

D2.10: Yearly Public Report Published

Grant Agreement Number: 713514

Project Acronym: ICARUS

Project title: Innovative Coarsening-resistant Alloys with enhanced Radiation tolerance and Ultrafine-grained Structure for aerospace application

Starting Date: 01/09/2016

Project Duration: 36 months

Project Officer: Adelina NICOLAIE

Project Coordinator: Dr. Santiago Cuesta-López (UBU-ICCRAM)

Author(s): Gloria Rodríguez, UBU-ICCRAM, grlepe@ubu.es
Rocío Barros, UBU-ICCRAM, rbarros@ubu.es
Santiago Cuesta-López, UBU-ICCRAM, scuesta@ubu.es

Contributing partners: Tamas Barczy, Admatis, pal.barczy@admatis.com
Francesco Delogu, CSGI, francesco.delogu@unica.it
Alvise Bianchin, MBN, research@mbn.it
Gréta Gergely, UNIMI, femgreta@uni-miskolc.hu
Michael Scheerer, AAC, Michael.Scheerer@aac-research.at
Ioannis Diamantakos, LTSM, diamond@mech.upatras.gr
Clio Drimala, EASN, clio.drimala@easn.net
Sabine Jung-Waclik, BRIMATECH, sjw@brimatech.at

Due Submission Date: 31/8/2017

Actual Submission Date: 31/8/2017



Status	
Draft	
Final	X

Type		
R	Document, report	X
DEM	Demonstrator, pilot, prototype	
DEC	Websites, patent fillings, videos, etc.	
OTHER		

Dissemination Level		
PU	Public	X
CO	Confidential, only for members of the consortium (including the Commission Services)	

Revision History

Date	Lead Author(s)	Comments
13/07/2017	Gloria Rodríguez, UBU-ICCRAM	First draft
28/07/2017	All partners	Contributions to the first draft
04/08/2017	Gloria Rodríguez, UBU-ICCRAM	Second draft
11/08/2017	All partners	Revision to the second draft
23/08/2017	Santiago Cuesta-López, UBU-ICCRAM	Final revision
30/08/2017	Gloria Rodríguez & Rocío Barros, UBU-ICCRAM	Final version

Glossary

Acronym	Meaning
FET	Future and Emerging Technologies
nc	Nanocrystalline
EC	European Commission
NASA	National Aeronautics and Space Administration
ESA	European Space Agency
CRM	Critical Raw Materials
RTD	Research, Technology & Development
SME	Small and Medium-sized Enterprises
TRL	Technology Readiness Level
PEDR	Development of the Plan for Exploitation and Dissemination
CSA	Coordination & Support Action
FEM	Finite Element Method
PVD	Physical Vapour Deposition
GB	Grain Boundaries
MD	Molecular Dynamics
WP	Work Package
GA	Grant Agreement
CA	Consortium Agreement
MIT	Massachusetts Institute of Technology
HEBM	High Energy Ball Milling
RVE	Representative Volume Elements
ACARE	Advisory Council for Aviation Research and Innovation in Europe
ESTEC	European Space Research and Technology Centre
TRP	Technology Research Programme
GSTP	General Support Technology Programme



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 713514

The statements made herein do not necessarily have the consent or agreement of the ICARUS consortium.

Copyright © 2016, ICARUS Consortium, All rights reserved.

This document and its contents remain the property of the beneficiaries of the ICARUS Consortium. It may contain information subject to intellectual property rights. No intellectual property rights are granted by the delivery of this document or the disclosure of its content. Reproduction or circulation of this document to any third party is prohibited without the consent of the author(s).

THIS DOCUMENT IS PROVIDED BY THE COPYRIGHT HOLDERS AND CONTRIBUTORS "AS IS" AND ANY EXPRESS OR IMPLIED WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE ARE DISCLAIMED. IN NO EVENT SHALL THE COPYRIGHT OWNER OR CONTRIBUTORS BE LIABLE FOR ANY DIRECT, INDIRECT, INCIDENTAL, SPECIAL, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO, PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY OUT OF THE USE OF THIS DOCUMENT, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.



Table of Contents

List of Figures 5

List of Tables..... 5

Abstract 6

Introduction..... 7

1. Summary of the context and overall objectives of the project 8

2. ICARUS Consortium 11

3. Work performed from the beginning of the project and main results achieved so far 13

 3.1. Work Packages 1 & 2..... 14

 3.2. Work Package 3..... 15

 3.3. Work Package 4..... 17

 3.4. Work Package 5..... 18

 3.5. Work Package 6..... 20

4. ICARUS progress 23

5. Expected final results and their potential impact and use..... 25

List of Figures

Figure 1: ICARUS Consortium 11

Figure 2: Interconnections between Work Packages of the project 14

Figure 3: Schematic description of a nanostructured metal alloy 16

Figure 4: Probability of observing thermodynamic stability in W-based nanostructured alloys..... 17

Figure 5: Representative RVE of a nanocrystalline material..... 20

Figure 6: ICARUS project progress 24

List of Tables

Table 1: List of Deliverables and deadlines 23



ABSTRACT

In general terms, the present Yearly Public Report (Deliverable 2.10) establishes an ICARUS general overview and summarises the activities performed during the first twelve months of the project, as well as the results achieved so far. It has a “public” “Dissemination Level”, hence, it is presented in an understandable format to enable direct publication by the European Commission (thus in line with the “Publishable Summary”), if appropriate. Additionally, diagrams or photographs illustrating and promoting the work of the project are provided. It is to highlight that this initial deliverable will be developed in a yearly basis and thus submitted in months 24 and 36 of the project.

The present document is structured in the following chapters: The first section includes a summary of the context and overall objectives of the project, where •the problems/issues addressed by the project and the important for society of the actions are underlined, while the second section presents the ICARUS Consortium. The third section focuses on the work performed and on the results achieved during the first year of the project. The fourth section shows the project of the progress against the foreseen chronogram and work plan. The fifth section highlights expected final results and their potential impact and use.



INTRODUCTION

According to the Horizon 2020 – Work Programme 2014-2015 for Future and Emerging Technologies (FET), the mission of this initiative is “to turn Europe's excellent science base into a competitive advantage by uncovering radically new technological possibilities”. In order to succeed in this mission, FET focuses on research beyond what is known, accepted or widely adopted and supports novel and visionary thinking to open promising paths towards new technologies and supports collaborative research projects to open up new and promising fields of research, technology and innovation.

