

Collection of Abstracts:

Development and qualification of accident-tolerant fuel (ATF) cladding materials: the H2020 IL TROVATORE approach

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The 2011 Fukushima Daiichi event has demonstrated the need for safer nuclear energy, prompting the development of accident-tolerant fuels (ATFs), which are expected to overcome the inherent technical shortcomings of the standard zircaloy/UO₂ fuels. The main objective of the H2020 project IL TROVATORE is to optimize and validate, in an industrially relevant environment (i.e., via a neutron irradiation in PWR-like water), some of the most promising ATF cladding material concepts for use in Gen-II/III light water reactors (LWRs). The innovative ATF clad concepts considered in IL TROVATORE must demonstrate significant improvement in performance when compared to the standard fuel cladding materials (i.e., zircalloys), thus helping to take a critical step towards an improved nuclear energy safety. IL TROVATORE is an international collaboration between Europe, the USA and Japan that combines academic excellence with industrial support, involving standardization bodies and nuclear safety regulatory authorities in order to accelerate the transfer of the envisaged innovation to market. The innovative ATF clads should satisfy the following 2 key requirements: (a) achieve a step enhancement in performance during nominal operation conditions & short-lived design-basis transients (<1200°C), and (b) maintain hermeticity for prolonged periods during beyond-design-basis accidents (>1200°C).

The ATF cladding material concepts studied in IL TROVATORE are: (a) SiC/SiC composite clads (various material concepts produced by different processing routes), (b) coated clads (MAX phase and nanocrystalline oxide coatings on zircaloy substrate clads), (c) GESA surface-alloyed clads (surface modification of zircaloy clads based on the GESA process), and (d) oxide-dispersed-strengthened (ODS) FeCrAl alloys. In order to reach its ambitious scientific & technical objectives within the short timeframe of 4.5 years, IL TROVATORE attempts to establish a culture of accelerated materials development (AMD). AMD strives for the expedited development and optimization of innovative nuclear materials by ensuring the constant communication between application-driven material design, material production, and material performance assessment in application-relevant conditions. The successful implementation of this approach relies on the use of high-throughput material screening tools capable of reliably assessing material performance prior to in-pile testing; one such tool is the use of ion/proton irradiation to assess material radiation tolerance.

Basic Principles of Thermal Spraying

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As compared to weld cladding, using a rather large distance of some tens of centimeters between the spray torch and the part and thus transferring limited energy into the surface, the relative low interface temperature during Thermal Spray processes avoids reactions to potentially brittle phases. Thus, Thermal Spray techniques are rather universal with respect to applicable spray materials, ranging from polymers, over all sort of metals and metal alloys up to ceramics, and a variety of different composites. Coating thickness is typically in a range of some hundreds of microns. The liquid phase droplet impact on rather cold substrates usually results in high quench rates of up to 10^4 - 10^5 K/s. The presentation summarizes the basic principles and differences for using wires or powders as feedstock, key influences on possible coating qualities, as well as examples for applications.

Electric arc discharge, a flame or a plasma provide the needed thermal energy to melt, or at least partially melt the feedstock material. Kinetic energy is supplied by the flow and expansion of less or more pressurized gas or/and the combustion products. The thermal history over the flight duration and the impact velocity of molten or semi-molten droplets on the substrate determine the possible pick-up of oxygen from the flame or environment as well abilities to close possible gaps on the surface, means avoiding porosity. Despite the rather short expose times of less than one of up to some milliseconds against environmental surrounding, surface oxidation is unavoidable, however can be reduced by adjusting lower temperatures for possible reactions and using higher velocities just minimizing the flight time. So called High Velocity Oxy-Fuel (HVOF) spray techniques operate at supersonic gas and particle velocities and, in addition to reduced oxidation, by the high kinetic energy upon impact on the substrate also result in low porosity coatings. For avoiding oxidation, an inert gas flow as obtained in plasma spraying has to be combined with vacuum conditions as vacuum plasma spraying (VPS). The term vacuum here refers to chamber of some tens of millibars, already causing a wider expansion of the plasma plume as compared to environmental surrounding, and resulting in a longer exposure of the spray materials to high temperatures.

