PROJECT FINAL REPORT

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1.1. Final publishable summary report

1.1.1. An executive summary

The macroscopic mechanical properties of silicon nitride depend on its microstructure. As it is possible to prepare Si_3N_4 with various microstructures, so it is also possible to obtain materials with different mechanical and/or damage properties. The complex relation between the microstructural properties and the macroscopic thermoelastic, fracture, and wear properties is neither well known nor well understood. This challenge was tackled in RoLiCer by employing computer simulation following a multi-scale paradigm, in which the simulation of the properties of silicon nitride is broken down in simulations on three different interconnected levels: the atomic scale, the micro and meso-scale, and the macro-scale. The simulations were backed-up by targeted model experiments.

The results of RoliCer enabled constructing a robust subroutine that models mechanical as well as thermomechanical wear in ceramic components by means of finite element method. Moreover, lifetimes predictions of ceramics were accomplished as fatigue life predictions.

Using cohesive zone modelling, crack nucleation and propagation for short crack in the range 10-100 µm was predicted. Fracture behaviour was successfully modelled for different silicon nitride grades by optimising traction separation parameters. Additionally, XFEM method was successfully applied and provided good results when bridging effects were not strong (i.e., for longer cracks).

The 3D microstructure of silicon nitride was modelled using EBSD as input for numerical models. For instance, the effective thermoelastic properties of silicon nitride were computed based on mean field and full field homogenization techniques. The fracture behaviour of silicon nitride was studied using finite element analysis and it was shown that damage initiates across the intergranular interface, thus, preceding transgranular fracture. Moreover, two macroscale damage models for silicon nitride were implemented in RoliCer; an analysis has been made under static and cyclic loadings.

The atomistic simulations in RoliCer focused on describing the properties of the grains, grain interfaces, and amorphous bulk and IGF materials. Ab initio simulations and molecular dynamics simulations were conducted. Ab initio simulations were used to study the cohesive strength of Si_3N_4 grains with and without defects and impurities. The results were further used to assess the accuracy and reliability of the empirical potentials. Furthermore, the adhesion between grains was studied by means of IGFs.

Two silicon nitride grades were tailored for bearing and wire rolling applications. The materials were fully characterised and compared to state-of-the-art silicon nitride grades.

In the prototype testing and demonstration of functionality phase of the project, ceramic rolls were used in hot wire-rolling experiments. The rolls were successfully used to roll approximately 150,000 kg of different steel qualities including an unprecedented quantity of nickel-base superalloys wires.

1.1.2. A summary description of project context and objectives

The objective of RoliCer is to boost the reliability and longevity of advanced ceramics by using extensive data from engineering applications, numerical simulations and targeted model experiments.

Studies on advanced ceramics have highlighted their exceptional superior mechanical, thermal and tribological properties for many engineering applications. Ceramics are especially well suited for modern rolling and sliding bearings, as well as for metalworking and cutting tools.

However, there are still concerns over the reliability and lifetime of ceramic materials. RoliCer as an EU-funded collaboration of companies that develop and manufacture ceramic materials and components and research institutes that conduct research by means of numerical simulations and experiments to assess materials on the different scales – works to bridge the gap in knowledge between damage, wear, reliability and lifetime of ceramics. The project investigates the damage and degradation of silicon nitride (Si_3N_4) by means of multiscale numerical simulations (atomistic, microscale, mesoscale and macroscale) as well as targeted model experiments. The outcomes of the project are validated through industrial testing.

The macroscopic mechanical properties of silicon nitride (Si_3N_4) depend on its microstructure: on the size and orientation of the Si_3N_4 grains, on the chemical composition of the glassy phase and on the inter-granular film (IGF) glassy phase which mediates the interaction and structure between nearby grains. As it is possible to prepare Si_3N_4 with different microstructures, so it is also possible to obtain Si_3N_4 materials with different mechanical or damage resistance properties. In principle, this enables the engineering of Si_3N_4 with specific properties by tailoring its microstructure. Unfortunately, the complex relation between the microstructural properties and the macroscopic thermoelastic, fracture, and wear properties is neither well known nor well understood. Knowing this relation would be of great practical importance in the development of Si_3N_4 based components for many advanced applications, including aerospace, energy production industries, metal rolling industries and much more.

This challenge was tackled in the RoLiCer project employing computer simulation following a *multi-scale* paradigm in which the simulation of Si_3N_4 is broken down in simulations on three different interconnected levels: on the *micro-scale*, the *meso-scale*, and the *macro-scale*.

One of the most challenging aspects of the methodology is that evolving from small-scale models to large-scale models involves several changes, including those related to time. There are many aspects involved in transferring information from the over-simplified, small-scale model of a very complex phenomenon into the larger-scale model and vice versa. For instance, calculations and simulations at the atomic level provide insight into phenomena and may explain what happens on larger scales. A clear example is fracture: the occurrence of fracture on the atomistic level shows the orientations and planes at which fracture is most likely to occur on larger scales. On the other hand the macro-scale fracture mechanics rely on concepts such as the stress intensity factor, which is an indicator of the stress state at the crack tip in ceramic materials. It is used to predict fracture, and hence failure, in ceramics. Stress gradients within the material may influence the stress intensity factor, directing towards certain design or loading recommendations.

Since ceramics are applied in various fields, no one material combination can be expected to portray a magic recipe. RoliCer is targeting two groups of applications: bearings and manufacturing tools. With bearings, the ceramic rolling components are subjected to severe mechanical contact stresses. With manufacturing tools, the ceramic tools undergo high mechanical and tribological stresses at high temperatures. The project aims at designing two distinct materials capable of sustaining the loading conditions pertaining to each type of application. This being said, both material combinations must be economically feasible for production as well.

Parallel to the numerical simulations, the research in RoliCer focuses on both material design and implementation in the industry. The testing phase will involve using material grades developed within the project to manufacture rolling components that will be examined in full-scale hybrid bearings tests and rolls that will be tested in a nickel-base superalloy wire rolling mill.

1.1.3. Description of the main S&T results/foregrounds

Silicon nitride ceramics are prime structural materials for several challenging assignments and applications such as automobile industry, bearings and cutting tools, among others. This is due to their outstanding high stiffness, high-temperature strength and, especially, their high fracture toughness. This interesting property profile is related to different aspects of the material on the micro level.

In order to better understand the behaviour of the material, the results obtained from both numerical simulations and experimental results were coupled to give new insights.

Atomistic approach

Initially, the properties of single microstructural elements, i.e., single grains having either a crystalline or amorphous structure, are described. The adhesion strength of grains separated by a thin layer of amorphous material, that is by an intergranular film (IGF), is also taken into accounts as it is found often between nearby grains, and therefore controls much of the damage growth through the material. All such microscale-properties can be described by looking at the local behaviour of relatively small number of atoms. In this case it is possible to employ atomistic scale calculations that provide qualitative and quantitative information, albeit on small sample systems, that can describe extended ones by proper boundary conditions on the mesoscale, simulations of the geometrical features of the microstructure, such as the size and distribution of grains, are explicitly taken into account. The average behaviour of a set of a few hundreds of grains under high stress or temperature is modelled, taking micro-scale parameters as basic input information for the physical behaviour of the single constituents of the microstructure. The result of this averaging on the microstructure (the so-called *homogenisation* procedure) is the constitutive equations that describe the material on the macro-scale. Constitutive equations can be used to simulate the macroscopic behaviour of Si_3N_4 tools under realistic load condition. This is the third and final step in the multi-scale simulations chain for silicon nitride. Within the RoLiCer project a multi-scale procedure was established for the predicting the interrelation between the microstructural properties and the performance of (macroscopic) industrial tools.

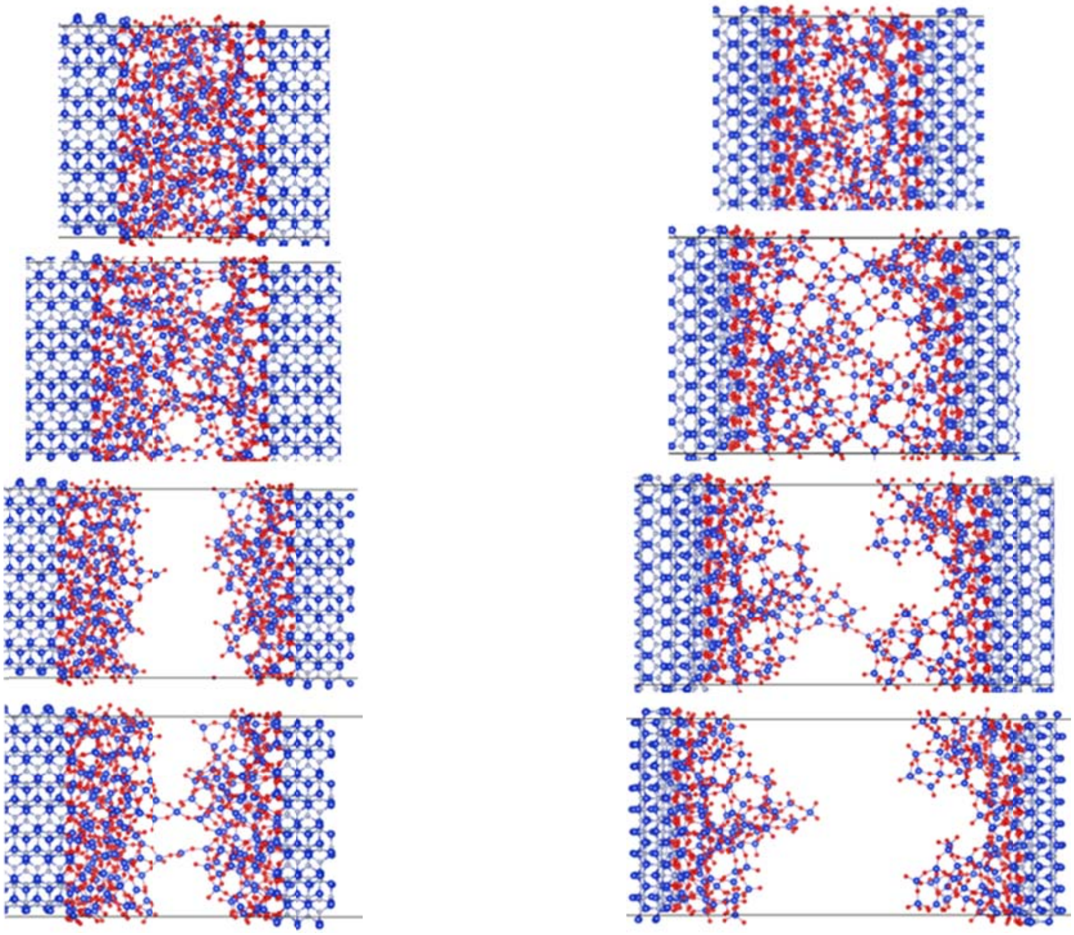
The atomistic simulations focused on describing the properties of the grains, grain interfaces, and amorphous bulk and IGF materials, and in particular on the development of simple, but reliable procedures to obtain information in all the cases where experiments are either not possible, or simply not yet available. This way we were able to compensate for the lack of information in existing experimental data and to provide a complete set of typical microstructural parameters to other work packages to enable completing the homogenization procedure.