In this context, ICARUS brings a radically novel scientific vision within a field that is completely unexplored. The project targets the identification, design and fabrication of novel thermodynamically stable nanocrystalline (nc) metal alloys resistant to coarsening, enabling its design and fabrication. This will result in new families of materials with unprecedented properties and performances, which will also have far-reaching consequences on the development of revolutionary technologies in near future, thus paving the way to applications ranging from structural engineering to catalysis and energy generation.

Starting from forefront of fundamental science knowledge and from the creation of a dynamic collaborative network acting as the first seed for the nucleation of a new research-based industry, ICARUS fosters Europe's leadership in strategic areas of materials science like aerospace, automotive and energy generation and catalyses. This process leads to successful addressing the societal challenges identified by the European Commission (EC).



1. SUMMARY OF THE CONTEXT AND OVERALL OBJECTIVES OF THE PROJECT

At a first glance, the fabrication of new nc alloys is not difficult and hundreds of examples exist. Nonetheless, none of them resists to even modest temperature rises. With this aim in mind, ICARUS proposes the first attempt of developing a new thermodynamic methodology able to identify the elements and the relative chemical composition allowing a nanocrystalline state to occupy a relative minimum of the Gibbs free energy, which makes the nanostructure reasonably stable against coarsening. Hence, ICARUS brings a radically new concept by addressing a still unsolved problem in the stabilization of nanocrystalline alloys.

This scientifically sound approach will open and boost the exploration route to a new horizon of discovery and exploration of multinary thermal stable nanocrystalline alloys, exhibiting superb tailored properties. The materials discovery approach of ICARUS will be synergistic with the forefront industrial production technologies of nanomaterials and alloys.

Results arising from ICARUS exploration will be materialized in specific demo compounds representative of carefully selected new alloys families that will change the present paradigm of the aerospace industry. The most promising nanocrystalline material identified will be synthesized and the obtained samples characterized toward the applicability in the aerospace sector. A proof of concept will be given and tested by experts and specialized industries working in the aerospace sector in close contact with NASA¹ and ESA². In particular, ICARUS will demonstrate its potential by producing innovative coarsening-resistant nanocrystalline alloys of superb strength and relatively low density, or potentially able to combine such mechanical properties with enhanced resistance to radiation damage.

Taking the satellite launching and manufacturing market as an example, when a satellite is launched into space, the customer (or taxpayer) pays approximately \$10,000 to \$20,000/kg. Every kilogram saved in the payload's weight means a kilogram less thrust needed from the booster, leading to a reduction of fuel consumption. The structural cost of an unmanned spacecraft is around \$5,000 per kg; hence, ICARUS weight reduction perspectives will boost space travel and growing satellite market.

In the aviation sector, the new ICARUS family of lightweight high resistance alloys, half dense but five times strengthen will be possible, and using it in critical components of a plane (i.e. bearings), implies less weight, what is equivalent to lower fuel consumption and therefore lower CO₂ emissions. Additionally, ICARUS will allow a substantial turbine operation temperature increment, which would lead to an increase of the engine

¹ <https://www.nasa.gov/>

² <http://www.esa.int/ESA>



efficiency, allowing less fuel to be burnt for the same thrust output. These reductions also result directly to a decrease in CO₂ emissions. Massive fuel savings and reduced costs lead to higher accessibility of flying for general population and thus improvement of mobility within EU and outside, boosting economy by easy transfer of people and skills will be also a medium term consequence.

In the space sector, apart from weight and fuel savings at launch, ICARUS will support the trend towards rapid-response micro-satellites and mini-satellites and will contribute to the EU Copernicus³ (aiming at achieving an autonomous, multi-level operational Earth observation capacity) and Sentinel ESA programs⁴ (which include radar and super-spectral imaging for land, ocean and atmospheric monitoring). Moreover, ICARUS new low-weight radiation shielding families of alloys will protect satellites from space radiation and solar flares in such an effective way, that the risk of global failure by a solar storm could be reduced in 80%.

Moving beyond current aerospace trends and with the ICARUS new generation of materials in the spotlight, presently unfeasible supersonic flights may become a reality because of materials structural and thermal resistance, or even the possibility of long exploratory space missions without radiation risks to the crew, allowing thus a new era for humankind.

In addition, ICARUS plays a major role in Critical Raw Materials (CRM) substitution, particularly in alloys under extreme conditions (i.e. super alloys, cement carbides - typically using Cr, W, Co, etc.). ICARUS is thus not only relevant to industrial leadership but is cross-cutting with the H2020 Societal Challenge "Climate action, environment, resource efficiency and raw materials"⁵. On the other hand, ICARUS alloys will impact sectors where the material specifications may be of interest (e.g. medical prosthesis, oil and gas, (petro) chemical, processing industry, etc.).

All in all, ICARUS is a 36-month project which aims particularly at developing a new thermodynamic approach to materials design that promises the discovery of entirely new classes of multi-component nanocrystalline metal alloys resistant to coarsening, with properties specifically tailored to application.

The specific objectives of the project are as follows:

1. To develop the conceptual framework necessary to design thermodynamically stable multi-component nc metal alloys resistant to coarsening.
2. To validate the statistical thermodynamic modelling by matching numerical simulation with experimental evidence.

³ <http://ec.europa.eu/growth/sectors/space/copernicus/>; <http://www.copernicus.eu/>

⁴ <https://sentinel.esa.int/web/sentinel/home>

⁵ <https://ec.europa.eu/programmes/horizon2020/en/h2020-section/climate-action-environment-resource-efficiency-and-raw-materials>



3. To provide a proof of concept by fabricating selected thermodynamically stable multi-component nc metal alloys resistant to coarsening of interest for specific aerospace applications.

To achieve these goals, ICARUS fosters a three-fold multidisciplinary strategy:

1. Thermodynamic modelling will make use of a statistical mechanical approach. Thermodynamic state functions and auxiliary quantities will be described mathematically in terms of chemical composition and atomic species distribution in both crystalline grains and intergranular disordered interfaces.
2. The validation of the thermodynamic model will require identifying suitable processing methods and optimizing experimental conditions. Depending on the number of components, developing innovative processing methods is necessary. For this reason, validation will be first performed on suitably selected test systems.
3. The fabrication of thermodynamically stable multi-component nc metal alloys resistant to coarsening and specifically addressed to meet the materials demand of aerospace, aeronautical and turbine industry will require a careful selection of materials.