New developments in thermal spraying work with lower flame temperatures as in High Velocity Air-Fuel spraying, the use of suspensions instead of powders in Suspension HVOF or plasma spraying, as SHVOF or SPS, or longer expose times in Low Pressure Vacuum Plasma Spraying (LP-VPS). The later is capable to evaporate the spray material; thus coating formation can be described as condensation, thus bridging the gap to thin film methods.

Internal coatings for accident tolerant fuel claddings: numerically assisted scale-up of the deposition process

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Abstract:

Internal coatings for nuclear fuel claddings in pressurized water reactor show a dual interest. First, they should mitigate pellet-cladding interaction in transient and nominal regimes. Second, in the case of a coolant-limitant accident, claddings made from zirconium alloys balloon and burst. An inner coating thus prevents the high-temperature steam oxidation of cladding internal surface and limits hydrogen generation. DLI-MOCVD, or direct liquid metalorganic chemical vapor deposition was developed in order to answer the geometrical constraints imposed by the internal coating of a nuclear fuel cladding. In addition to a traditional design of experiments, the deposition process was numerally modeled thanks to a multi-physics approach. This coupled development assisted in the scale-up of a DLI-MOCVD chamber, from a 0.3 m cladding segment, to a 1 m long segment, to three 1 m long segments and finally to a bundle of sixteen 1 m long cladding segments. A set of optimized deposition parameters (thermal field, pressure, vapor flow rates) was obtained with 3D computational simulations that led to the growth of a homogeneously thick coating inside 1 m long cladding segments.

Deposited coating consists in amorphous chromium carbide CrC_x exhibiting a glassy microstructure without grain boundaries. A benchmark among other Cr-based coatings revealed that amorphous chromium carbide show a better resistance to high-temperature oxidation.

After shortly detailing the specifications leading to the selection of DLI-MOCVD process for the internal protection of nuclear fuel claddings, the numerical-experimental coupled development will be presented along with the scale-up of the process.

Keywords:

Accident tolerant fuels; Chromium carbide coating; Internal protection; DLI-MOCVD scale-up

Development of MAX phase-based coatings deposited by HiPIMS to improve the high-temperature oxidation behavior of Zr-based alloy

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Abstract:

Following the Fukushima Daiichi accident in 2011, international efforts focus on the development of accident-tolerant fuels (ATF) claddings for light water reactors. Several short-term solution have been proposed worldwide, implying surface modifications and various types of coatings on Zr-based material. In order to resist to high-temperature steam environment, Al-containing MAX phases, as Cr₂AlC, are considered to be a promising solution due to the formation of a dense and adherent alumina scale. In this work, MAX phase-based coating deposited by HiPIMS (High Power Impulse Magnetron Sputtering) and subsequent thermal annealing were investigated as protective coating on Zr-based alloys.

Partially crystallized Cr₂AlC thin films were obtained by a 500°C annealing of as-deposited Cr-Al-C coatings. As the metallurgical properties of the zirconium-based substrates is preserved, this two-step process is a viable solution to protect the last generation of nuclear fuel claddings with Cr₂AlC coating. The behavior of as-deposited and annealed coatings with respect to high-temperature oxidation slightly differs for short oxidation times but converges for longer durations. Both coatings revealed significant protective effect against rapid oxidation under dry and wet air at high temperatures (up to 1200°C) owing to the formation of a continuous oxide layer. During the first stages of oxidation, this layer is made of α-Al₂O₃ and Cr₂O₃ for as-deposited coating while only α-Al₂O₃ is present for the annealed one. Because of Al depletion, coatings later deteriorate and form a residual and porous intermediate chromium carbide (Cr₇C₃) layer which further fully oxidizes. It was shown that the inward diffusion of Al with Zr also accelerates the coating deterioration. Self-healing capability is also observed for submicronic defects.

In addition, thanks to the flexibility of the modern industrial HiPIMS facilities, different multilayered architectures were deposited in a single deposition chamber, aiming to improve the performance of the coating during both normal and accident conditions. Molybdenum interlayer were proposed as diffusion barrier to enhance the lifespan of MAX phase-based coating under high temperatures while Cr outer layer was deposited on the top to eliminate potential fast hydrothermal dissolution of Al during normal operation. Globally, the results indicate that Cr₂AlC MAX phase-based thin films obtained by HiPIMS process are promising candidates for ATF cladding coatings.

Keywords: HiPIMS; Accident tolerant fuels; Cr₂AlC MAX phase coating; High-temperature oxidation; Self-healing.