Two different kind of atomistic simulations were employed, according to specific needs: *the first are ab initio* simulations, which provide a highly accurate and reliable technique in which the forces between atoms are computed directly form quantum mechanical first principles methods, and the second are empirical molecular dynamics simulations, where the interatomic forces are modelled by empirical laws. Empirical potential offer the advantage of shorter simulations time, and are capable of dealing with larger model as compared with *ab initio* simulations albeit with less quantitative accuracy.

Ab initio simulations were used to study the cohesive strength of Si_3N_4 grains with and without defects and impurities. The results were further used to assess the accuracy and reliability of the empirical potentials. Thermoelastic properties of ß- Si_3N_4 at finite temperature, in the range T=300-1500 K, were computed by means of empirical potentials employing the so called quasi-static approximation, complementing existing experimental data (i.e. high temperature expansion coefficients and bulk modulus). With the same technique also the temperature dependence of a model amorphous Si_3N_4 was computed. These data can be used in the homogenization procedure to find the effective thermoelastic behaviour of macroscopic materials. Reliable thermoelastic constitutive equations are a fundamental piece of information, because it allows estimating and locating the peak of stress in the silicon nitride, i.e., when and where the tools are most likely to fail.

We further investigated how the adhesion between grains is mediated by the IGFs. To this end we produced models of IGF of the typical thickness of about 1.8 nm, with three different compositions: SiO_2, Si_3N_4, and Si-O-N with Al impurities. The IGF models were produced between the two main crystallographic planes of the crystalline ß-Si_3N_4: the basal and the prismatic one. On these models we performed atomistic stress-strain experiments by pulling the samples at constant speed (ca. 0.1 Å/ps) and measuring the component of the stress along the pulling direction. These experiments were done at several temperatures in the range T=300 K to 1500 K in order to assess the influence of high (operating) temperature on intergranular cohesion. In Fig. 1 we report a series of illustrative snapshots of the breaking mechanism of a silicon dioxide IGF at room temperature (T=300 K). By evaluating the relative strength of different IGF and the weakening of cohesion due to high temperatures, we provided reference points for the parametric studies of fracture propagation performed on the mesoscale.

The multi scale approach we developed proved to work well in the prediction of thermoelastic and fracture resistance properties of Si_3N_4 at low and high temperature, resulting in a useful tool for the optimization of ceramic materials by the tailoring of their microstructure.



(a) SiO_2-IGF between basal planes

(b) SiO_2-IGF between prismatic planes

Fig. 1. Snapshots of computational tensile experiment on a diffuse interface with a SiO_2 IGF at room temperature (T=300K). The small gray spheres indicate Nitrogen atoms, the dark blue Silicon atoms, and the red ones Oxygen. Left panel (a): IGF between Si_3N_4 basal planes. Right panel (b): IGF between Si_3N_4 basal planes. The top panels show the unstrained IGF

Materials microstructure characterisation

Throughout RoliCer, four silicon nitride materials (two reference grades and two newly developed grades) were characterised from the microstructural point of view using several methods.

The homogeneity of the material is an essential aspect of the macroscopic characteristics of silicon nitride. In this case, the distribution of the so-called "snowflakes" is of major importance. Snowflakes can be described as localised patches that exhibit a lack of glassy phase; thus, creating spots with increased microscopic porosity. The visible light used in low magnification optical microscopy is the optimal method for snowflake observation, thanks to light scattering on the micro-pores, which in turn create white spots. However, such micro-porosity can be clearly identified as well using sophisticated methods possessing higher resolution such as scanning electron microscopy (SEM).

The grain size distribution was determined by image analysis where thousands of grains were analysed for each material. Back scattered electron SEM images were used for the analysis; the contrast between silicon nitride grains and its glassy phase is significantly higher in the back scattered more than in its secondary electrons mode counterpart. Maximum (grain length) and minimum (grain width) grain size characteristics were determined and the aspect ratio was calculated. The characteristics obtained by this method can be described as indicative due to the fact that two-dimensional cross sections of randomly oriented grains are not able to provide accurate information about the real grain shape (especially in highly elongated grains) even when the orientation is known using methods such as the electron back scatter diffraction (EBSD).

Grain triple points and the glassy phase presented in the grain boundaries were characterized using atomic force microscopy. Thanks to its non-contact mode, it was possible to distinguish between silicon nitride grains and amorphous glassy phase, which cannot be evaluated using EBSD.

Moreover, X-ray diffraction was employed to determine exact phase composition of the materials in addition to lattice parameters of individual phases. The lattice parameters were later used for enhancement of the grain orientation indexing used in the three-dimensional EBSD analysis.

3D EBSD microstructure reconstruction

The microstructure of silicon nitride consists mainly two phases: crystalline prismatic β-Si_3N_4 grains, which can have elongated shapes and the glassy phase located in the inter-granular spaces (such information can be obtained from X-ray diffraction analysis). The prismatic β-Si_3N_4 grains with various lengths and aspect ratios are randomly oriented and located within the microstructure. Whereas, the glassy phase is formed from the sintering additives; it usually consists of silicon dioxide enriched by other sintering additives like yttrium oxide, alumina, etc. Additionally, residual porosity is also present in the microstructure.

As previously mentioned, the 2D microstructural parameters are not suitable for realistic 3D numerical modelling of such complicated microstructure. Therefore, 3D microstructure reconstruction was needed; hence, 3D EBSD was selected for this task. No relevant literature data was available and therefore the methodology used for metals was adjusted for silicon nitride. It was necessary to solve plentiful obstacles starting with the non-conductive nature of silicon nitride, its high hardness compared to metals, and its dual-phase microstructure. The combination of 2D EBSD mapping and focussed ion beam (FIB) slicing of specially prepared thin sample was employed. The whole procedure was automated thanks to the support of both Tescan and Oxford Instruments companies. Finally, the obtained 2D EBSD data of individual consequent slices were combined to create a 3D form using both commercial (HKL Viewer) and open source (Dream 3D) software packages. The commercial one was found more intuitive, whereas the open-source option more adjustable, however, both provided suitable results for numerical simulations, see Fig. 2.

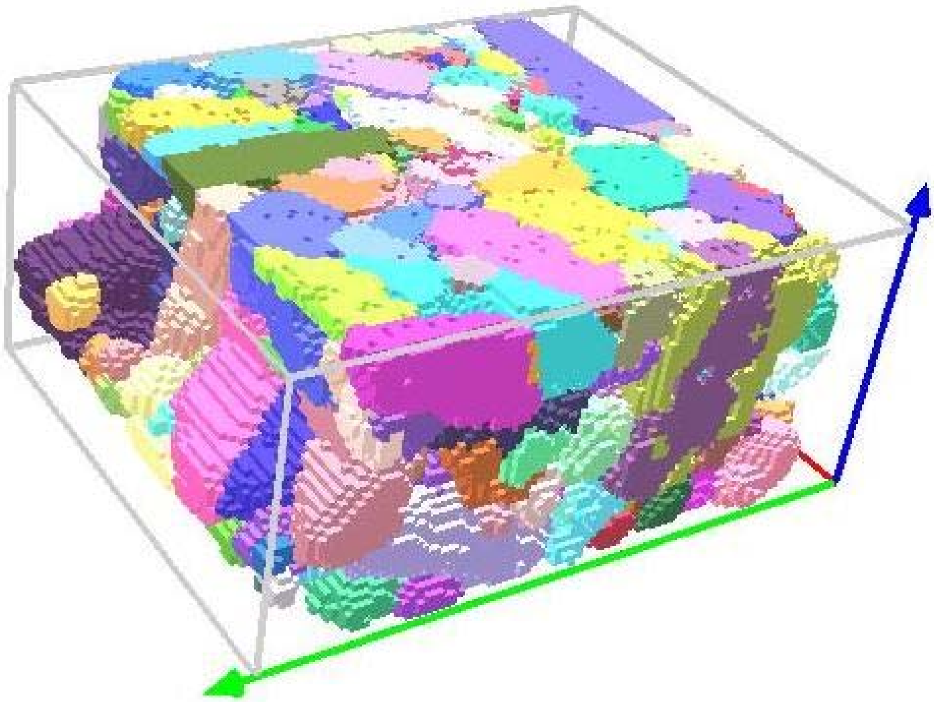


Fig. 2. An example of the 3D reconstruction of the microstructure from the stacked 2D EBSD data for silicon nitride

Microstructural 3D modelling

The microstructure reconstruction employing the 3D EBSD data gathered by application of newly developed procedure at IPM were used for creation of realistic model of the microstructure further used for numerical calculation of both elastic, thermal and fracture behaviour.