Specific attempts will be carried out in connection with the needs pointed out by the SMEs involved in ICARUS. In this regard, the project focuses on materials with the following target properties:

- Enhanced radiation resistance by self-healing mechanisms, aimed at withstanding the extreme conditions undergone by materials exposed to cosmic radiation, at lengthening the life cycle of aerospace materials and microelectronics and at protecting the health status of human beings in manned spacecraft missions.
- Enhanced thermal resistance, aimed at enabling stable performances under high-temperature conditions, high heat conduction and low thermal expansion, and at enhancing materials performances in dynamic thermal environments with temperature varying approximately in the range from -80 and 100 °C.
- High mechanical strength to reduce the total weight associated with structural materials, keeping mechanical performances unchanged, which results in lighter construction elements and directly lower fuel consumption in aerospace industry.



2. ICARUS CONSORTIUM

ICARUS brings together a fully multidisciplinary team with long experience in materials science, integrating Research, Technology & Development performers (RTDs) and industries to exploit synergies in order to achieve the project objectives. The industrial part of the consortium includes 4 SMEs leaders in materials production and engineering related to aerospace applications; plus 2 SMEs, leaders in knowledge transfer into industry.

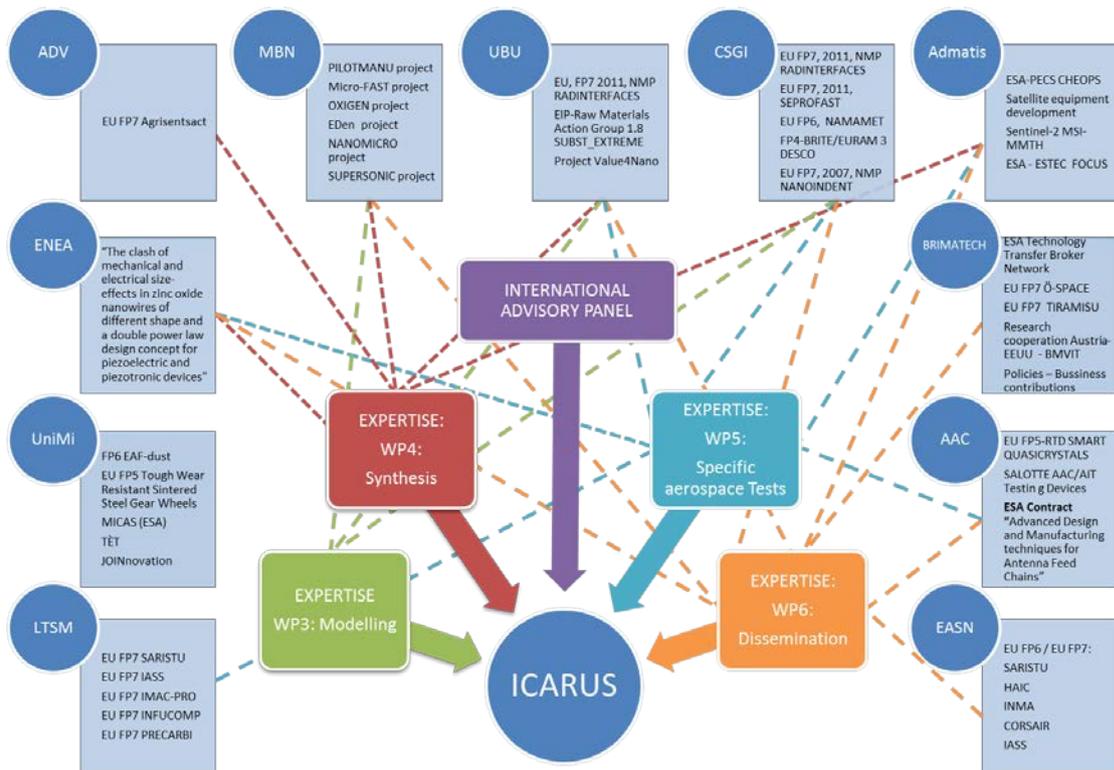


Figure 1: ICARUS Consortium

The following eleven partners constitute the consortium that is executing ICARUS project:

- **UBU-ICCRAM** (lead partner), specialized in materials, nanosafety and multiscale modelling;
- **ENEA**, leading the multiscale characterization of structures and properties of materials;
- **CSGI**, expert in thermodynamic modelling, laboratory synthesis, fabrication of dense nc alloys and mechanical behaviour evaluation under extreme conditions;



- **UniMi**, leading researcher in nano-Calphad and finite element method (FEM) Simulation, production of crystalline amorphous composite materials and microstructure characterization;
- **LTSM**: research group specialized in continuum modelling of materials and characterization of mechanical properties.

On the other hand, SMEs and Industries bring the following expertise:

- **MBN**, expert SME in producing the nano-alloys of interest on the pilot scale;
- **Advamat**, leader in fabrication of thin films by physical vapour deposition (PVD);
- **Admatis** brings space environment definition (focus on satellite business) and mechanical/thermal design, analysis, production, assembly and test for flight hardware;
- **BRIMATECH**, ESA broker and partner of its technology transfer program will contribute with the assessment/review of the performance of the proposed alloys with space experts, as well as the exploitation/dissemination activities;
- **AAC**, created as a spin-off from the Austrian Institute of Technology is a leading SME in development, characterization, testing & qualification of space materials, advanced test methods and analysis of materials & surfaces;
- **EASN**, a SME that will be a clue contributor in dissemination & diffusion to industry, Academia and research establishments & general public (with BRIMATECH).

Additionally, an International Advisory Board was set-up and is constituted by world-wide experts in forefront prediction of nc-alloys and thermodynamic prediction of new phases; nonetheless, other experts can be identified during the project, and will be properly invited to follow the project.

This group of experts acts as proposer body bringing the external developments to the consortium attention and gives regular nonbinding feedback. The Advisory Board is normally invited to all ICARUS scientific discussions, and some of the scientists are also contributing in-kind to the project, since they are already in close scientific cooperation with key members of the consortium.



3. WORK PERFORMED FROM THE BEGINNING OF THE PROJECT AND MAIN RESULTS ACHIEVED SO FAR

ICARUS core strategy involves a relatively simple approach based on a few logically connected steps:

1. Development of a theoretical and mathematical tool interlinked complementarily with a new Nano-Calphad approach, and able to identify new thermodynamically stable nc metal alloys based on a suitable exploration of parameters space, by involving a description the statistical mechanics of multi-component nc- solid solutions involving multiple chemical species segregation at disordered grain boundaries (GBs), relating local enthalpic and entropic contributions to the overall Gibbs free energy Parametric calculations will be replaced by the construction of realistic multi-dimensional Gibbs free energy surfaces specific to selected cases, which requires estimating the fundamental physical quantities either by numerical methods such as ab initio and molecular dynamics (MD), or by the use of experimental information.
2. Experimental verification of the thermal stability of nc alloys identified theoretically.
3. Selection and optimization of the most suitable methods for fabricating the thermodynamically stable nc alloys identified theoretically and tested experimentally.