Preparation and characterization of rhombohedral metal-oxide thin films on c-plane α -Al₂O₃ substrates

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Rhombohedral metal-oxide thin films are grown on c-plane α -Al₂O₃ (0001) single crystal substrates at low substrate temperatures by non-reactive radio frequency magnetron sputtering. Phase formation and composition are characterized by X-ray diffraction (XRD) and Raman spectroscopy analysis. Additional information such as in-plane and out-of-plane lattice parameters, strain relaxation and texture are obtained by reciprocal space mappings (RSMs) and pole figure measurements. Transmission electron microscopy (TEM) has been carried out in order to study the microstructure and further confirm the orientation and epitaxial relationship between films and substrates.

Science of Kinetic Spraying: From Discovery and Basic Principles to Applications

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This presentation gives an overview concerning basic principles of Cold Spraying (CS) and Aerosol Deposition (AD) for making the methods suitable for applications. As powder spray techniques dealing with solid impacts, both methods result in coatings of high purity and unique properties, not attainable by other spray methods.

Cold Spraying deals with supersonic velocity (400 – 900 m/s) impacts of deformable metal powders in sizes typically between 15 and 50 μm , as attained by acceleration in an expanding, high pressure (10-50 bar) gas jet, realized by respective converging/diverging nozzle design, just operating under environmental conditions. With cold spraying, thick deposits of up to several centimeters can be build-up, applicable as additive manufacturing technique. Already in the early works, exceeding a material dependent critical velocity was identified as key parameter for successful coating build-up. Supported by modelling, reaching and exceeding the critical velocity, and thus coating quality, is associated with the occurrence of adiabatic shear instabilities, means thermal softening over-compensating strain and strain rate hardening, at particle-substrate and particle-particle interfaces, as occurring under severe, high strain rate plastic deformation. Applications are mostly found in electronics, mechanical part repair and additive manufacturing.

Aerosol deposition deals with high velocity impacts of ceramic particles in sizes of typically less than one micron and impact velocities of typically 100 to 500 m/s. At such small sizes, ceramic materials show a different deformation and fracture behavior than in large bulk shape, allowing for some plasticity. For avoiding interaction with the surrounding atmosphere and possible particle deceleration, the coating process has to be performed in vacuum. Since small particles easily adopt the velocity of the gas stream, low pressures (typically < 1 bar) and straight nozzle outlets are sufficient to reach needed velocity for bonding. Coating formation is typically associated by a grain refinement as compared to the feedstock powder, probably caused by deformation. By AD, coatings with some tens of microns in thickness be build up, so far bridging the gap between thin film technics and powder spraying. Applications are mostly found in electronics.

The presentation summarizes current models and key parameters for both techniques to achieve and to improve bonding and coating qualities, and gives examples for applications.

An overview of thin-film processing of MAX phase coatings

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$M_{n+1}AX_n$ phases (“MAX phases”, where $n=1, 2, \text{ or } 3$) are a class of hexagonal-structure ternary carbides and nitrides (“X”) of a transition metal (“M”) and an A-group element comprising >80 ternary members. What makes the MAX phases fascinating and potentially useful is their remarkable combination of chemical, physical, electrical, and mechanical properties, which in many ways combine the characteristics of metals and ceramics. For example, MAX phases are typically resistant to oxidation and corrosion, elastically stiff, but at the same time they exhibit high thermal and electrical conductivities and are machinable. These properties stem from an inherently nanolaminated crystal structure, with MX slabs intercalated with pure A-element layers. This talk gives an overview of the history and reviews recent developments in the MAX-phase field with focus on thin-film physics and surface engineering. A brief overview of thin-film processing methods (sputtering, arc deposition, CVD) will be given, with an emphasis on the characteristic attributes of each method and especially how they relate specifically to processing of MAX phases. New approaches such as spraying techniques and aerosol deposition will also be discussed. The thin film research in the area of MAX phases will also be discussed in correlation to the rapidly emerging field of two-dimensional MXene materials derived from bulk and thin-film MAX phases.

Low temperature growth strategies for nanolaminate thin films

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Cr-Al-C and Mo-B-C thin films were deposited by magnetron sputtering. The formation temperatures for Cr₂AlC and Mo₂BC during sputter deposition are compared to the amorphous – crystalline transition temperatures in these material systems. The transition temperatures are determined by DSC and XRD. Based on the significantly lower synthesis temperature for Cr₂AlC and Mo₂BC during vapor phase condensation compared to the bulk diffusion mediated amorphous – crystalline transition temperatures surface diffusion is identified as the atomic scale mechanism enabling the low temperature synthesis.