The modelling of silicon nitride microstructure is an important field of research. An important classical approach, adopted to carry out microstructure modelling, is the use of a unit cell that is assumed to represent the geometrical and material information of the considered bulk material. Assuming statistical representative microstructure, the unit cell is often called a representative volume element (RVE). The best way for creating such a unit cell is the direct usage of experimental data. In case of silicon nitride, tomographic observations cannot be used due to the extremely challenging preparation techniques. Consequently, a different approach is considered. In a first approach, a simplified algorithm for the generation of virtual periodic three dimensional silicon nitride-like structures has been introduced. Its primal result is the creation of microstructural models for micromechanical finite element simulations. The microstructure generator is based on a sequential adsorption procedure, which is enriched with growth of particles, steric hindrance and overlapping and preserves high aspect ratios and grain volume fractions. In order to give an insight into the behaviour of the model, the pseudo-time evolution of mean aspect ratio and grain volume fraction have been discussed for different parameter sets of a periodic ensemble of 1050 grains, which have been adsorbed in approximately 100 steps. It has been shown that the mean aspect ratio in generated microstructures decreases after a temporary peak at approximately 20% grain volume fraction due to steric hindrance. Realistic grain volume fractions have been adjusted by variation of the grain overlapping. The adjusted ensembles have been considered with respect to the probability density of the aspect ratio and grain length. A clear redistribution of the densities to longer grains and with higher aspect ratios was caused by increased grain growth anisotropy. The significance of the model has been shown by a comparison of the grain length and the aspect ratio distribution with literature values showing reasonable correspondence. Hereby, a general accordance of the stereological SEM image evaluation with the data provided by the structure generator was observed. Aside from these issues, the microstructure generator reproduced the main features of a real silicon nitride microstructure, which has been shown by a comparison of a SEM micrograph of SL 200 BG and a synthetic microstructure. Based on the aforementioned results, it can be concluded that the algorithmic structural model can, in general, be applied for generating silicon nitride microstructures to be used in computational micromechanics. The model appears as a reasonable approximation for the complex geometry of the silicon nitride microstructure.

A second approach consists in the employment of 3D electron backscatter diffraction technique (EBSD) measurement followed by reconstruction of silicon nitride microstructure as a geometrical input for finite element simulations. The electron backscatter diffraction technique allows direct examination of the individual grains, grain boundaries and grain orientations. It has been used by a large number of researchers for the microstructural representation of polycrystalline materials. In this work, 3D EBSD data has been provided by the subproject WP6. A first three dimensional voxel-based finite element mesh of silicon nitride microstructure has been generated using a self-written regular mesh generator. One set of EBSD measurement provide the data about the spatial distribution and the orientations of phases as a voxel array. The microstructure has been meshed with linear hexahedral elements which were attributed to the glassy phase and the 48 grains according to the array input data. The non-uniformity of the crystallographic orientation is negligible within one single grain of the microstructure. Accordingly, each element of the grain, representing a voxel, was assigned the average crystallographic orientation of the concerned grain. A second finite element mesh has been used within the micromechanical approach. For that a second set of EBSD reconstructed slices is used as input data for the commercial microstructure generator and meshing tool

ScanIP. The microstructure has been meshed with linear tetrahedral elements, distributed over the amorphous phase and the grains. Numerical convergence has been tested for different mesh sizes.

Among the tasks accomplished within work are the determination of the effective thermoelastic properties and the statistical characterization of stress fluctuations in silicon nitride local phases. For that purpose, a full field finite element solution has been considered. The two meshes, generated by making use of 3D Electron Backscatter Diffraction (EBSD) data of silicon nitride, has been used for the full-field computations. A second-order mean field homogenization scheme, consisting in Hashin-Shtrikman bounds, has been also considered additionally. Ab-initio simulations have been performed in order to determine the temperature dependent elastic properties of the local phases. It was observed that the anisotropy ratio is approximately equal to one, which implies that silicon nitride microstructure is isotropic. This finding has been confirmed by the crystallographic analysis of observed grains during 3D EBSD measurement. According to the pole figure constructed for the c-plane, no evident grain orientation anisotropy was present in the material under investigation. The analysis of the temperature variation between 20 °C and 950 °C of the effective Young modulus of silicon nitride, showed that experimental data and prediction by finite element method (FEM) of the latter effective property are in a very good agreement and they are bounded between Hashin-Shtrikman lower and upper bounds,. As for the effective shear modulus, the experimental data were very close to HS+. Prediction by FEM was in accordance with experimental results and lies between the bounds. In addition to the determination of the temperature-dependent effective properties, the analysis of stress fluctuations under mechanical loading, shows that the amorphous phase is the most vulnerable to fracture. The analysis of thermal residual stresses, after cooling from 950 °C down to 20 °C, has shown that the amorphous phase is subjected to tensile stresses. This phase is the most vulnerable to micro-cracks initiation due to high stress concentrations. It was shown also that the residual stress fluctuations in this phase are anisotropic. The analysis of thermal residual stresses showed also that β-Si_3N_4 grains are subjected to compressive residual stresses. These stresses are heterogeneous from one grain to another with high stress discontinuities concentrated around grain boundaries. The analysis shows an isotropic stress fluctuation within these grains. Small grains are subjected to higher residual stress fluctuation, compared with large grains.

The structural use of silicon nitride ceramics is restrained because of the limitation of its reliability and the occurrence of damage phenomenon under severe working conditions. In the research project, the weakest link model has been extended to account, not only for the volume defects, but simultaneously for the damage across the interface between silicon nitride phases. The model brings a significant improvement over the classical weakest link approach. It is based on a multivariate approach and is used in conjunction with the second-order estimates of the local fields. The second-order moment and covariance of the local fields have been formulated and computed numerically, based on a finite difference two point formula. The required effective properties have been computed based on Hashin-Shtrikman bounds. The failure probability of silicon nitride has been computed by integration of the local stress and traction fields over the

phase volumes and interfaces. An exhaustive parametric study has been carried out, for the cases of shear and uniaxial tension loadings, on the basis of the variation of four non-dimensional parameters and the definition of two error measures. The minimization of the two error measures allowed the determination of the range of the appropriate parameters. A parameter study has shown that the failure in silicon nitride is always controlled by the phase which constitutes the weakest microstructural element. In fact, it was shown that Weibull scale parameter of silicon nitride fits with the smallest among Weibull microscopic scale parameters of the phases and accordingly Weibull shape parameter. Hence, by comparing Weibull scale parameters estimated by the parametric study, it comes out that the failure probability of silicon nitrite is controlled by the failure probability of β-Si_3N_4 grains which constitute the weakest microstructural element.
A micro-scale fracture as well as a macro-scale damage models for silicon nitride has been proposed. The micro-scale model accounts for both transgranular and inter-granular fracture modes. Maximum principle stress theory has been used as failure criteria for the transgranular fracture mode. Anisotropic and isotropic fracture models have been suggested for both β-Si_3N_4 grains and the amorphous phase, respectively. A cohesive zone model has been used for the modelling of the inter-granular fracture. The model is based on the extension of Coulomb friction law, combined with a dissipation approach The fracture strength of the local phases and the cohesive strength of the interface has been determined by means of ab initio simulations. 3D EBSD measurement followed by the reconstruction of silicon nitride microstructure has been used as input for the finite element simulations. An analysis of crack patterning has been carried out. The analysis of inter-granular crack paths shows the dominance of interface fracture around glassy pockets, the transgranular fracture pattern has been also investigated. It showed that the fracture usually initiates along grain boundaries then it propagates inside the grain with sharp and straight shape. The influence of a defect (e.g., microscopic pore) on the fracture pattern has been analysed. It has been shown that the inter-granular fracture usually initiates within the micro-pore, and then it propagates along grain boundaries. It has been shown also that this mode of fracture initiation and propagation is similar for single and multiple micro-pores and is independent from the porosity of the material. In addition to fracture patterning analysis, the influence of fracture modes on stress fluctuation has been also carried out. The study shows the significant effect of transgranular fracture on increase of stress heterogeneity. In addition to the microscale fracture model for silicon nitride, a microscale damage model has been also proposed. Two phenomenological damage models concerning monotonous and cyclic loading have been implemented as a UMAT in Abaqus. To account for the effect of a direction change of the principal stresses the monotonous model has been generalized in terms of non-constant eigenprojections. In addition, crack closure mechanisms have been incorporated.
The cyclic damage model is based on a micromechanical slow crack growth law for non-interacting cracks. Using this power law as an evolution equation for the damage, a dissipation potential can be formulated in the sense of a generalized standard material. Derivations of this potential yield the evolution equations for

the compliance and the internal variable describing the amount of damage. A numerical implementation scheme based on the implicit Euler time integration has been used. The issues related to numerical problems resulting of using non-smooth functions as the maximum stress damage criterion and the crack closure formulation which essentially is a step function have been addressed. Moreover, stability of the Newton-scheme with respect to the initial values has been improved by using a homotopy scheme. Furthermore, to decrease the computation time for the cyclic damage model a cycle-jump approach has been implemented.

Both models have been identified based on data of the micromechanical simulations or data available from experiments. Whereas the Young's modulus and the Poisson's ratio predicted by the micromechanical model are in good accordance with values which can be found in literature, the tensile strength overestimates the crack energy.

Model problems have been examined which show the typical behaviour of a brittle material. The cyclic damage model has been validated by a four-point bending test. The result in regard of the cycles until failure is in accordance with the available experiment.

Crack propagation description

The knowledge of the fracture behaviour is critical in the case of structural ceramic materials. Silicon nitride is an excellent material from the point of view of its self-reinforcing ability trough the presence of elongated grains in the microstructure. This ability ensures that present cracks or those that have just nucleated under mechanical or thermal loading will grow stably without catastrophic consequences. The fracture behaviour on the microstructural (grain size) level was observed using analysis of indentation cracks using Vickers indenter. The crack behaviour and crack path development was observed from the two main views. The first one was related to the construction of a dependence of the crack opening displacement (COD) on the current crack length. This dependence characterises the increasing resistance against crack propagation and can be used for validation of developed FEM models. The material developed for rolling elements exhibits the best results followed by the reference material employed in hybrid-bearing balls. All obtained results show that the significant rise of the so called J-Δa curve is acting at the maximum crack length in the range of 100 μm. The second approach focused on the observation of the micro-fracture features and behaviour of the crack in the vicinity of grains, grain boundaries, triple points, pores and snowflakes. Two main fracture mechanisms: the grain de-bonding and grain fracture were identified. This observation was complemented with the finding that each material exhibited different amount of de-bounded and fractured grains, which allowed the development of new damage models described further in detail.