The activity is distributed into the following Work Packages (WP):

- WP1: Ethics requirements.
- WP2: Management and Coordination.
- WP3: Development of a new thermodynamic materials by design approach for designing new stable multicomponent nc metal alloys.
- WP4: Fabrication and processing optimization of binary and multinary alloys as radically new materials solution for extreme-conditions aerospace applications.
- WP5: Physicochemical, structural and mechanical characterization of the alloys. Specific performance tests under extreme operating conditions.
- WP6: Exploitation, dissemination, communication.

The structure combines horizontal activities (i.e. ethics, management, Intellectual Property Rights, human resources, dissemination, training, etc.) and vertical activities (i.e. modelling, synthesis, aerospace tests, etc.). The project activities are further grouped according to the following interconnections:



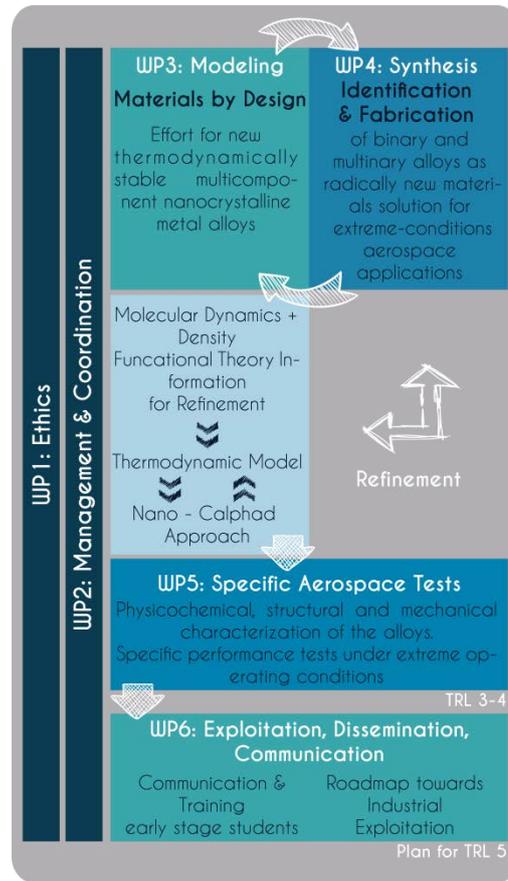


Figure 2: Interconnections between Work Packages of the project

The figure above attempts at a global view of all interconnections between the foreseen activities. The integration between different WPs appears as links connecting some of them. Results obtained in linked activities will mutually influence each other and will help achieve project objectives and turn out in long-term sustainable effects.

During the first twelve months of the project, a substantial amount of effort has been devoted to the following WPs and activities:

3.1. WORK PACKAGES 1 & 2

In WPs 1 & 2 (M1-36, led by UBU-ICCRAM), the project coordinator has dealt with the ethic requirements and has worked to ensure the proper management of day-to-day project activities as described in the Grant Agreement (GA).

Additionally, the drafting of the Consortium Agreement (CA), the production of all due deliverables, IPR and scientific management, as well as the coordination activities and meetings held can be considered as main results of WPs 1 & 2.



During the first year of the project, two Consortium Meetings have been organised: the Kick-off Meeting and the 6M Consortium Meeting.

The Kick-off Meeting of the project took place in Burgos (Spain) on September 8th and 9th, 2016. It was organised and hosted by the Project Coordinator, the University of Burgos-ICCRAM (UBU-ICCRAM). The 6M Consortium Meeting took place in Miskolc (Hungary) on March 29th-30th, 2017. It was co-organised and hosted by the University of Miskolc (UniMi) and ADMATIS in coordination with UBU-ICCRAM.

Additionally, different call conferences have been organised to track the progress of certain activities and to define specific action plans for the Work Packages, especially for WP3.

During the first twelve months of the project, the following deliverables have been produced in these WPs:

- D1.1, "DU – Requirement No. 1". It considers the potential dual use implications of the project and risk-mitigation strategies (with a view on the publication and dissemination of findings) and establishes the ICARUS Ethics Protocol.
- D2.1, "Yearly Consortium and Board Meeting 1". It contains an overview of the Consortium Meetings organised so far in the framework of ICARUS Project.
- D2.6, "Internal and main external communication channels". It establishes the different kinds of communication channels, both internal and external, with the aim of clarifying the treatment of information treatment, evaluating the communication flow and improving and avoiding the problems that could arise as a result of a lack of communication among partners.
- D2.7, "IPR Strategy". It describes the IPR strategy regarding the expected project results and its way of exploitation.
- D2.8, "Data Management Plan". It describes the data management life cycle for the data to be collected, processed and/or generated throughout the project.
- D2.10, "Yearly Public Report Published 1". Present document.

3.2. WORK PACKAGE 3

WP3 (M1-24, led by CSGI) focuses on a reliable theoretical methodology based on a multidisciplinary approach integrating theoretical thermodynamics, Nano-Calphad method, and multiscale modelling data. The main goal of this WP is to create a predictive tool for exploring and designing new binary and multinary nc alloys with enhanced thermal, mechanical and irradiation damage self-healing properties.

Nanostructured metals exhibit a three-dimensional mosaic microstructure comprising nanometer-sized crystalline grains separated by relatively diffuse and disordered grain boundaries characterized by excess volume. Due to the different structural arrangement of atomic species in grain boundaries, and the corresponding variation of local chemical



bond energies, nanostructured metals exhibit unusual and unexpected physical and chemical properties.

Excess volume at grain boundaries allows higher atomic mobility, which makes internal interfaces susceptible of evolution under thermal input. Specifically, nanocrystalline grains tend to coarsen in the attempt of reducing interface energy contributions and, thus, minimizing Gibbs free energy.

Whereas thermal instability is intrinsic in elemental metals, which undergo coarsening at relatively low homologous temperatures, in nanocrystalline alloys it can be somehow depressed, or even suppressed, by solute enrichment at grain boundaries. First hypothesized in 1993, thermodynamic stabilization of nanostructured metal alloys by chemical segregation found support in empirical evidence.

Based on the available literature, ICARUS provides an improved description of the thermodynamics stabilization scenario allowed by solute partitioning between grain interior and grain boundaries. The theoretical work performed during the first year of the project aims at relaxing most severe assumptions concerning dilution and segregation. Starting from the analytical model proposed in 2009 by Massachusetts Institute of Technology (MIT)⁶ researchers J. R. Trelewicz and C. A. Schuh, ICARUS developed a thermodynamic approach integrating classical and statistical thermodynamics to predict the relative stability of non-dilute metal alloys, relating grain boundary energy to the thermodynamic quantities governing mixing in solid solutions.

