1. PUBLISHABLE SUMMARY

Summary of the context and overall objectives of the project (For the final period, include the conclusions of the action)

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.
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. 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.

Work performed from the beginning of the project to the end of the period covered by the report and main results achieved so far (For the final period please include an overview of the results and their exploitation and dissemination)

WORK PACKAGES 1 & 2: Ethics requirement, Management and Coordination
In WPs 1 & 2, 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).
WORK PACKAGE 3: Development of a new thermodynamic materials by design approach for designing new stable multicomponent nc metal alloy.
WP3 aims 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. Starting from the analytical model proposed in 2009 by Massachusetts Institute of Technology (MIT) 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.

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 Image 3 ("W-based nanostructured alloys), where the probability of observing stability in W-based alloys is shown as a function of alloy elements.

WORK PACKAGE 4: Fabrication and processing optimization of binary and multinary alloys as radically new materials solution for extreme-conditions aerospace applications

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.

WORK PACKAGE 5: Physicochemical, structural and mechanical characterization of the alloys. Specific performance test under extreme operating conditions

Though this WP has not yet officially started, a series of actions regarding spec possibilities has performed, 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.

WORK PACKAGE 6: Exploitation, dissemination, communication

The main activities related with exploitation achieved in the period covered are: development of the PEDR, development of the questionnaire and conducting first interviews with project partners, development of a matrix comprising relevant properties of materials used in space and aviation and participation in exploitation activities. Regarding the dissemination and communication, an effective and sustainable dissemination and communication strategy respecting the H2020 rules for open access publication and the IPR protection issues has been developed. Additionally, the “International Spring School on Forefront Alloys and Advanced Materials for Extreme Conditions“ (http://icarus-alloys.eu/spring-school/icarus-supermat-spring-school) took place during 15th-17th May 2017 in Chia (Sardinia, Italy).

Progress beyond the state of the art, expected results until the end of the project and potential impacts (including the socio-economic impact and the wider societal implications of the project so far)

In this section goes the detailed information on how the project is going beyond the state of the art and is influencing positively on the potential impact.

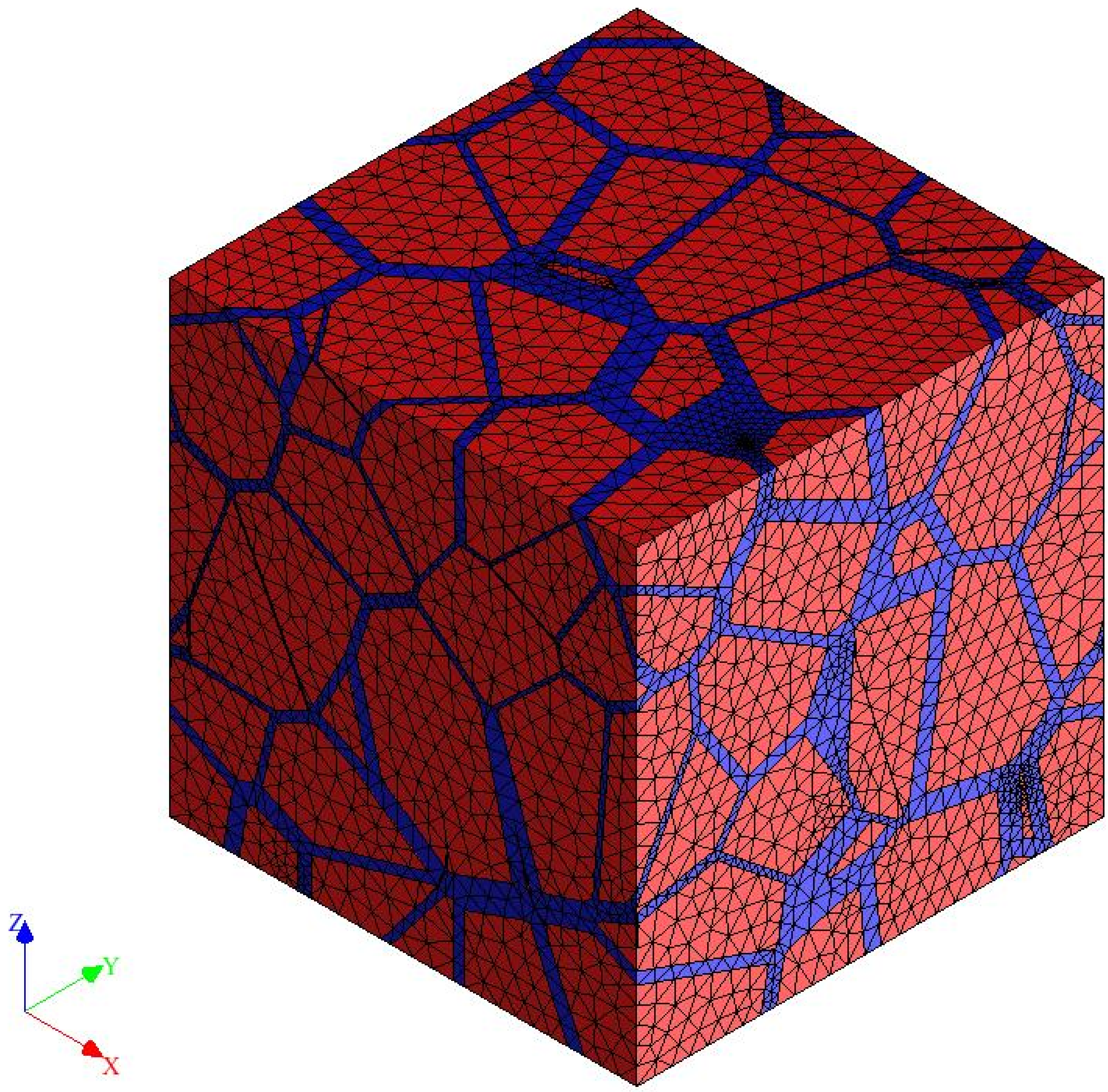
• Development and validation of a novel methodology for the numerical prediction of nanocrystalline materials mechanical behavior, based on the FE method, will be exploited for the choice of appropriate material micro-structure characteristics, so that the required mechanical properties are obtained. 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 of the total aircraft mass and CO_2 emissions.