Crack growth modelling

Crack growth modelling achieved great success and progress during the last decade. Finite element and boundary element methods where used in material research for quite a long time. These methods have been modified, e.g., parallel approach implementation. Of great importance is the finite element method with procedures based on the fracture mechanics approach derived basically from knowledge of global parameters such as the stress intensity factor and J integral.

Based on FEM and microstructural analysis, the crack growth model describing crack behaviour in the initial stage has been developed. As the microstructural analysis showed, the bridging mechanisms have been detected in the beginning stage of crack growing. Mechanisms like crack bridging can provide substantial increase in toughness coupled with strength in silicon nitride ceramics. Thus, cohesive (bridging) law was incorporated into the standard finite element package Abaqus using a user subroutine and the test of crack nucleation and crack propagation for various conditions was accomplished.

As an example of the special element responding to damage and crack growth are the “cohesive elements”; they are similar to contact elements and are based on the vanishing elements and new surface creation. The phenomenological description characterizing material behaviour is realized using the traction-separation law, and consequently the local damage can be predicted. Many models published within last years can be found in literature for laminates, composites, long fibre composites etc. The area below the traction-separation curve whether for tangential or for normal direction gives us the energy dissipated by the cohesive element. A schematic diagram for the bridging law can be seen in Fig. 3.

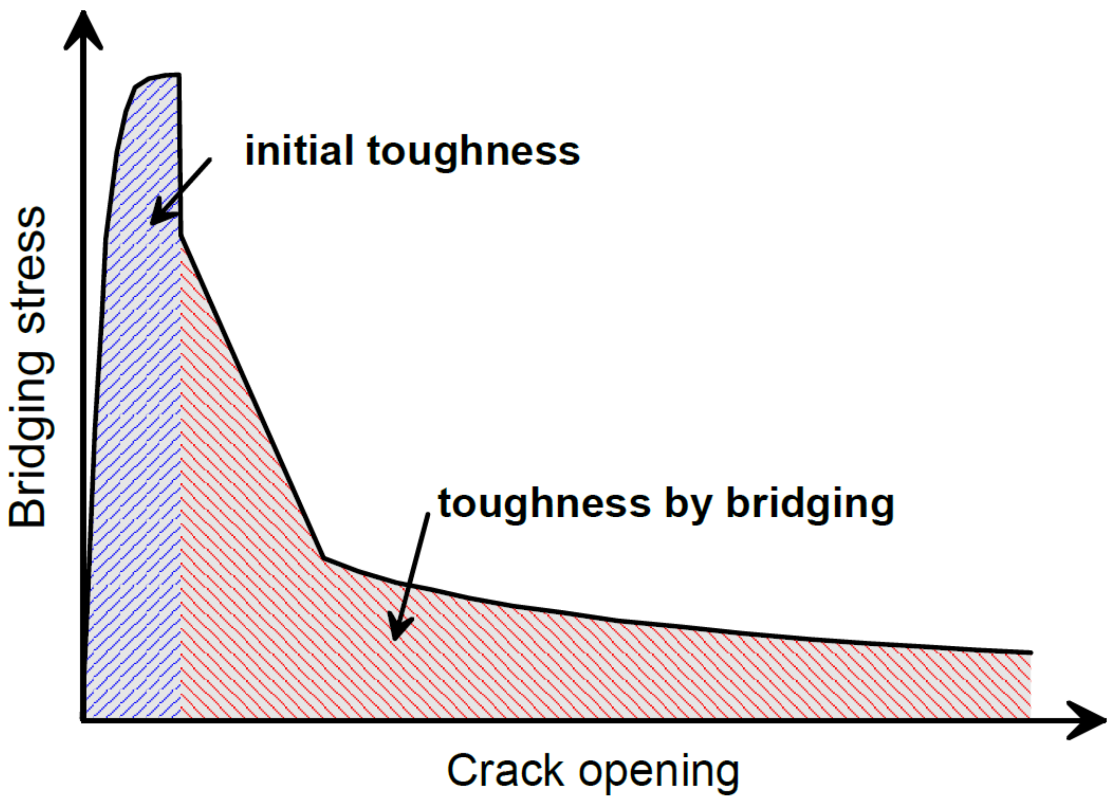


Fig. 3. Shape of the bridging law

The input parameters of the traction separation law describe the shape, which can be optimized for a given material based on the fracture behaviour; however, they are not easy to be measured. It is possible to obtain them using optimization procedures, which reflect the measured COD versus σ_a curve (described earlier). As a comparable method the standard XFEM procedure implemented in the FEM package Abaqus has been selected. This procedure works only with the simple linear (with or without softening) traction-separation law. The formulae and laws that govern the behaviour of the XFEM cohesive segments for crack propagation are very similar to those used for cohesive elements with traction separation law. The similarities extend to the linear elastic traction separation model, damage initiation criteria and similar damage evaluation law.

Based on the numerical simulations results and after a necessary parameter optimisation procedure it was possible to compare both methods for crack propagation prediction and come to the following conclusions:

(1) Saturation in the *J–R* curve was reached for XFEM modelling substantially later than for the cohesive zone approach (usually when the crack length was greater than 20 µm). This observation is predicable because the XFEM model does not incorporate the bridging mechanism into the cohesive law.

(2) The expected behaviour of the *J–R* curve based on literature data should be a bit different and the saturation was expected for the smaller crack lengths, roughly about 10 µm. The discrepancy comparing literature with our results can be seen in the different microstructure and/or due to numerical oscillation, which can lead to the underestimation of *K* values.

(3) The optimised parameters for traction-separation (bridging) law enables *J–R* prediction, for precise prediction seems to be essential to determine at least the maximum stress σ_0 experimentally. It is important to guess the scale where the bridging mechanisms are active.

The results can explain the fracture behaviour in the initial stage of the crack growth of silicon nitride ceramics with respect to microstructural parameters such as the grain size, grain orientation and presence of glassy phase; they can provide us with a method to optimize silicon nitride microstructure for high strength and fracture toughness and/or it allows the prediction of crack behaviour for various loading states based on the real application of the component.

Probabilistic damage model for the crack path prediction

The microstructural constitution of silicon nitride possesses the ability to enhance fracture properties by changing the grain shape parameters and change the glassy phase composition. The composition of the glassy phase plays significant role in the grain formation. Usually, the elongated beta silicon nitride grains homogeneously distributed within the microstructure formed from equiaxed grains create significant obstacle for the propagating crack. The fracture mechanisms identified during detailed fracture patterns observation act competitively based on the number of factors. The obstacle in the modelling based on physical principles of the crack behaviour is the determination of material parameters as the grain de-cohesion energy dependence on the glassy phase or single-crystal strength as well as rather complicated local stress state around the crack tip. The suggested approach tries to eliminate outlined difficulties by simplification of necessary independent variables with addition of probabilistic approach necessary for realistic results. An extensive evaluation of the microstructural parameters performed during the crack behaviour observations pinpointed the important characteristics allowing prediction of the crack propagation with the given probability. Proposed new model was tested using four silicon nitride materials under investigation. It was found that decision between both mechanisms is strongly dependent on the angle between the crack direction and the main axis of grain together with the grain length distance from the crack tip and the grain thickness. Additionally, the existence of a critical angle was proved; if it is exceeded, no grain fracture occurs and only the grain de-bonding can take place. The statistical description was implemented and Weibull distribution was identified as suitable for sufficient description of probability assigned to the individual fracture mechanisms. The grain de-bonding is well described by a two-parameter Weibull distribution function and the grain fracture by the three-parameter function. The proposed damage model can be easily constructed for newly developed materials with a minimal experimental effort and utilised in the crack propagation modelling on the microstructural level.

Macroscopic wear in silicon nitride

Studying wear in ceramic materials has gained importance due to their potentially wide application spectrum, especially under severe tribological loading. Here, a distinction is made in the wear behaviour of ceramics undergoing rolling-contact and sliding contact. The former is observed in applications such as roller bearing, in which mechanical stresses are extremely high due to the non-conforming nature of contact. Sliding friction, on the other hand, can be observed in applications such as sliding bearings and cutting tools. Two different regimes can be distinguished in sliding friction, the first of which is gross sliding, which includes large relative displacements and the second is micro-slip or micro-sliding, which can be observed in most contact conditions, especially conforming contacts that include plastic deformation, example of which is metalforming processes such as wire rolling.

In RoliCer, finite element based simulations of wear were constructed and carried out using ABAQUS/Standard. The two distinct cases mentioned above were modelled.

In the case of rolling-sliding contact (with a very high slip ratio exceeding 0.2 to accelerate wear), the simulations were able to accurately predict the wear profile after short running periods (e.g., up to 3-hour running time tests); in this case, an discrepancy between the simulation results and the experimental results mainly stems from the mesh density, so that the finer the mesh the closer the results will become. For longer periods of time (as shown in a 10-hour tests), the wear profile obtained from the simulations clearly deviates from the experimental one in terms of its shape, although the wear volume predicted by the simulation corresponds to the adopted wear coefficient. In such accelerated simulations, this can be explained by the considerable change in the geometry of counter surface, leading to changes in the contact configuration. In these simulations, the wear in the counter surface was assumed to be negligible.

The important aspect of these simulations is to show how contact stresses are affected by the geometrical changes due to progressive wear, see Fig. 4.

