloys for hot and aggressive environment
17. joining processes

Mechanical and functional properties

A strong overlap should be created between interface and plasticity projects. In the field of plasticity the following areas of fundamental interest were identified.

1. collective behaviour of structural defects
2. scale-bridging plasticity and failure concepts in materials simulation and experiment
3. elasticity and plasticity in confined, layered, graded, and nanoscaled materials
4. effects of solute elements on work hardening
5. anisotropic elasto-plasticity of polycrystalline matter
6. internal stresses in conjunction with plasticity and transformation
7. void nucleation and coalescence
8. mechanics of entangled and percolated systems: metal wool, cellular solids, dendritic structures, scale and gradient effects in plasticity
9. textures at the micro- and nanoscale: coupled stress and texture determination
10. interaction between environment and plasticity
11. high strength - high conducting composites
12. grain cluster mechanics
13. mechanical, transformation, and precipitation fundamentals of novel lightweight Mg, Be, Al, Fe, and intermetallic based lightweight alloys under to complex loadings
14. mechanical properties of alloys and intermetalics doped with rare earth elements
15. integrated structure and materials optimisation: integrating design and materials properties
16. mechanical-functional materials properties as inverse problems, i.e. back-extrapolation of optimum thermodynamics and microstructures from desired final properties

Conclusions

Metals and composites represent the most important group of structural and functional materials. Facing and solving the scientific and engineering challenges associated with their further development will open the door to an improved fundametal insight into the nature of these materials and entail essential further discoveries and developments in all fields which rely on high performance materials assigning metals and composites a key pole in our modern societies.

The asic scientific challenges lie particularly in pursuing fundamental and long-term oriented research in this field with aiming at the development of well-tailored solutions and insights which serve society with respect to **sustainable progress**, **ecological benefits**, **advanced safety demands**, and **improved productivity**. The most prominent challenges along these lines lie in understanding and developing the fundamentals of lightweight structural materials and design solutions, self-organising microstructures, failure-tolerant materials systems, smart materials, and enhanced materials for ground and aerospace transportation.

The basic scientific means of achieving these ambitious goals are extensive scientific investments in the fields of

- computational materials science and
- experimentation on model systems.

Key issues in the field of computational materials science are:

- prediction of novel structural and functional materials
- computer-tailoring of complex materials / design solutions
- simulation of materials synthesis, processing, microstructures and properties
- development of history–dependent and of scale-bridging multi–scale simulation concepts
- integration of electronic and atomic level as well as continuum scale approaches

Key issues in the field of experimentation on model systems:

- consequent application of novel experimental tools and/or advanced combinations of experimental tools exploiting observation methods that have not yet matured to their full potential
- addressing fundamental long-term problems of existing structural and functional metallic materials concepts by use of model experiments which

are the basis of our economy but are not covered by applied or industry research

- creation of experimental model systems heading beyond conventional approaches, focussing particularly on so far less investigated combinations of different material classes, microstructures and property profiles
- design of model systems should be particularly pursued in projects with highly interdisciplinary character closely integrating concepts and approaches from materials physics, materials engineering, materials chemistry, mathematics, information technology, and/or biology.

Topical key issues are in the fields:

- Interface science and microstructure design
- Thermodynamics and kinetics
- Synthesis and processing
- Mechanical and functional properties