Specifically, ICARUS provides a Gibbs free energy function for binary metal alloys based on pairwise nearest-neighbour interactions. The thermodynamic model of the nanostructured metal alloy makes use of a structural description involving three different regions, i.e. grain interior, intergranular zone and grain boundary. Microstructure is schematically depicted in Figure 3.

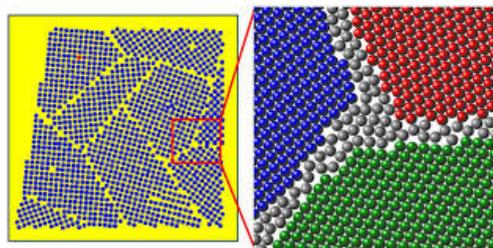


Figure 3: Schematic description of a nanostructured metal alloy

Using the regular solution approach and assuming a random site occupation, the intergranular zone is allowed to exhibit energy and composition different from grain interior. An equilibrium grain size is shown to exist for any given chemical composition

⁶ <https://web.mit.edu/>



due to thermodynamic stabilization effects connected with solute segregation at grain boundaries. Able to reduce to the standard case of grain boundary segregation in the limit of infinite grain size, the model allows considering binary systems weakly segregating and away from the dilute limit. Enabling a comparative analysis of different binary alloys, ICARUS model provides improved guidelines for the design of nanocrystalline binary metal alloys.

The model predicts the existence of thermodynamically stable nanocrystalline binary metal alloys for a relatively broad spectrum of elemental combinations. Specifically, it shows that specific binary alloys exhibit a minimum in the Gibbs free energy surface for grain size values in the nanometre range. It follows that new families of potentially stable binary alloys can be identified by the exploration of the parameter space. A typical result is given in Figure 4, where the probability of observing stability in W-based alloys is shown as a function of alloy elements.

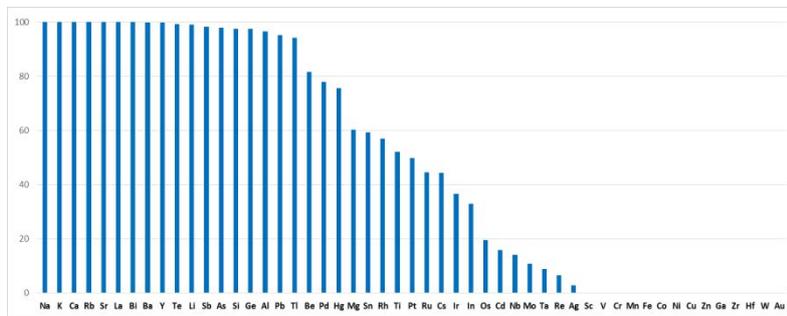


Figure 4: Probability of observing thermodynamic stability in W-based nanostructured alloys

This thermodynamics mathematical model and characterisation of the multi-dimensional Gibbs free energy surface is gathered in Deliverable 3.1, “Thermodynamics based predictive model for materials design”, developed by CSGI in collaboration with other partners involved in WP3. Though already finalised and taken into account for related activities, this deliverable has not yet been submitted, as a series of final revisions are still to be made.

3.3. WORK PACKAGE 4

WP3 runs in synergy and continuous feedback with WP4 (M12-30, led by MBN) with the aim of fabricating binary and multinary alloys radically new in concept and with tailored composition and properties. After selecting the most promising thermodynamically stable nc alloys potentially exhibiting superior mechanical, shielding and self-healing properties to meet the challenge associated to aerospace, aeronautical industrial needs, the best synthesis methodology ensuring quality homogeneity, future standardization and future scale up of the production in the proper suitable way for the target applications will be defined in WP4.



Though the activities in WP4 are planned to start in project month 12 (August 2017), some synthesis routes are already used in WP3 for the screening of the possible material phases. Trial tests have been made with some modelled systems, in particular synthesis trials of, W-Ti, Nb-Based, Ti-Based systems have been performed with High Energy Ball Milling (HEBM) in the hundreds of grams scale, while PVD has been used for synthesis trials with W-Ti systems.

During the scientific research carried out by UniMi, the obtained metal powders are milled with a high energy ball mill to a state where the constituents of the metal powder mix are turned into an amorphous state. These powder mixes then are sintered into shapes.

The core of WP4 activities for the development of processing routes will start after the selection of the most promising systems emerging from modelling and screening.

3.4. WORK PACKAGE 5

WP5 (M18-26, leaded by ADMATIS) has a two-fold aim, to provide a full characterization of the physical, chemical and mechanical properties of the new alloys specimens arising from the exploration (WP3) and subsequent synthesis/production (WP4) and to carry out specific tests in the selected specimens to demonstrate the advantages of ICARUS families of nc alloys when operating at harsh conditions.

Though this WP has not yet officially started, ADMATIS, as WP5 leader, has performed a series of actions regarding spec possibilities, with the aim of collaborating with the theoretical team in the very difficult work of material selection. Starting from the space industry requirements and learning the promises and limitations of planned nanocrystalline materials, preliminary feasibility studies on the predictable material properties were worked out. As the stability expansion was declared as preferred quality, one summary was given about stability limits under various interactions and environment with special attention on space conditions.

A dedicated study has been performed by ADMATIS focusing on radiation fundamentals and the radiation environment in space missions. Due to the lack of protection of atmosphere, the chance of material degradation is significantly increasing in space. To handle this fundamental problem, specific materials are required. One survey of the preferable fields inside space technology was also provided. Low temperature and high temperature application were analysed. Some relevant test procedures were prepared.

Furthermore, some partners (i.e. AAC) have already started collecting materials and its properties typically used in space application. The literature survey included documents such as:



- “Materials and Processes for Spacecraft and High Reliability Applications”, Barrie D. Dunn.
- “ECSS Q 70-71” regarding stress corrosion cracking and standard material properties.

At this respect, examples of Metal Matrix Composites from the ESA project: “High SSM - High Specific Stiffness Materials for Space Applications” coordinated by AAC have been also analysed. The type of required qualification tests for different space applications such as vacuum and thermal compatibility (e.g. outgassing, thermal cycling), static and dynamic mechanical properties in relevant environment (i.e. vacuum, temperature, radiation), susceptibility to stress corrosion cracking were investigated.

Additionally, during this first year, University of Patras (LTSM) efforts have been focused in WP5 concerning the mechanical characterization of the novel nanocrystalline materials to be produced in the frame of the project and the use of numerical simulations for the prediction of their mechanical properties.