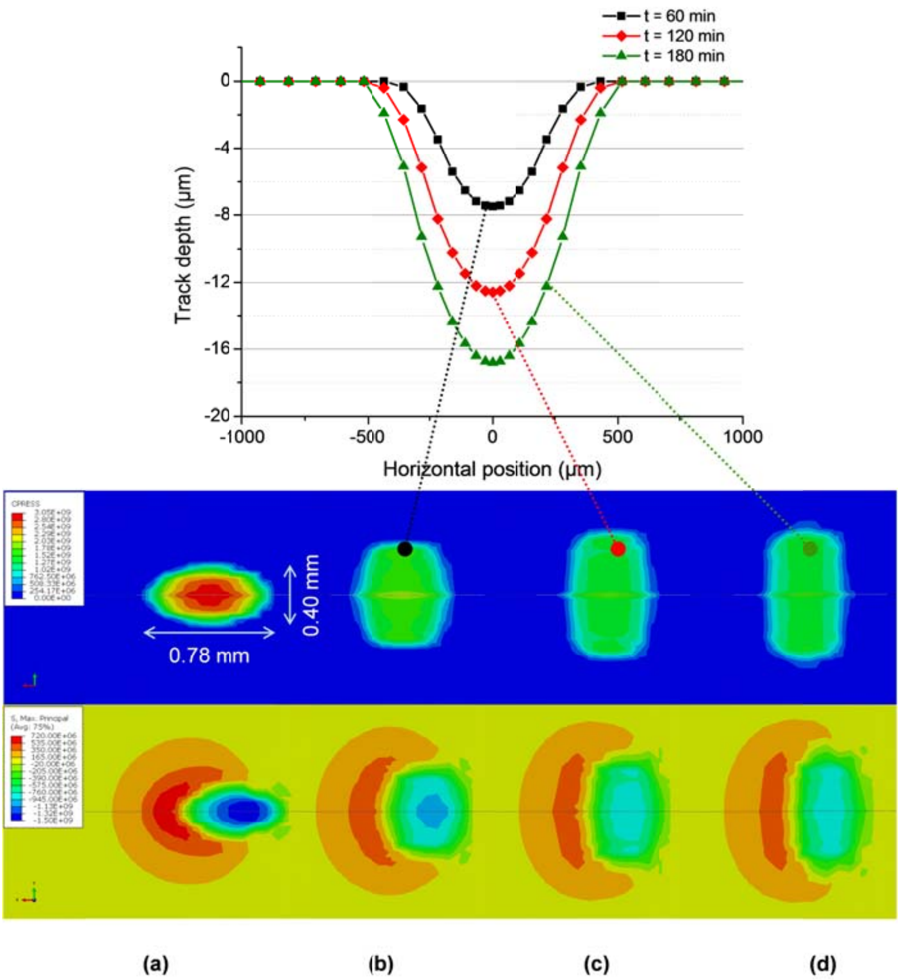


Fig. 4. FEM results showing (a) unworn configuration, p_{max}=3.1 GPa, peak of S_{max}=720 MPa; (b) after 60 min, p_{max}=2.1GPa, peak of S_{max}=680MPa; (c) after 120 min, p_{max}=1.8GPa, peak of S_{max}=540 MPa; (d) after 180 min, p_{max}=1.6GPa, peak of S_{max}=470 MPa

Sliding contact was modelled using a coupled thermal-mechanical two-dimensional plane-strain finite element simulation in ABAQUS/Standard. The ceramic sample was moved along the metal substrate after initiating contact between both objects with prescribed contact velocities Dry sliding contact causes a rise in the contact temperature. Contact temperature may reach values that are high enough to change the mechanical and chemical properties of the materials. While changes in the mechanical properties were considered in the mechanical model, the chemical behaviour of the contact partners may be very difficult, if not impossible to consider. Therefore, wear was modelled using two different approaches; the first is to calculate to volume loss as a function of the contact pressure, which in turn is dependent on the contact temperature. The second approach is to calculate wear based on a thermo-mechanical wear model, which was first proposed by Trigger and Chao[2] and later applied by Usui et al.[3].

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[2] Trigger, K. J. and Chao, B. T., "The Mechanism of Crater Wear of Cemented Carbide Tools" TRANS ASME, Vol. 78, No. 5 (1956) 1119-1126.
[3] E. Usui, T. Shirakashi, T. Kitagawa, Analytical Prediction of Three Dimensional Cut-ting Process, Transactions of the ASME 100 (1978) 236-243.

Lifetime evaluation of ceramic components

One of the goals in the project was the development of a convenient method for the lifetime evaluation of components (or specimens) under contact loading conditions. Such loading situations occur for example when metal wires are rolled with ceramic tools, in hybrid bearings or in specific wear tests like in rolling contact fatigue testing. It is known that fatigue growth of incipient cracks that popped-in during loading is the dominating mechanism, which will eventually lead to failure of the component. In principle, it is possible to evaluate fatigue crack growth by means of FE analysis if a crack growth law has been incorporated. For complicated components and cyclic loading condition this may require huge 3D-FE models and unrealistic computational time. A much faster approach was developed within the project. It is based on the pre-knowledge of the following information:

(1) The approximate location of incipient cracks and their growth path. This knowledge can be gained from model experiments or by obtaining stress fields combined with experimental evidence
(2) The crack growth law (Paris law) for the material. Such a law can be obtained experimentally for relevant environmental (humidity, temperature, etc.) conditions. It relates the crack growth velocity (or: amount of crack growth per loading cycle) of a crack to the stress acting on the crack (characterized by the stress intensity factor, SIF)
(3) The stress distribution in the un-cracked component, specifically the section stresses at the location of the cracks. It can be obtained from the FEM analysis used during the design procedure. In certain cases, a refinement of the used mesh at these locations (see (1)) may be necessary

The problem under consideration addresses cyclic loading and considerable crack growth (i.e., many calculation increments) the analysis of crack growth using this approach requires the evaluation of the stress intensity factor (SIF) for many combinations of crack length and stress, i.e., several millions of times. Therefore, the weight function method was used to calculate the SIFs. This approximate approach allows the evaluation of SIFs for specified cracks loaded by an arbitrary stress profile normal to the crack faces by an analytical or numerical integration. A standalone program suitable for the calculation of SIFs for various crack geometries and stress gradients was established (SIF tool). An additional speed-up of the calculation was achieved by implementing a routine that adjusts the input crack lengths for which a calculation is performed: a large spacing of evaluation points is chosen if no or only very little crack growth takes place, while successively smaller increments are evaluated as the crack growth rate increases. As a result, a single plot is delivered which allows reading the length of starting cracks with different sizes as a function of load cycles.

The development of the calculation procedure was accompanied by several experimental investigations. A multitude of experiments was conducted to determine the relevant material properties which were needed for the FEM stress evaluation and the lifetime analysis, e.g. Young's modulus, thermo-elastic properties, strength, fracture toughness. The cyclic crack growth behaviour of two silicon nitride grades was investigated under various loading conditions (swelling and alternating loads) and environments in order to deliver the crack growth laws. It turned out that for a given maximum stress, cracks grow several orders of magnitude faster under alternating load than under swelling load, see Fig. 5.

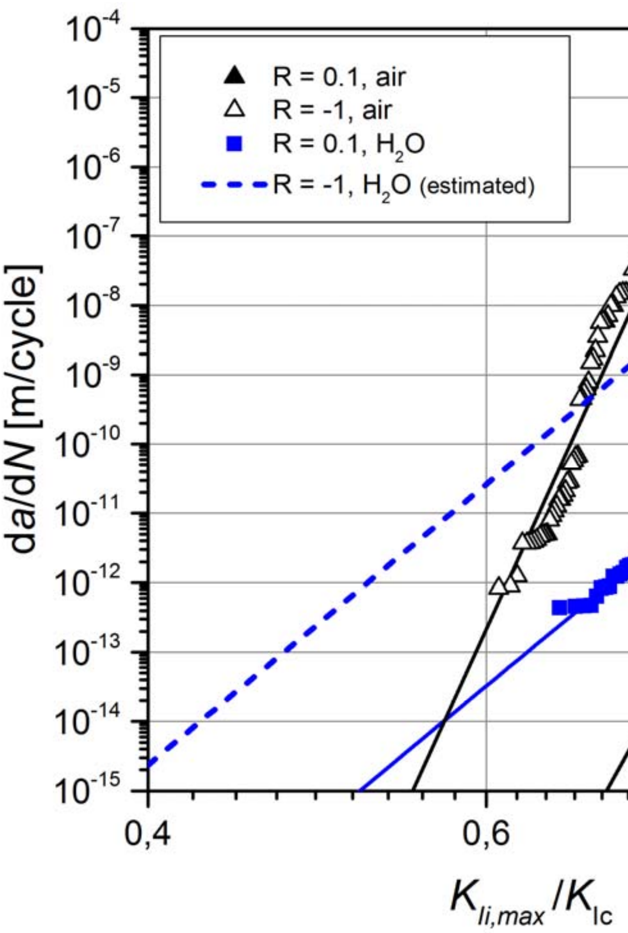

Fig. 5. Cyclic fatigue behaviour of one of a model silicon nitride material tested under two loading ratios (R = 0.1 and R = -1) and two different environmental conditions

A fractographic analysis allowed investigation of microstructural mechanisms that are responsible for the fatigue crack growth. Material features were identified that act as nucleation sites for fracture or contact damage. Additionally, demonstrators were examined to deliver the necessary information on damage and incipient cracks that appears during service. Static contact fracture experiments using very simple loading configurations were conducted to verify the SIF calculation method. For a fast evaluation of these experiments, a visualization tool for contact stresses was programmed.

Finally, the lifetime evaluation method was applied to two cases for which the necessary background (stress calculations and experimental) was delivered in the project: (1) one of the targeted model experiments and (2) the wire rolling field test.

(1) A twin-disc test set-up was used for the investigations of the rolling contact fatigue behaviour. During the experiments it turned out that cracks appear in the contact zone if the normal load was increased above a certain level. A considerable extension of these cracks normal to the surface into the material was detected. For this experimental set-up a crack growth analysis was performed.

Since the FEM stress calculations are less time consuming for this configuration (as compared to the design of the wire rolling set-up) a study was performed to elaborate the requirements for a suitable FE mesh. It could be shown, that considerable growth of these cracks is only possible above certain loads and if the cracks appear in a distinct region about the contact patch: it is not only the tensile stresses at the surface which are important but mainly the load history: regions with alternating tension-compression loading are much more endangered than regions experiencing only tensile loads, cp. Fig. 6. This is a direct consequence of the different crack growth laws.