Pulsed Laser Deposition of ductile amorphous oxides and their key enabling role in liquid metal fast reactors and thermonuclear fusion

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Pulsed Laser Deposition is a unique technique to produce out-of-equilibrium materials not accessible by conventional techniques. We will discuss how PLD can give access to a new class of materials key for the development of next generation nuclear systems: ductile amorphous oxides. In fact, we recently demonstrated (E. Frankberg et al. Science, 2019) that defect-free amorphous alumina, by PLD, exhibits an elastoplastic response under both tensile and compressive *in situ* TEM tests at room temperature. A yield stress as high as 4 GPa (tensile and compressive) has been measured, with a plastic deformation as high as 7% in tension and 100% in compression. Such a performance has never been observed before, especially for a ceramic under a tensile stress condition. For comparison, it is 4 times stronger than the best high strength steels available at a fraction of the density (3.5 g/cm³). Whilst the exact microscopic mechanism is still unknown, we observed that the plastic deformation of the material resembles viscous flow, in which no observable necking occurs and the stress is proportional to strain rate with no other strengthening mechanisms observed. This initial finding suggests that viscous creep of amorphous materials can be activated even at room temperature if sufficiently high stress levels can be reached, hence inducing yielding instead of brittle fracture. Microscopically, the high mechanical stress breaks the Al-O bonds, which are instantly reformed with different neighbours. As a comparison, we also simulated a typical silica glass finding a similar mechanism but on a much smaller scale: in α -Al₂O₃ bond switching occurs for as much as 50 % of all atoms at 15% elongation, while in α -SiO₂ just for 2%, right before brittle fracture occurs. We hypothesize that the higher rigidity of the α -SiO₂ network, coupled with the intrinsic presence of nanoscale voids (up to 65.7 Vol. % compared to 8.7% in α -Al₂O₃), might be the atomistic explanation of the different behaviours of the two amorphous materials. Hence, the experimental and theoretical work performed so far portrait a scenario in which three conditions seem to be necessary: structural homogeneity; high mass/atomic density; absence of defects down to the nm range; bonds flexible enough to undergo changes in coordination number as well as of neighbour. SEM *in situ* micromechanical tests suggest that this elastoplastic behaviour is maintained even for volumes of several microns cube. These unconventional mechanical properties seems not to be unique to alumina, but PLD deposited Cr₂O₃, Y₂O₃ hold the same promise and are currently under investigation. Indeed, we will show how these materials, in the form of coatings on structural materials like zirconium alloys or steels, are key for next generation nuclear systems, like accident tolerant light water reactors, liquid metal cooled fast reactors and magnetically confined nuclear fusion, enabling the design of innovative and economically attractive power plants.

Highly-performant nano-ceramic coatings: an innovative approach for present and next generation nuclear systems

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In the framework of future generation nuclear reactors, newly designed systems are meant to outperform current ones, by providing disruptive solutions in terms of non-proliferation, fuel cycle efficiency, radioactive waste management and safety. However, the eventual development of future power plants is directly linked to the availability of suitable materials for the most demanding conditions. Among the different solutions, ceramic coatings are a promising candidate to tackle the most relevant issues. Indeed, the deposition of ceramic coatings on traditional structural materials can provide surface engineering without affecting mechanical requirements and structural integrity. It is worth highlighting that protective coatings are already being considered as a near-term option for accident tolerant fuels in Light Water Reactors (LWRs) while, in the case of Generation-IV (GIV) fission concepts and fusion systems, coatings could be used to mitigate high-temperature heavy liquid metal corrosion and tritium permeation. The great interest around these solutions has been already manifested and worldwide partners have gathered in high-impact international projects. Here, we present a brief summary of all the activities performed by the Istituto Italiano di Tecnologia (IIT) on the materials for advanced nuclear systems. Ceramic and composite coatings are grown on relevant structural alloys such as austenitic AISI316 and 1515-Ti in the case of GIV fast reactors, while ferritic/martensitic T91 and EUROFER-97 for fusion systems. Coatings are designed and processed by a peculiar Physical Vapour Deposition (PVD) method, namely Pulsed Laser Deposition (PLD). PLD is particularly well suited for growing high-quality ceramic thin films in the form of metal oxides. In respect to fission systems, specifically lead-cooled fast reactors, alumina (Al_2O_3)-based coatings have been characterized as anti-corrosion radiation-resistant barriers. In particular, the compatibility of PLD-grown Al_2O_3 in molten lead and lead alloys has been proven in up to 8'000 hours of exposure time, with no degradation. For what concerns fusion reactors, yttria (Y_2O_3) as well as alumina coatings have been evaluated as possible solutions against Pb-Li corrosion and tritium permeation. Nevertheless, the tritium permeation reduction of PLD films is in the order of 10^4 - 10^6 , well above the design requirements (*i.e.* 1'000). Last but not least, Al_2O_3 -based coatings have been tested also under heavy ions irradiation, at damage levels relevant for fusion and fast fission reactors (up to 450 dpa). The ceramic film under irradiation preserves its integrity and stability, evolving structurally from an amorphous to an almost-completely crystalline state. This mechanism grants an unusual radiation tolerance to the tested materials. To conclude, engineered coatings deposited by the PLD technique represent promising candidates to face the major issues related to future nuclear technologies and allow the design of innovative and economically attractive power plants.