• Participation in a project where atomic modelling is used to find stable nanocrystal alloy is a great challenge. The progress in that way means deeper understanding of all worldwide used common alloys have been developed long time empirical way. Collaborating people from theoretical and industrial side of the materials science created a strong driving force existed never before. One real progress was also to learn how real materials obey or not on any newborn thermodynamic rules and how they changes on effect of new developed production technology.
• Due to the favourable distribution of roles and functions among ICARUS partners and to their variety in size and location (from SMEs to universities, from standardization bodies to research centres all over Europe), the R&D achievements of the project are expected to escalate both geographically and economically fields.

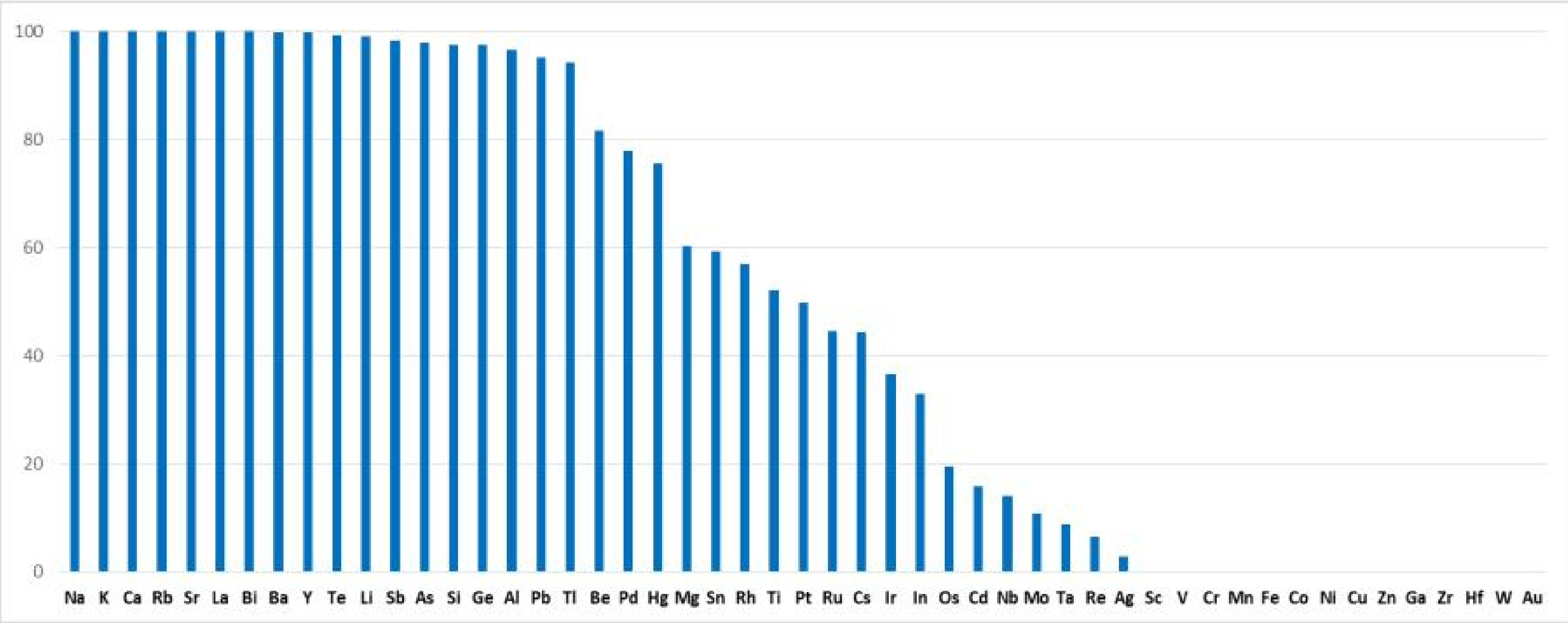
Address (URL) of the project's public website