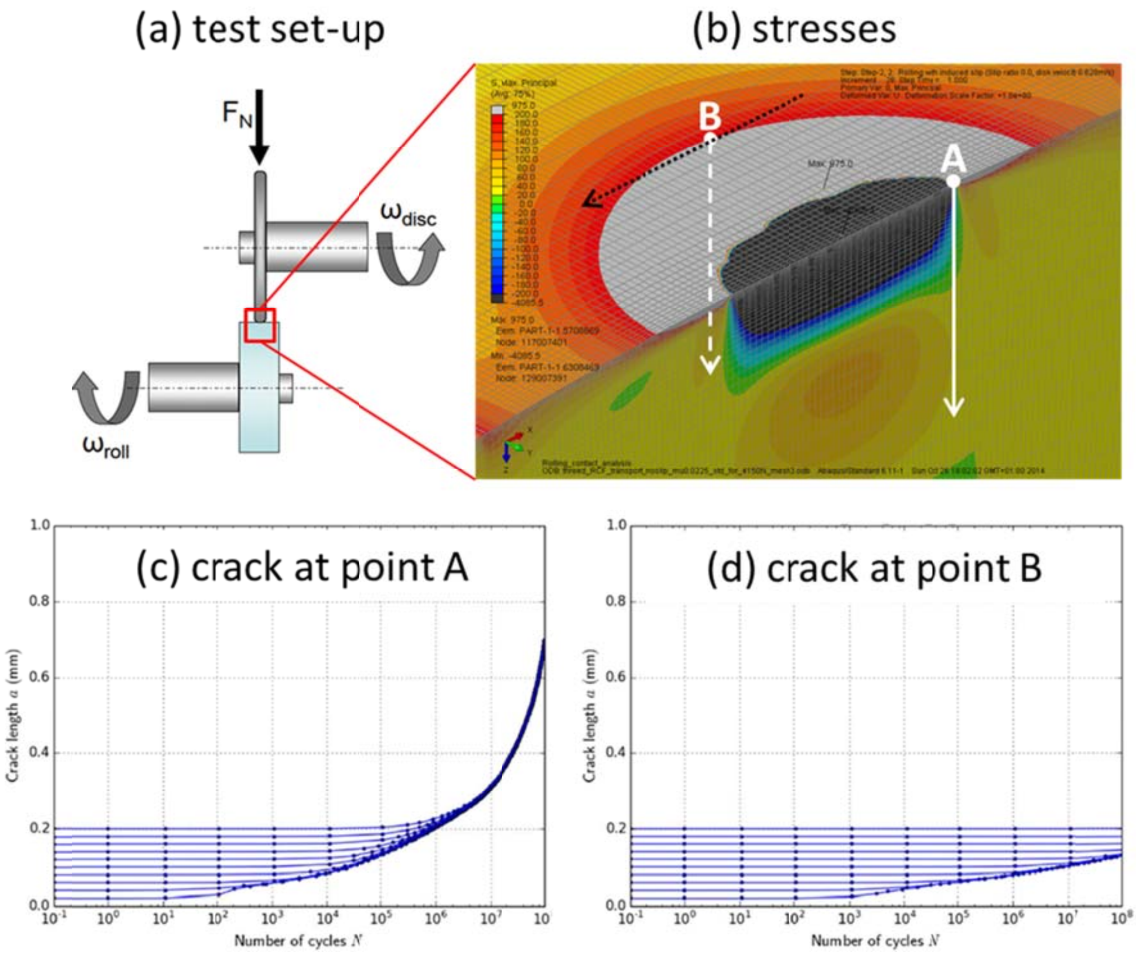

Fig. 6. Crack growth in twin-disc rolling contact fatigue experiments. (a) Schematic of the test set-up. (b) Maximum principal stress distribution near the contact zone. Two possible crack paths A and B are marked by white lines. The load history during rotation for each path can be evaluated by moving the path through the model along the direction indicated by the black dashed arrow. (c) and (d) Crack length as functions of the number of load cycles for edge cracks of different starting length at positions A and B. At Point A all cracks grow. At point B only small cracks grow but will stop once they reach a length of approx. 150 µm

(2) A similar analysis was made for the demonstrator rolls which were used for the industrial field tests. For the rolls, a full 3D-FEM stress calculation of the rolling process was performed comprising several time steps. Two crack paths were investigated on which different loading conditions prevail: cracks on one path experience alternating as well as swelling loads, while cracks on the other one see only swelling load. In this case too, the calculations revealed that cracks on the “alternating load path”

are much more dangerous. But, since the stresses in the chosen optimized design of the roll are generally low, it can be expected that even cracks with a depth of up to 400µm may not lead to fatigue failure of the rolls.

Industrial testing

The main reasons for considering ceramic based monolithic and/or composite materials in the production of metal forming tools and machine components is their drastic wear and contact fatigue resistance. This enables producing components with enhanced reliability, prolonged lifetimes and superior performance. In metal forming this also results in fabricating high quality end-products with supreme surface finish and highly tight dimensional tolerances.

In the prototype testing and demonstration of functionality phase of the project, a test under industrial conditions was conducted. A pair of ceramic rings was implemented in stand DB03 of the finishing block. The lifetime of previously tested ceramic rings was limited due to damage caused by thermal stress, in addition to using an inadequate rolling unit. Moreover, deep surface cracks appeared in the rolling groove when rolling nickel based alloys causing complete failure of the rolls after rolling a maximum of 3 wire rod coils.

In order to accomplish a successful installation of the rings, the rolling unit in the roll stand was completely re-designed. The outcomes of numerical simulations indicated certain aspects of the proposed design that had to be reconsidered in order to reduce the stresses on the rolling unit and to accomplish a clamping configuration that ensure prolonged lifetimes of the ceramic components (i.e., ceramic-friendly design). The major advantage of the redesigned rolling unit is to induce compressive stresses on the sides of the ceramic rolls.

1.1.4. Potential impact

Apart from the important research findings reached in RoliCer, the project resulted in developing two silicon nitride ceramic grades to satisfy the requirements of two completely different sets of loading regimes; by itself this is considered as a commercial advancement within the portfolio of a European ceramic manufacturer. The industrial testing of silicon nitride rolls in hot wire-rolling of superalloys confirmed that ceramics are a promising class of materials for metalworking applications. Further improvements and industrial tests succeeding the project have been committed by the project partners.

The work conducted by the RoliCer team is on track to be translated for application in industrial and technical settings. The outcomes of RoliCer will help to broaden the range of technical applications significantly, because there will be opportunities for fast and efficient design of robust high performance systems using ceramic components. In addition to providing new insights into ceramics, the RoliCer project has also provoked new questions that will guide future research.

From the dissemination activities within RoliCer, many students and young researchers within the European Union have had the opportunity to get into contact with professionals within the field of engineering and materials science through the organization of several workshops and many seminars and through participation in numerous conferences, including having a RoliCer-Symposium within the proceedings of the fourth MSE "Materials Science and Engineering" Congress, which took place between the 23rd and the 25th of September 2014 in Darmstadt, Germany. Additionally, the involvement of many young researchers within the R&D activities throughout the project has helped them to broaden their horizon and deepen their knowledge within their respective fields. In addition to several small research topics and master theses, six PhD candidates were involved in the project. As regards the consortium of RoliCer, the project has enhanced and strengthened the networking, share of knowledge and know-how amongst professionals within the European Union and amongst research institutes, higher education establishments and companies.

RoliCer: Enhanced reliability and lifetime of ceramic components through multi-scale modelling of degradation and damage

RoliCer is an EU-project (ID: 263476) funded by the 7th Framework Programme under the call "Nanosciences, Nanotechnologies, Materials and new Production Technologies NMP”. RoLiCer is a collaborative research project with a total budget of 3.2 million € running from Dec. 1st 2011 until Dec. 1st 2014.
http://www.rolicer.eu/

1.2. Use and dissemination of foreground

Section A (public)

TEMPLATE A1: LIST OF SCIENTIFIC (PEER REVIEWED) PUBLICATIONS, STARTING WITH THE MOST IMPORTANT ONES										
NO.	Title	Main author	Title of the periodical or the series	Number, date or frequency	Publisher	Place of publication	Year of publication	Relevant pages	Permanent identifiers[4] (if available)	Is/Will open access[5] provided to this publication?
1	A study on the wear of silicon nitride in rolling-sliding contact	I. Khader, D. Kürten, A. Kailer	Wear	296 [1-2]	Elsevier B.V.		2012	pp. 630-637	http://dx.doi.org/10.1016/j.wear.2012.08.010	no
2	Structure and fracture property relation for silicon nitride on the microscale	J. Wippler, T. Böhlke	Computational Materials Science	64	Elsevier B.V.		2012	pp. 234-238	http://dx.doi.org/10.1016/j.commatsci.2012.02.042	no
3	A Two-Scale Weakest Link Model for Silicon Nitride	T. Böhlke, Y. Othmani	Computational Materials Science	80	Elsevier B.V.		2013	pp. 43-50	http://dx.doi.org/10.1016/j.commatsci.2013.04.018	no
4	A micromechanically motivated finite element approach to the fracture toughness of silicon nitride	J. Wippler, T. Fett, T. Böhlke, M.J. Hoffmann	Journal of the European Ceramic Society	33 [10]	Elsevier B.V.		2013	pp. 1729-2736	http://dx.doi.org/10.1016/j.jeurceramsoc.2013.01.013	no
5	Zyklische Ermüdung technischer Keramiken in wässrigen Medien	C. von der Wehd, T. Lube, I. Khader, A. Kailer, U. Degenhardt, K. Berroth	Fortschritte in der Werkstoffprüfung für Forschung und Praxis		Verlag Stahleisen GmbH	Düsseldorf	2013	pp. 379-384		no
6	Crack growth modelling in the silicon nitride ceramics by application of the cohesive approach	V. Kozák, Z. Chlup	Material Structure & Micromechanics of Fracture	7	Trans Tech Publications Inc.	Durnten-Zurich	2014	pp. 193-196		no

[4] A permanent identifier should be a persistent link to the published version full text if open access or abstract if article is pay per view) or to the final manuscript accepted for publication (link to article in repository).

[5] Open Access is defined as free of charge access for anyone via Internet. Please answer "yes" if the open access to the publication is already established and also if the embargo period for open access is not yet over but you intend to establish open access afterwards.

