European Commission

ACCMET Report Summary

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Final Report Summary - ACCMET (Accelerated Metallurgy - the accelerated discovery of alloy formulations using combinatorial principles)

Executive Summary:
The five year Accelerated Metallurgy Project set the ambitious goal of transferring the novel approaches of High Throughput synthesis to the field of metallurgy and demonstrate this concept in an integrated pilot facility by the end of the project.

Using the laser based Additive Manufacturing approaches as the main basis, novel rapid synthesis approaches for making alloy formulations of up to 8-compenents were achieved. To show the widest impact of this development, over a 1000 alloy formulations were selected and synthesised for a wide range of application areas, covering the automotive, aerospace and energy fields. High accuracy of control towards the target compositions have been shown and the potential has been demonstrated through synthesis of library of formulations within defined compositional phase diagrams.

The extensive involvement of end-users and industry in validating the approach has been ensured by the network of well-defined application focused clusters. This has laid the basis for listing up a range of over 20 exploitable results.

The successful scale-up has been demonstrated for selected alloy formulations, in different application areas, generated using the miniaturised High Throughput synthesis approach.

In parallel, the Virtual Alloy Library platform has been established and structured to integrate with the network of physical and virtual tools developed by the partners. Using the initial standards as basis, the VAL platform has the potential to be positioned as a leading European repository for alloy formulations, which would make it a valuable tool for planning and validating developments in multi-component alloy formulations. With over ten thousand alloy formulations already accumulated in the library, the potential of the VAL is already demonstrated.

The culmination of the Accmet project activities has been through a full demonstration in the form of an integrated pilot facility. This has involved the construction of a fully automated alloy synthesis unit in pre-commercial form. This facility is integrated with the Virtual Alloy Library for planning of formulations to be synthesised and for uploading of the complete sample history, as well as being linked to a robot sample handling system for archiving libraries of samples.

Extensive activities with respect to exploitation and dissemination of results has been achieved, including over 74 scientific publications, 23 external presentations over 26 documented exploitable results and 4 patents. Outreach to schools and public has been achieved through resources packs for museums, "Space case" and "Materials Monopoly" for use in schools. A major initiative within the field of metallurgy has been promoted, through the European Metallurgy Roadmap, which is now being implemented through the Metallurgy Europe EUREKA cluster, now setting up the first research programs.

Project Context and Objectives:
Additive manufacturing is an exponentially growing approach which aims to achieve a paradigm shift with respect to advanced manufacturing. One major aspect of this approach is the potential for accelerating the workflow from concept to object. The concepts for AM are now been seen as a platform for other applications that can bring equivalent acceleration of workflow. High Throughput approaches aim to implement parallel / accelerated approaches to the development and testing of new chemical and materials as a fast track to development of new products.

The core concept of the Accelerated Metallurgy project is to unite the two technology areas of Additive Manufacturing and High Throughput to achieve a combined acceleration in the workflows for the development and optimisation of new alloy formulations. The demonstration of this approach by Accelerated Metallurgy is through the delivery of an integrated pilot-scale facility for the High Throughput synthesis and testing of many thousands of unexplored alloy formulations. This facility is the first of its kind in the world and represents a significant advance for the field of metallurgy.

The novel technology that enables the integration of Additive Manufacture and high throughput technology in an automated HTT facility is based on the use of elemental wires that are accurately and directly fed into a laser's focal point, heated by the laser beam, and deposited on a substrate in the form of a melt pool. Through advanced automated control, this melt poll solidifies to create a homogeneous fully-dense alloy button given the precise target stoichiometry. With this automated, robotic approach - alloy synthesis that is 1000 times faster than conventional manual methods are achieved. Once produced, these discrete millimetre sized samples are submitted to a range of automated, standardised tests that evaluate the chemical, physical and mechanical properties of the new formulations in order to determine their potential for target applications.

One major advantage of this High Throughput alloy production and evaluation, is that large amounts of information can be generated. Within the Accelerated Metallurgy project, a second "virtual platform" has been established, so that this flow of information is recorded in a "Virtual Alloy Library" that will ultimately be a major standalone datamining resource. The coupling of the automated allow synthesis with computer codes such as neural network models, provides sophisticates methods to extract and map out the key trends linking process, composition, structure and properties. Within the project, the most promising alloy formulations are scaled-up and further tested for exploitation by the 20 end-users within Accelerated Metallurgy. Industrial interests include:
• new lightweight fuel-saving alloys (<4.5 g/cm3) for aerospace and automotive applications
• new higher-temperature alloys (stable>1000 degC) for rockets, gas turbines, jet-engines, nuclear fusion
• new high-Tc superconductor alloys (>30K) that can be wire-drawn for electrical applications
• new high-ZT thermoelectric alloys for converting waste heat directly into electricity
• new magnetic and magnetocaloric alloys for motors and refrigeration
• new materials for bio-medical devices
The main objectives of Accelerated Metallurgy project are:

Scientific Objective:
• to reveal a profound and quantified understanding of the links between the process conditions (including heat treatment), composition, phases, micro- and nano-structures, and the final mechanical, chemical and physical properties of newly-explored alloy formulations. This will be well supported by modern computational techniques, such as neural networks, data-mining, density functional theory, genetic algorithms and Calphad models, in order to better predict these composition-structure-property relationships. The ultimate scientific aim is to enable “material mapping”, for both equilibrium as well as metastable phase transformations.