During the project evolution, it has been obvious that the production of nanocrystalline materials in the frame of the project will remain limited. Materials quantity requirements, related to the mechanical characterization experimental campaign originally planned in the project have been examined by LTSM. The tests commonly applicable for aeronautical materials and the respective specimens’ dimensions have been gathered and reported to the ICARUS Consortium. Furthermore, a procedure has been introduced based on micro-hardness measurements in order to pre-screen the nanocrystalline materials, which will be developed with regards to their potential for mechanical performance.

Additionally, an extensive literature survey has been performed by LTSM concerning efforts for the development of nanocrystalline materials having a potential for aeronautical applications.

Furthermore, the survey revealed that, although atomistic simulation methods provide unprecedented insight into the structural behaviour of nanocrystalline materials, their exploitation for predicting the respective material properties is very difficult due to inherent restrictions of the methods. Therefore, in LTSM a multi-scale numerical model of nanocrystalline materials is under development, which aims to provide a tool for the design-by-analysis of the essential nanocrystalline material microstructural features in order to obtain the desired mechanical behaviour.

The proposed approach is based on the development of Representative Volume Elements (RVE) of the nanocrystalline material. In each RVE detailed three-dimensional modelling of the grain and grain boundaries as randomly-shaped sub-volumes is performed (see Figure 5), proper material laws at each sub-volume are assigned and the RVE is loaded under representative loading conditions. Thus, the basic mechanical



properties of the material (Young's Modulus of Elasticity and Yield Strength) can be numerically predicted without the need to perform an extensive mechanical test campaign. For validation purposes, a limited number of experiments is necessary.

The developed methodology will provide the means to design the essential nanocrystalline material microstructure based on the required material properties.

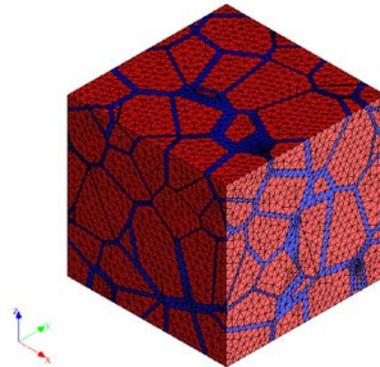


Figure 5: Representative RVE of a nanocrystalline material

Also, a wide range of characterization method and main principles of the methods and sample specifications were presented to the partners by UniMi during the 6M Meeting in Miskolc.

3.5.WORK PACKAGE 6

In WP6 (M2-36, leaded by BRIMATECH), expert brokers from ESA and aerospace industry takes care of the proper dissemination and management of scientific and technological results, paying attention to plan, for the selected materials, a future EU industrial roadmap beyond the Technology Readiness Level (TRL) 3-4 that ICARUS will achieve.

Objectives of WP6 comprise to foster exploitation, collect needs & requirements, identify challenges for implementation, summarise impact and to develop the exploitation plan & exploitation strategy. In this respect, main activities and results achieved in the period covered by this report are:

- Development of the Plan for Exploitation and Dissemination (PEDR).
- Development of the exploitation plan and summary of exploitation activities which is described in D6.1 “Dissemination and Exploitation plan and Annual Dissemination Report 1”.
- Development of the questionnaire for interviews with project partners and conducting first interviews with project partners.



- Development of a matrix comprising relevant properties of materials used in space and aviation. This matrix summarises the collected information from the project partners in WP5 (see above) about materials and properties relevant for applications in space and aviation. It provides a basis for interviews with stakeholders.
- Participation in exploitation activities: in the course of the EBN congress taking place from 5th-7th July 2017 in Enghien-les-Bains (France), an ICARUS project partner participated in a meet & match event of FETs and BICs and presented the ICARUS project in a one day start-up and FET project exhibition.
- Identification of exploitation options during the project: the FET Innovation Launchpad is a Coordination & Support Action (CSA) which aims at funding further innovation related work. It allows ICARUS project partners to verify and substantiate the innovation potential of the ideas arising from the project and to support the next steps in bringing them closer to the market. As a result, application for the call is planned for the next cut-off date in 2018.
- Identification of relevant conferences, which resulted in a conference list that is displayed in D6.1.

Regarding the dissemination and communication of results, an effective and sustainable dissemination and communication strategy respecting the H2020 rules for open access publication and the IPR protection issues has been developed. In this sense, the following activities and results were achieved during this first year of the project:

- D6.6, "Website and Project Logo" was delivered on time. The deliverable reports about the actions realized towards the development of the project's website and logo. It particularly includes considerations related to the messages to be communicated and the audiences targeted. Special considerations were taken during the website development, in order to ensure that it is able to contain all the necessary information in an easily-digestible language, being able to engage the visitors' interest whereas in the case of the project logo, several alternatives were developed before selecting the most appropriate choice.
- Website, project logo and templates for deliverables and presentations were designed and implemented within the first 3 months of the project. Further dissemination material (i.e. project flyer, poster, banner, etc.) was prepared within the first year. Printed versions of the ICARUS leaflet and poster were sent to all project partners for dissemination purposes.
- Establishment of the ICARUS project Private Area, a secure password-protected e-collaboration platform, which was developed for the needs of the project in order to facilitate the internal communication and document exchange among partners.
- Establishment and maintenance of the "International Spring School on Forefront Alloys and Advanced Materials for Extreme Conditions" - mini website as well as



design and production of the dissemination materials for the ICARUS and SUPERMAT International Spring School.

- Dissemination approval process. To monitor the dissemination activities and to prevent IP conflicts a “Dissemination e-Approval Tool” was set up.
- PEDR: Development of the Plan for Exploitation and Dissemination, which is a document for monitoring the exploitation and dissemination activities. The PEDR was circulated among all partners and resulted in the documentation of exploitation & dissemination activities in D6.1.
- D6.1, “Dissemination and Exploitation plan and Annual Dissemination Report 1” delivered on time. It describes the first version of the dissemination and exploitation strategy and summarizes all dissemination, communication and exploitation activities that took place in the first year of the project.
- Implementation of social media accounts and continuous update (LinkedIn⁷, Twitter⁸).
- Publication of project related information to the EASN portals (Periodic EASN Association Newsletter, EASN Association Portal, EASN-TIS Company Website).

Additionally, as part of the tasks envisaged for the empowerment of high potentials, and though according to the Grant Agreement this task starts in M18 (March 2018), the “International Spring School on Forefront Alloys and Advanced Materials for Extreme Conditions”⁹ took place during 15th-17th May 2017 in Chia (Sardinia, Italy). This event was organised by UBU-ICCRAM in collaboration with EASN and BRIMATECH. The Spring School was shared with another H2020 project (i.e. SUPERMAT10). Through this experience, students, partners and other attendees had the opportunity to be specifically trained on the cutting edge science and technology intrinsic to the ICARUS and SUPERMAT projects by leading researchers. This 3-day event included 19 lectures of project partners and a best poster award. A keynote was given by Frank Salzgeber, Head of ESA TTPO.