7	Ermüdungsbruch in Siliziumnitrid", 14. Internationale Metallographie-Tagung 2014, Leoben, Austria, 17. bis 19. September 2014	T. Lube, I. Khader, A. Kailer, U. Degenhardt, K. Berroth	Fortschritte in der Metallographie	46	Inventum GmbH	Bonn	2014	pp. 353-358		no

TEMPLATE A2: LIST OF DISSEMINATION ACTIVITIES								
NO.	Type of activities[6]	Main leader	Title	Date/Period	Place	Type of audience[7]	Size of audience	Countries addressed
1	Conference Presentation	A. Kailer	IUVSTA-ASEVA Workshop WS-66: "Friction under controlled environments"	9 -12 July, 2012	Avíla, Spain	Scientific community		International
2	Conference Presentation	V. Kozák, Z. Chlup	Material Structure & Micromechanics of Fracture – MSMF	1-3 July, 2013	Brno, Czech Republic	Scientific community		International
3	Conference Presentation	I. Khader, D. Kürten, A. Kailer	World Tribology Congress 2013	September 8 – 13, 2013	Torino, Italy	Scientific community		International
4	Conference Presentation	T. Lube, I. Khader, A. Kailer, U. Degenhardt, K. Berroth, K.-H. Lang, C. Wörner	Fractography of Advanced Ceramics IV, FAC2013	Sept. 29th – Oct.2nd, 2013	Slovak Republic	Scientific community		International
5	Conference Presentation	J. Ruck, Y. Othmani, T. Böhlke, I. Khader, A. Kailer	GAMM2014	10th -14th March 2014	Erlangen, Germany	Scientific community		International
6	Conference Presentation	T. Böhlke, V. Müller, Y. Othmani, F. Rieger	International Scientific Conference Advances in Micromechanics of Materials	8-11 July 2014	Rzeszów, Poland	Scientific community		International
7	Conference Presentation	S. Rasche, T. Lube	European Conference on Fracture - ECF 20	30th June - 4th July 2014	Trondheim, Norway	Scientific community		International
8	Conference Presentation	Z. Chlup, P. Tatarko, H. Hadraba, V. Kozák, I. Dlouhy	European Conference on Fracture - ECF 20	30th June - 4th July 2014	Trondheim, Norway	Scientific community		International
9	Conference Presentation	T. Lube, I. Khader, A. Kailer, U. Degenhardt, K. Berroth	14. Internationale Metallographie-Tagung 2014	17. bis 19. September 2014	Leoben, Austria	Scientific community		International
10	Conference Presentation	V. Kozák, Z. Chlup, P. Padělek	MSE 2014	23 - 25 September, 2014	Darmstadt, Germany	Scientific community		International
11	Conference Presentation	F. Colonna, A. Hashibon, C. Elsässer	MSE 2014	23 - 25 September, 2014	Darmstadt, Germany	Scientific community		International
12	Conference Presentation	I. Khader, A. Renz, A. Kailer, U. Degenhardt	MSE 2014	23 - 25 September, 2014	Darmstadt, Germany	Scientific community		International

[6] A drop down list allows choosing the dissemination activity: publications, conferences, workshops, web, press releases, flyers, articles published in the popular press, videos, media briefings, presentations, exhibitions, thesis, interviews, films, TV clips, posters, Other.

[7] A drop down list allows choosing the type of public: Scientific Community (higher education, Research), Industry, Civil Society, Policy makers, Medias, Other ('multiple choices' is possible).

13	Conference Presentation	R. Raga, I. Khader, A. Kailer, Z. Chlup	MSE 2014	23 - 25 September, 2014	Darmstadt, Germany	Scientific community		International
14	Conference Presentation	Y. Othmani, T.A. Langhoff, T. Böhlke, Z. Chlup, F. Colonna, A. Hashibon, I. Khader, A. Kailer, T. Lube	MSE 2014	23 - 25 September, 2014	Darmstadt, Germany	Scientific community		International
15	Conference Presentation	S. Rasche, T. Lube	MSE 2014	23 - 25 September, 2014	Darmstadt, Germany	Scientific community		International
16	Conference Presentation	T. Lube, S. Rasche, I. Khader, R. Raga, A. Kailer	MSE 2014	23 - 25 September, 2014	Darmstadt, Germany	Scientific community		International
17	Poster	C. von der Wehd, T. Lube, I. Khader, A. Kailer, U. Degenhardt, K. Berroth	Werkstoffprüfung 2013	28.- 29.11.2013	Neu-Ulm, Deutschland	Scientific community		International
18	Poster	T. Lube, S. Rasche, W. Harrer, P. Supancic	WerWasWo.Forschung@MUL2012	12. - 23.3.2012	Leoben, Austria	Scientific community, civil society, medias		International
19	e-Poster	S. Rasche, T. Lube	European Conference on Fracture - ECF 20	30th June - 4th July 2014	Trondheim, Norway	Scientific community		International
20	Conference Sesssion	IWM, MUL	Modelling Material Behaviour, Degradation and Reliability of Advanced Ceramics	September 23 - 25, 2014	Darmstadt, Germany	Scientific community	approx. 80	International
21	Workshop	MUL	Bruchmechanik spröder Werkstoffe	2. - 3.5.2013	Montanuniversität Leoben, Austria	Scientific community	32	Germany, Austria
22	Workshop	SKF	Bearing Reliability	12. - 13.2.2014	SKF, B.V. (Engineering and research centre-ERC), Nieuwegein, NL	Scientific community	32	Netherlands, Belgium, Sweden, Germany
23	Workshop	KIT	Multiscale Lifetime Modeling for Ceramics	September 29 - 30, 2014	Karlsruhe Institute of Technology	Scientific community	14	Germany, Austria
24	Workshop	IPM	Fracture in ceramic matrix composites	October 15th, 2014	Institute of Physics of Materials, Academy of Sciences of the Czech Republic	Scientific community	33	Czech Republic
25	Article popular press	Kleine Zeitung	Werkstoff wird optimiert	7.12.2011		civil society		
26	Article popular press	Wanted	Neues EU-Projekt am Institut für Struktur- und Funktionskeramik "RoLiCer"	März 2012		civil society		
27	Article popular	Triple M	Neues EU-Projekt am Institut für Struktur-	Issue 1, 2012		civil society		

	press		und Funktionskeramik					
28	Presentation	T. Lube	Förderungen im Umfeld industrieller Technologien	5.6.2012	Leoben, Austria	scientific community	50	Austria
29	Thesis	G. Kolb	Oberflächenrisse unter Kontaktbelastung	4.11.2013	Institut für Struktur- und Funktionskeramik, Montanuniversität Leoben			
30	Electronic article	RoLiCer Consortium	Modelling in ROLICER 263476	2012	What makes a material function? Let me compute the ways… Modelling in FP7 NMP Programme Materials projects	Scientific community, civil society, medias		International
31	Electronic article popular press	A. Kailer, H. Klemm	Risiken von Keramiklagern werden oft überschätzt	12.7.2013	MaschinenMarkt - Das Industrieportal	industry, civil society, medias		Germany, Austria , Switzerland
32	Homepage	IWM	www.rolicer.eu					
33	Conference paper	I. Khader, D. Kürten, A. Kailer	Proc. of World Tribology Congress 2013	September 8 – 13, 2013	Torino, Italy	Scientific community		International

Section B (Confidential[8] or public: confidential information to be marked clearly)
Part B1

TEMPLATE B1: LIST OF APPLICATIONS FOR PATENTS, TRADEMARKS, REGISTERED DESIGNS, ETC.					
Type of IP Rights[9]:	Confidential Click on YES/NO	Foreseen embargo date dd/mm/yyyy	Application reference(s) (e.g. EP123456)	Subject or title of application	Applicant (s) (as on the application)

[8] Note to be confused with the "EU CONFIDENTIAL" classification for some security research projects.

[9] A drop down list allows choosing the type of IP rights: Patents, Trademarks, Registered designs, Utility models, Others.

Part B2

Type of Exploitable Foreground[10]	Description of exploitable foreground	Confidential Click on YES/NO	Foreseen embargo date dd/mm/yyyy	Exploitable product(s) or measure(s)	Sector(s) of application[11]	Timetable, commercial or any other use	Patents or other IPR exploitation (licences)	Owner & Other Beneficiary(s) involved

[19] A drop down list allows choosing the type of foreground: General advancement of knowledge, Commercial exploitation of R&D results, Exploitation of R&D results via standards, exploitation of results through EU policies, exploitation of results through (social) innovation.
[11] A drop down list allows choosing the type sector (NACE nomenclature) : http://ec.europa.eu/competition/mergers/cases/index/nace_all.html

1.3.Report on societal implications

A	**General Information** *(completed automatically when **Grant Agreement number** is entered.*
Grant Agreement Number:	263476
Title of Project:	Enhanced reliability and lifetime of ceramic components through multi-scale modelling of degradation and damage
Name and Title of Coordinator:	Dr. rer. nat. Andreas Kailer

B Ethics	
1. Did your project undergo an Ethics Review (and/or Screening)?	***NO***
• If Yes: have you described the progress of compliance with the relevant Ethics Review/Screening Requirements in the frame of the periodic/final project reports?	O*Yes* O*No*
Special Reminder: the progress of compliance with the Ethics Review/Screening Requirements should be described in the Period/Final Project Reports under the Section 3.2.2 *'Work Progress and Achievements'*	
2. Please indicate whether your project involved any of the following issues (tick box) :	***YES***
RESEARCH ON HUMANS	
• Did the project involve children?	
• Did the project involve patients?	
• Did the project involve persons not able to give consent?	
• Did the project involve adult healthy volunteers?	
• Did the project involve Human genetic material?	
• Did the project involve Human biological samples?	
• Did the project involve Human data collection?	
RESEARCH ON HUMAN EMBRYO/FOETUS	
• Did the project involve Human Embryos?	
• Did the project involve Human Foetal Tissue / Cells?	
• Did the project involve Human Embryonic Stem Cells (hESCs)?	
• Did the project on human Embryonic Stem Cells involve cells in culture?	
• Did the project on human Embryonic Stem Cells involve the derivation of cells from Embryos?	
PRIVACY	
• Did the project involve processing of genetic information or personal data (eg. health, sexual lifestyle, ethnicity, political opinion, religious or philosophical conviction)?	
• Did the project involve tracking the location or observation of people?	
RESEARCH ON ANIMALS	
• Did the project involve research on animals?	
• Were those animals transgenic small laboratory animals?	
• Were those animals transgenic farm animals?	
• Were those animals cloned farm animals?	
• Were those animals non-human primates?	
RESEARCH INVOLVING DEVELOPING COUNTRIES	
• Did the project involve the use of local resources (genetic, animal, plant etc)?	
• Was the project of benefit to local community (capacity building, access to healthcare, education etc)?	
DUAL USE	

• Research having direct military use	0 Yes 0 No
• Research having the potential for terrorist abuse	

C Workforce Statistics

3. Workforce statistics for the project: Please indicate in the table below the number of people who worked on the project (on a headcount basis).