Technological Objectives
• to implement a brand-new technique for the high-speed synthesis of ternary and higher-order alloys, based on robotic direct laser deposition (DLD) fed with elemental feedstock. A single alloy sample will take 2 minutes to produce. Hence, the alloy production rate will be over 250 times faster than conventional alloy manufacturing methods;
• to deliver a modular suite of automated high-throughput characterisation techniques able to measure the specific material properties of interest to the end-user community (see again Table 2), and to develop experimental design strategies, work-flows, standardised HTT protocols and software;
• to provide and maintain a secure “Virtual Alloy Library”, containing all process and property data;
• to integrate all of the above technology into a pilot-scale combinatorial facility at a single location, while also benefiting from the analytical support from a wide network of HTT laboratories across the EU;
• to finally deliver an HTT processing/screening capability of 10 alloy systems per day. The objective of processing 10 alloy systems per day, by the end of the project, would permit about 3000 alloy systems per year. Spread out over 5 years, and perhaps using 2 facilities, this would cover almost all possible processable ternary alloy combinations (»32,000, as stated on page 2).

Commercial Objectives
• to reduce alloy development time from 5-6 years to less than 1 year (excluding end-user validation);
• to discover a range of new alloy formulations, with superior properties compared with today’s systems, especially for the 6 application areas listed in the preceding section;
• to protect the most promising alloy compositions by means of patenting. More than 5 “composition-of- matter” and “HTT” patent applications are expected before 2015, and these will be publicised as success stories;
• to maximise the commercial output of the combinatorial facility and the associated network of European laboratories, and to be in pole-position for future HTT commercialisation.

Environmental Objectives
• to compile an inventory of eco-data for upstream production for each of the selected elements of major relevance to AccMet, primarily according to Abiotic Depletion Potential, Global Warming Potential, SO2/NOx Acidification Potential and Human Toxicity Potential. This data will therefore quantify for each element the effects on resource depletion, greenhouse gas emissions, acid rainfall and human safety; and will permit the partners to calculate a sustainability index, or “environmental footprint”, for all new alloy formulations;
• to perform a Life-Cycle Analysis (LCA), following ISO guidelines, for the new alloys relative to conventional materials. This will allow the team to design strategies to make cleaner, safer and more sustainable alloy products, in line with EC commitments such as REACH, RoHS and Kyoto Protocol.

Project Results:
Novel approaches to accelerated synthesis of multi-element alloy formulations:
A core result of the Accmet project has been to develop, validate, demonstrate and implement novel approaches to

High Throughput alloy synthesis. Using the platform of Additive manufacturing, approaches allowing the rapid synthesis of alloys with up to 8-different elemental components has been successfully demonstrated, with 1000's of alloy formulations generated for investigation in a range of application areas. Great accuracy in the control of the target compositions has been achieved, producing homogeneous samples that can be rapidly screened for a range of target properties. Great flexibility in the approach has been met, allowing the handling of high melting elements.

Rapid analytical techniques for screening of alloy libraries:
Through the involvement of the leading groups with experience of a range of analytical approaches, a wide range of accelerated techniques have been developed and tested for screening of the most relevant properties of the library of alloy formulations generated by the High Throughput synthesis. This has in many cases involved innovations to alloy automated handling of the small sized samples, in order to accumulate Chemical, Physical and Mechanical properties, matching the throughput of the synthesis step.

Virtual Alloy Library:
The development of a dedicated Alloy Materials database has been a cornerstone of the Accmet project in order to set the basis of the Virtual Alloy Library. Through automated integration with the alloy synthesis step, the foundations are there for making the Virtual Alloy Library into a vast repository of millions of alloy formulations with an associated rich set of property information. This includes an interface to a variety of modelling approaches, allowing the VAL to be populated with both theoretical as well as experimental data. Advanced search methodologies provide tools for mapping relevant properties, searching for new correlations or mapping the basis for defining the compositional space for making new alloy formulations.

Integrated Combinatorial facility (ICF):
Through the involvement of Renishaw, a leading player in the production of Additive Manufacturing systems, the final goal of establishing an integrated pilot for High Throughput synthesis of multi-component alloy formulations has been achieved. This is in the form of a pre-commercial fully automated pilot unit, integrated with the Virtual Alloy Library.