A deliverable not foreseen in the GA was developed by WP6 leader together with project partners and is assigned to Task 6.1 “Sustainable impact and exploitation”. Objective of this deliverable is to further elaborate on the rationale for concentrating on the aerospace sector and to report on basic needs of aerospace industry and the characteristics of materials currently used, as well as the requirements new materials shall fulfil. The deliverable includes input from project partners experienced in the relevant application fields. It summarises internal documents produced by project partners, a review of relevant parts of the ESA material databases, presentations held in the course of the ICARUS Spring School and findings from first interviews. It gives indications for selecting base materials and binary alloys that might be promising for industry.

⁷ <https://www.linkedin.com/groups/13523454>

⁸ https://twitter.com/ICARUS_ALLOYS

⁹ <http://icarus-alloys.eu/spring-school/icarus-supermat-spring-school>

¹⁰ <http://imnr.ro/supermat/>



4. ICARUS PROGRESS

In general, the action has fully achieved its objectives for the first year with relatively minor deviations, and the most important milestones and deliverables (See Table 1 below) scheduled for the first twelve months of ICARUS project have been fully achieved. Although some minor reports have not been fully finalised on time, all project partners concur in the assessment that the slight delays so far incurred are not substantial and they are to be expected in a complex project like this, with multiple WPs, tasks and deliverables and with a relatively large number of partners.

WP	DELIV.	TITLE	LEADER	DEADLINE
6	D6.6	Website and Project Logo	UBU	Done
1	D1.1	DU-Requirement No.1	UBU	Done
2	D2.6	Internal and main external communication channels operating	UBU	Done
2	D2.8	Data Management Plan. Adhesion to the Open data Pilot (scientific data not in conflict with military applications - ethics)	UBU	Done
2	D2.1	Yearly Consortium and Board Meeting 1	UBU	Done
2	D2.10	Yearly Public report Published 1	UBU	Done
6	D6.1	Dissemination and Exploitation Plan and Annual Dissemination Report 1	EASN TIS	Done
3	D3.1	Thermodynamics based predictive model for materials design	CSGI	30 Apr. 2017
2	D2.7	IPR Strategy	UBU	31 Aug. 2017
2	D2.4	Action/Review check meeting 1	UBU	31 Oct. 2017
3	D3.2	Exploration map of new stable nc alloys	UBU	30 Nov. 2017
4	D4.1	Report specifying the most promising candidates in terms of challenging properties under extreme conditions and feasibility of fabrication	CSGI	30 Nov. 2017
2	D2.2	Yearly Consortium and Board Meeting 2	UBU	31 Aug. 2018
2	D2.11	Yearly Public report Published 2	UBU	31 Aug. 2018
3	D3.3	Report of the experimental validation and refinement of the proposed theoretical approach	CSGI	31 Aug. 2018
6	D6.2	Dissemination and Exploitation Plan and Annual Dissemination Report 2	EASN TIS	31 Aug. 2018
4	D4.2	Report assessing the most convenient processing routes, SWOT analysis for the production of new alloys	CSGI	31 Dec. 2018
4	D4.3	Full production of representatives demo probes of selected nc-multinary-allots	MBN	28 Feb. 2019
6	D6.5	Empowerment of high potentials: Dedicated summer/winter school	UBU	28 Feb. 2019
5	D5.5	Report on Safety and LCA for ICARUS materials	UBU	31 Jul. 2019
2	D2.3	Yearly Consortium and Board Meeting 3	UBU	31 Aug. 2019
2	D2.5	Action/review check meeting 2	UBU	31 Aug. 2019
2	D2.9	Data Management Plan updated	UBU	31 Aug. 2019
2	D2.12	Yearly Public report Published 3	UBU	31 Aug. 2019
5	D5.1	Micro/nano physicochemical and structural characterization of the new alloys	UniMi	31 Aug. 2019
5	D5.2	Mechanical Characterization of the new NC-alloys	LTSM	31 Aug. 2019
5	D5.3	Report about the behaviour of the alloys specimens under specific standard aerospace test	ADMATIS	31 Aug. 2019
5	D5.4	anticipation of the materials behaviour by ICE under service/operation	LTSM	31 Aug. 2019
6	D6.3	Dissemination Plan and Annual Dissemination Report 3	EASN TIS	31 Aug. 2019
6	D6.4	Impact Areas and Exploitation Plan	BRIMATECH	31 Aug. 2019

Table 1: List of Deliverables and deadlines



During the first twelve months of the project, the collaboration among all project partners has been relentlessly gaining momentum in an atmosphere of collegiality and partnership, to the point that currently there is a smooth project implementation and an intensive collaboration among all project partners on all WPs, and there is a lot of excitement about the project and the benefits ICARUS will bring to the European aerospace industry and to the consolidation of the European leadership in this very promising field in the world.

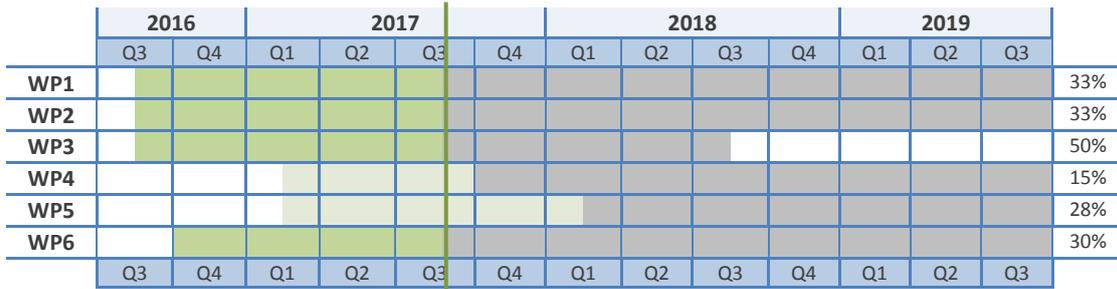


Figure 6: ICARUS project progress

Though WP4 and WP5 are expected to start in month 12 and month 18 respectively, as stated in [Section 3.3](#) and [Section 3.4](#), a series of activities are being developed since month 6 by some of the partners involved in order to advance work on the fabrication of alloys and on the mechanical characterization and modelling of the materials that will be produced.