Type of Position	Number of Women	Number of Men
Scientific Coordinator	0	1
Work package leaders	2	5
Experienced researchers (i.e. PhD holders)	3	23
PhD Students	1	5
Other	3(IWM:3)	75

4. How many additional researchers (in companies and universities) were recruited specifically for this project?	
Of which, indicate the number of men:	5

D Gender Aspects

5. Did you carry out specific Gender Equality Actions under the project?

⊙ Yes
○ No

6. Which of the following actions did you carry out and how effective were they?

		Not at all effective → Very effective
☑	Design and implement an equal opportunity policy	○ ⊙ ○ ○ ○
❑	Set targets to achieve a gender balance in the workforce	○ ○ ○ ○ ○
❑	Organise conferences and workshops on gender	○ ○ ○ ○ ○
❑	Actions to improve work-life balance	○ ○ ○ ○ ○
○	Other:	

7. Was there a gender dimension associated with the research content – i.e. wherever people were the focus of the research as, for example, consumers, users, patients or in trials, was the issue of gender considered and addressed?

○ Yes- please specify

⊙ No

E Synergies with Science Education

8. Did your project involve working with students and/or school pupils (e.g. open days, participation in science festivals and events, prizes/competitions or joint projects)?

○ Yes- please specify

⊙ No

9. Did the project generate any science education material (e.g. kits, websites, explanatory booklets, DVDs)?

⊙ Yes- please specify: Website

○ No

F Interdisciplinarity

10. Which disciplines (see list below) are involved in your project?

⊙ Main discipline[12]: 2.3
○ Associated discipline[12]:
○ Associated discipline[12]:

G Engaging with Civil society and policy makers

11a Did your project engage with societal actors beyond the research community? *(if 'No', go to Question 14)*

⊙ Yes
○ No

11b If yes, did you engage with citizens (citizens' panels / juries) or organised civil society (NGOs, patients' groups etc.)?

○ No
○ Yes- in determining what research should be performed
○ Yes - in implementing the research
⊙ Yes, in communicating /disseminating / using the results of the project

[12] Insert number from list below (Frascati Manual).

11c In doing so, did your project involve actors whose role is mainly to organise the dialogue with citizens and organised civil society (e.g. professional mediator; communication company, science museums)?	○ ⦿	Yes No

12. Did you engage with government / public bodies or policy makers (including international organisations)

- ⦿ No
- ○ Yes- in framing the research agenda
- ○ Yes - in implementing the research agenda
- ○ Yes, in communicating /disseminating / using the results of the project

13a Will the project generate outputs (expertise or scientific advice) which could be used by policy makers?

- ○ Yes – as a **primary** objective (please indicate areas below- multiple answers possible)
- ○ Yes – as a **secondary** objective (please indicate areas below - multiple answer possible)
- ⦿ No

13b If Yes, in which fields?

Agriculture Audiovisual and Media Budget Competition Consumers Culture Customs Development Economic and Monetary Affairs Education, Training, Youth Employment and Social Affairs		Energy Enlargement Enterprise Environment External Relations External Trade Fisheries and Maritime Affairs Food Safety Foreign and Security Policy Fraud Humanitarian aid		Human rights Information Society Institutional affairs Internal Market Justice, freedom and security Public Health Regional Policy Research and Innovation Space Taxation Transport	

13c If Yes, at which level?

- ○ Local / regional levels
- ○ National level
- ○ European level
- ○ International level

H Use and dissemination

14. How many Articles were published/accepted for publication in peer-reviewed journals?	**7**
To how many of these is open access[13] provided?	**0**
How many of these are published in open access journals?	**0**
How many of these are published in open repositories?	**0**
To how many of these is open access not provided?	**7**
Please check all applicable reasons for not providing open access:	
❑ publisher's licensing agreement would not permit publishing in a repository ❑ no suitable repository available ❑ no suitable open access journal available ❑ no funds available to publish in an open access journal ☑ lack of time and resources ❑ lack of information on open access ☑ other[14]: the Journals, in which the work was published did not offer open access at the time of budgeting the project, i.e., no resources were planned for this options. Additionally, no agreed open access policy available at partner organisations	

15. How many new patent applications ('priority filings') have been made? *("Technologically unique": multiple applications for the same invention in different jurisdictions should be counted as just one application of grant).*		**0**
16. Indicate how many of the following Intellectual Property Rights were applied for (give number in each box).	Trademark	**0**
	Registered design	**0**
	Other	**0**
17. How many spin-off companies were created / are planned as a direct result of the project?		**0**
Indicate the approximate number of additional jobs in these companies:		

18. Please indicate whether your project has a potential impact on employment, in comparison with the situation before your project:

❑ Increase in employment, or	❑ In small & medium-sized enterprises
❑ Safeguard employment, or	❑ In large companies
❑ Decrease in employment,	☑ None of the above / not relevant to the project
❑ Difficult to estimate / not possible to quantify	

[13] Open Access is defined as free of charge access for anyone via Internet.
[14] For instance: classification for security project.

19. For your project partnership please estimate the employment effect resulting directly from your participation in Full Time Equivalent (*FTE = one person working fulltime for a year*) jobs:	*Indicate figure:*
Difficult to estimate / not possible to quantify	☑

I Media and Communication to the general public

20. As part of the project, were any of the beneficiaries professionals in communication or media relations?

○ Yes ⦿ No

21. As part of the project, have any beneficiaries received professional media / communication training / advice to improve communication with the general public?

○ Yes ⦿ No

22 Which of the following have been used to communicate information about your project to the general public, or have resulted from your project?

☑	Press Release	☑	Coverage in specialist press
☑	Media briefing	❑	Coverage in general (non-specialist) press
❑	TV coverage / report	❑	Coverage in national press
❑	Radio coverage / report	❑	Coverage in international press
☑	Brochures /posters / flyers	☑	Website for the general public / internet
❑	DVD /Film /Multimedia	☑	Event targeting general public (festival, conference, exhibition, science café)

23 In which languages are the information products for the general public produced?

☑	Language of the coordinator	☑	English
❑	Other language(s)		

***Question F-10*:** Classification of Scientific Disciplines according to the Frascati Manual 2002 (Proposed Standard Practice for Surveys on Research and Experimental Development, OECD 2002):

FIELDS OF SCIENCE AND TECHNOLOGY

1. NATURAL SCIENCES

1.1 Mathematics and computer sciences [mathematics and other allied fields: computer sciences and other allied subjects (software development only; hardware development should be classified in the engineering fields)]

1.2 Physical sciences (astronomy and space sciences, physics and other allied subjects)

1.3 Chemical sciences (chemistry, other allied subjects)

1.4 Earth and related environmental sciences (geology, geophysics, mineralogy, physical geography and other geosciences, meteorology and other atmospheric sciences including climatic research, oceanography, vulcanology, palaeoecology, other allied sciences)

1.5 Biological sciences (biology, botany, bacteriology, microbiology, zoology, entomology, genetics, biochemistry, biophysics, other allied sciences, excluding clinical and veterinary sciences)

2 ENGINEERING AND TECHNOLOGY

2.1 Civil engineering (architecture engineering, building science and engineering, construction engineering, municipal and structural engineering and other allied subjects)

2.2 Electrical engineering, electronics [electrical engineering, electronics, communication engineering and systems, computer engineering (hardware only) and other allied subjects]

2.3. Other engineering sciences (such as chemical, aeronautical and space, mechanical, metallurgical and materials engineering, and their specialised subdivisions; forest products; applied sciences such as geodesy, industrial chemistry, etc.; the science and technology of food production; specialised technologies of interdisciplinary fields, e.g. systems analysis, metallurgy, mining, textile technology and other applied subjects)

3. MEDICAL SCIENCES

3.1 Basic medicine (anatomy, cytology, physiology, genetics, pharmacy, pharmacology, toxicology, immunology and immunohaematology, clinical chemistry, clinical microbiology, pathology)

3.2 Clinical medicine (anaesthesiology, paediatrics, obstetrics and gynaecology, internal medicine, surgery, dentistry, neurology, psychiatry, radiology, therapeutics, otorhinolaryngology, ophthalmology)

3.3 Health sciences (public health services, social medicine, hygiene, nursing, epidemiology)

4. AGRICULTURAL SCIENCES

4.1 Agriculture, forestry, fisheries and allied sciences (agronomy, animal husbandry, fisheries, forestry, horticulture, other allied subjects)

4.2 Veterinary medicine

5. SOCIAL SCIENCES

5.1 Psychology

5.2 Economics

5.3 Educational sciences (education and training and other allied subjects)

5.4 Other social sciences [anthropology (social and cultural) and ethnology, demography, geography (human, economic and social), town and country planning, management, law, linguistics, political sciences, sociology, organisation and methods, miscellaneous social sciences and interdisciplinary , methodological and historical S1T activities relating to subjects in this group. Physical anthropology, physical geography and psychophysiology should normally be classified with the natural sciences].

6. HUMANITIES

6.1 History (history, prehistory and history, together with auxiliary historical disciplines such as archaeology, numismatics, palaeography, genealogy, etc.)

6.2 Languages and literature (ancient and modern)

6.3 Other humanities [philosophy (including the history of science and technology) arts, history of art, art criticism, painting, sculpture, musicology, dramatic art excluding artistic "research" of any kind, religion, theology, other fields and subjects pertaining to the humanities, methodological, historical and other S1T activities relating to the subjects in this group]