http://icarus-alloys.eu/

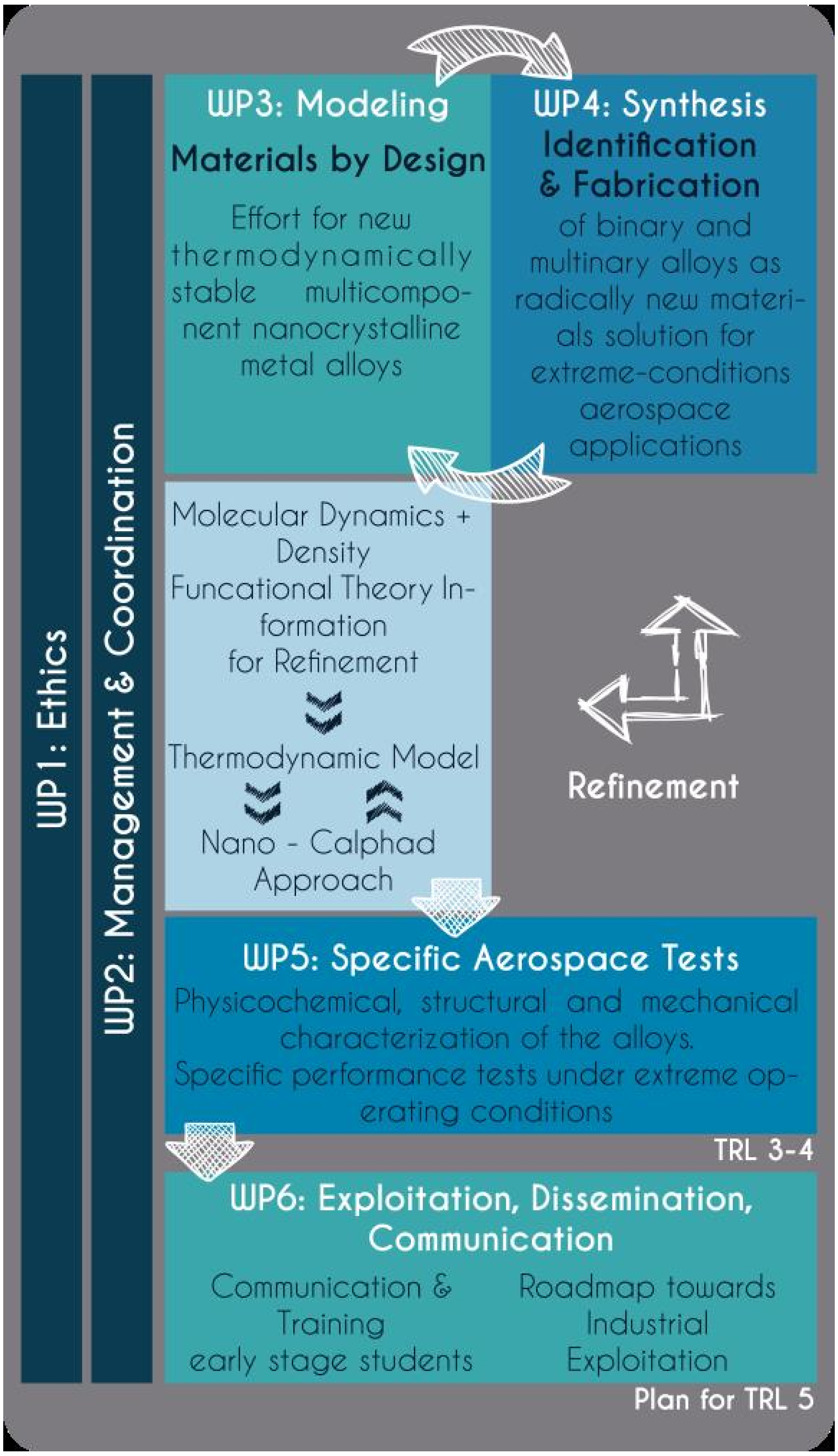
Representative RVE of a nanocrystalline material



Probability of observing thermodynamic stability in W-based nanostructured alloys



Interconnections between Work Packages of the project



Schematic description of a nanostructured metal alloy