5. EXPECTED FINAL RESULTS AND THEIR POTENTIAL IMPACT AND USE

While the alloys developed and the method to design them will have a broad application spectrum, ICARUS will focus on the needs and requirements in two areas, namely aeronautics and space.

In the space exploration and satellite sector, ICARUS will address space materials and process qualifications driven by high reliability, performance and harsh space environment (radiation, temperature etc.). This is combined with limited availability of raw materials and low volumes in terms of units, yet with sometimes very complex manufacturing processes.

In the aeronautics sector, the high level drivers set out by the Advisory Council for Aviation Research and Innovation in Europe (ACARE) lead to materials technology requirements related to reduction in mass, increased temperature capabilities, and reduced cost through the use of new materials with low density, mechanical properties unaffected by high temperatures and simpler production and maintenance processes, so as to be used in primary and secondary structures, cabin elements and engine structures.

In this regard, ICARUS will strongly impact the aerospace sector providing a new methodology for exploring and tailoring properties “a la carte” for new families of super alloys.

In particular, ICARUS will provide an answer to the high temperature present challenges in aviation: improved materials for engines, and lightweight temperature resistant materials for supersonic flight regimes.

The new generations of alloys deriving from ICARUS will have the following impacts on the aviation industry:

- More efficient use of resources and energy.
- Reductions in aviation’s negative environmental impact through the use of lighter and recycle structures in aviation.
- Reduction in manufacturing and maintenance costs and lead time.
- Reduction in the certification/standardisation costs.

Focusing on project-specific activities, as far as WP3 (modelling) is concerned, the thermodynamic model, in its final version, is expected to enable the identification of potential thermodynamically stable nanostructured metal alloys by design. In particular, it can be expected that the model allows for a systematic screening of binary and multinary



metal alloys in search of those nanocrystalline systems able to exhibit a minimum in the Gibbs free energy.

Therefore, the full development of the thermodynamic modelling approach can be expected to beneficially impact materials science and engineering, providing a tool for exploring the thermodynamic properties of possible alloys of interest for specific technological applications, and identifying candidate materials by design.

WP4 is showing promising results considering the W-Ti system, already known from literature. With this system the first synthesis trials have been already performed both by HEBM and PVD with good results. The sintering route for the powder obtained by HEBM is not yet optimized and it will lead to the production of specimen suitable for mechanical tests and material assessment for use in the aerospace sector. Notwithstanding this, the W-Ti system could be exploited also in other market sectors as radiation shielding material.

Since WP4 has not yet formally started, it is difficult to draw any conclusion, but the preliminary activities, done so far with the better known W-Ti system, have proved that the route defined in the ICARUS project is promising and that we should expect more systems to be released for exploitation in aeronautics, space and other sectors. Also, it is expected that the exact methods and technical specifications regarding the powder metallurgy based manufacturing of metal alloys, which will be backed up by the WP5 examinations, are clarified throughout the project.

Regarding WP5, the most perfect final result will be a new material with reliable production technology and extreme advantageous properties. Furthermore, a measurement procedure able to characterise new alloys will be successfully developed. Though the way from laboratory research toward production is always difficult and takes long time, the most appropriate solution is being sought. In this sense, the final material is predicted for long term space missions where the stability requirements have special priority. Geostationary satellites for GPS services are designed for 10 years operation time. The 20 years long PLATO mission for exoplanet observation was accepted by ESA in 2017 June. Other European space missions are also under preparation (Mars mission, Jupiter mission). In ESA Non-dependence strategy 2018-20 the material of combustion chamber is selected as the most focussed material problem. These are just examples indicating potential impacts. Also, one further success (potential impact) will be to generate more motivation to work out thermodynamic independent (nonequilibrium) structure-property predictive models.

Additionally, the expected final result with respect to space applications is a validated temperature stable nano-structured material under the following simulated space relevant conditions:



- No degradation of the mechanical properties (and microstructure) after thermal cycling under vacuum (100 cycles between -160°C and 160°C) according to ECSS Q-ST-70-04.
- No degradation of the mechanical properties (and microstructure) after thermal exposure under vacuum (-196°C and 160°C).
- No susceptibility to stress corrosion cracking according to ECSS-Q-ST-70-37A.

Based on the achieved results (i.e. mechanical, thermal, etc., properties and their stability under space conditions), potential space application fields will be further discussed with the relevant responsible people from ESA (Quality department from ESTEC¹¹) to launch further development studies (pre-qualification campaigns) under, for instance, ESA programs such as TRP¹² or GSTP¹³.

Additionally, the development and validation of a novel methodology for the numerical prediction of nanocrystalline materials mechanical behaviour, based on the FE method, will be exploited for the choice of appropriate material micro-structure characteristics, so that the required mechanical properties are obtained. Thus, new nanocrystalline materials stable at high temperatures and high specific mechanical properties can be designed and produced. The use of such materials in aircraft structures is expected to reduce the total aircraft mass and CO₂ emissions.

As far as WP6 is concerned, expected results with regards to exploitation are the following ones:

- Final materials and processes developed in ICARUS are not yet certain. Therefore, the concretisation of the exploitation plan and strategy will continue throughout the project, as R&D outcome materialises. Results will be summarised in D6.4 “Impact Areas and Exploitation Plan”, to be due in M36, comprising:
 - Clear understanding and description of relevant ICARUS exploitation target groups (from among dissemination target groups) tailored to the ICARUS project results.
 - Understanding and description of the needs and requirements of the defined user groups.
 - Plan for exploitation after ICARUS: identification of promising exploitation options after the FET project ICARUS (future roadmap). Potential strategies for exploiting ICARUS results after the project end comprise further internal research, collaborative research, internal product development, internal service development, licensing, assignment, joint venture, spin-off, etc.

¹¹ http://www.esa.int/About_Us/ESTEC

¹² http://www.esa.int/Our_Activities/Space_Engineering_Technology/Shaping_the_Future/About_the_Technology_Research_Programme_TRP

¹³ http://www.esa.int/Our_Activities/Space_Engineering_Technology/Shaping_the_Future/About_the_General_Support_Technology_Programme_GSTP



Regarding dissemination and communication, the following results are expected:

- Continuously updated public website.
- To enhance the connection among the consortium members, the stakeholders of the related scientific fields, and the general public to the concept, achievements and activities performed within the project.
- Knowledge sharing, transparency and education to be promoted.
- The potential of market uptake and commercial exploitation of the project results to be considerably increased.
- A large number of people from different stakeholder groups aware of the ICARUS project.

Last but not least, the expected result with regards to the empowerment of high potentials is to engage a new generation of researchers to consider doing research in Forefront Alloys and Advanced Materials for Extreme Conditions.