Potential Impact:
The vision of the Accelerated Metallurgy project has been to establish the technology that can make previously unattainable multi-component alloy formulations available for evaluation for their potential in a wide range of applications. With metallurgy's major role in the economy of Europe, the impact of new unique formulations can be significant. To achieve the widest potential impact, the Accmet project has structured it's activities to test development of novel alloy formulations for three major industrial segments in Europe. This has, included the close involvement of major stakeholders in the research and evaluation of results:

- Aerospace (AIRB, Norsk Titanium, AVIO, Rolls Royce)
- Automotive (CRFI, ArcelorMittal)
- Energy (CCFE, BEAS)

Through extensive in-depth scientific activities, partners in the project have already generated over 74 publications in leading scientific journals in addition to participation in a wide range of dissemination activities, including at least 23 documented presentations towards scientific conferences, museums, schools and other public initiatives. These dissemination activities have culminated, among other things, in a resources for schools (a «materials monopoly» game) which has been produced in collaboration with other large metallurgy research projects. These are being freely made available to schools in the UK, with the aim of providing resources for teachers to develop students' interest in Materials.

The core of the Accmet vision has been the two main platforms, which are to be the basis of further innovation – the Virtual Alloy Library (VAL) and the Integrated Combinatorial Facility (ICF). Specific focus has been given to laying the basis for the exploitation of these two platforms in a pathway that can realise the vision of the Accmet project. An number of models for exploitation of the VAL have been identified, both as an integrated part of the ICF, as well as the potential of a future European information repository. This can be catalysed by the over 16 thousand data points that have been generated through the Accmet research activities; going in parallel with the development of the platforms. This identifies novel business models that would aim to make this platform self-sustainable and be a hub for linking research organisations to industrial partners.

The development of the alloy synthesis technology has been at the heart of the final demonstration of the ICF with an innovative application of additive manufacturing technology. This has been successfully demonstrated for a range of applications through the installation at the University of Birmingham. With this platform and the expertise developed over the 5 year period, this lays the basis for a service continuing the development of novel alloy compositions, together with the network of technologies established across the consortium. The potential for a second European "node" for high throughput alloy development has also been identified and is currently being evaluated. The objective of putting the technology for high throughput synthesis of alloys into the marketplace as a product for purchase by industrial end-users has been evaluated. Current assessments do not appear to be support a business case for this in terms of the market interest and the high level of investment needed to finalise the commercial unit.

With respect to exploitation of the results generated in the research activities, a documented inventory of at least 26 exploitable results has been identified, including the current status of ownership, contribution of partners in terms of relevant foreground. At least 4 of these exploitable results have been taken forward and patents have been.

Dissemination to Schools & Universities
A strategy to promote materials and engineering to young Europeans has been developed at the Education Department at Nottingham Trent University. This initiative is called the 'Space-Case', provides everything needed for pupils to investigate a range of materials with a space-craft theme. The materials are aimed at pupils in upper key stage two (Years 5 and 6). The case includes a CD with a PowerPoint presentation which introduces children to their challenge: to perform a range of investigations to find the material that will be best suited for use in Space on a satellite. Children are encouraged to explore and to use their investigative skills to record their findings and draw their own conclusions. A message directly from one of the scientists working for ESA will excite children and introduce them to a real-world context for scientific exploration.

The Space Case aims to inspire school students (Primary Schools with children aged 8-11years) to study physical sciences and pursue research careers. and is being disseminated as follows:
• There has been Press, TV & Radio Coverage in the UK
• An Exhibition Stand was held at the 2014 Farnborough Airshow
• A Presentation/Demonstration was given at Education Conference in York, UK
• The ESA & Nottingham Trent University Education Departments are further developing it for general introduction across Europe

The European Research Roadmap, Metallurgy Europe

One of the main legacies from the AccmMet project, has been the activities focused on the European Research Roadmap. The vision of the Roadmap is to help solve the grand challenges facing society through establishing a vibrant, well-coordinated and large-scale 'Metallurgy Europe Research' Programme that can design, develop and deploy the next set of revolutionary alloys and composites for key industrial applications, including energy, renewables, mobility and health. The goals of Metallurgy Europe aim:

• to lay the technical foundation for the design and discovery of next-generation alloys, compounds and composites that can be processed into higher- performance metallic components for industrial end-users
• to establish new high-tech start-ups and pilot-scale factories in Europe
• to develop a talent pipeline of well-trained post-docs, PhDs, masters students, apprentices and school children, who will eventually be part of the much- needed metallurgy workforce of Europe
• to create 100,000 jobs within a decade, comprising both manufacturing and adjacent service jobs
• to develop 1000 patents in order to secure European independence in metallurgy, as well as the protection of crucial intellectual property for new materials and processes;
• to make a positive contribution to Europe's GDP and societal wellbeing.

This Roadmap has evolved into a partnership between 260 companies and research organisations throughout Europe which is now established as an EUREKA Network. This program aims to raise up to a 1 billion Euro of funding for metallurgy research throughout Europe over the next 7 years and has been through its first round of applications for setting up projects within the three key areas of:
• Material discovery
• Novel design, metal processing and optimisation
• Fundamental understanding of metallurgy

List of Websites:
http://www.sintef.no/en/projects/accmet-accelerated-metallurgy-the-accelerated-disc/

Related information

Result In Brief	A 'genome project' for metal alloys

Contact

Tove Lillian Hønstad, (Controller/Financial officer)
Tel.: +4798243437
Fax: +4773597043
E-mail

Subjects

Innovation and Technology Transfer