The Pulsed Electron Beam Facility GESA: Device and Physics

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Pulsed electron beam treatment is used to modify the surface layer of metal targets while leaving the bulk material unchanged. Appropriate for such treatment are pulsed electron accelerators of the GESA family. A high voltage pulse, typically around 100 kV, is generated and applied to a large-area cathode. The extraction voltage of the triode system controls the electron emission. The electron beam is then transported in a guiding magnetic field and focused on the target. Beam-target interaction leads to melting of the target surface up to a depth of tens of micrometres. After termination of the electron beam, rapid cooling and re-solidification results in a modified surface layer with improved properties.

In this presentation, the pulsed electron beam devices GESA are introduced. An overview on the physics of their operation is given, including electron emission, beam formation and transport, and interaction of the electron beam with the target. Finally, heat transfer in the target is considered and specifications of the treatment such as melt depths and cooling rates are given.

GESA, pulsed electron beam facility – Surface modification, surface alloying– Applications

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Intense pulsed electron beams are used for the surface modification of materials since several years. An improvement of properties like wear, corrosion and oxidation resistance is obtained due to pulsed electron beam treatment of mainly metallic materials. Different modification modes can be distinguished: rapid melting and solidification, surface alloying of coatings into the bulk and surface-fusing of coatings to the bulk. All three surface treatment processes were and are investigated using the GESA (Gepulste Elektronen Strahl Anlage) facilities having following parameters: accelerating voltage 80–400kV; power-density 2 – 6MW/cm²; beam-diameter 4–10cm; pulse-duration 4– 250µs. Such pulses applied on material surfaces lead to a change in microstructure and in the case of surface alloying also to a change in chemical composition resulting in surface graded materials.

This presentation give an overview on the potential applications of this surface modification technology. Increase of wear and fatigue resistance for gears and blade materials, oxidation resistance for gas turbines and mitigation of corrosion attack in liquid metals. To achieve corrosion resistance in liquid metals alloying of strong oxide formers like Al is the selected process. Such surface alloyed steel and metals can improve the corrosion resistance against liquid b or PbBi and water significantly and are therefore also discussed in the frame of Accident tolerant fuel claddings.

Thermal stability enhancement of Cr₂AlC coatings on Zr by utilizing a double layer diffusion barrier

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Decomposition of Cr₂AlC deposited onto a Zr substrate and vacuum-annealed is observed at 800°C as Al diffuses from the MAX phase into the Zr substrate. A double layer of ZrN and AlN has been predicted by CALPHAD calculations to act as diffusion barrier between the Zr substrate and Cr₂AlC. Experimental thermal stability investigations corroborate this prediction by confirming that the proposed double layer diffusion barrier coatings suppresses the decomposition of Cr₂AlC at temperatures of up to 1000°C.

Aerosol Deposition of MAX-Phase Phase Coatings

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The rather new material class of MAX-phases combines properties of covalent bonded, brittle ceramics with those of metals. The metallic properties as machinability and electrical conductivity are due to atomic metal layers in the crystallographic structure. The general formula $M_{n+1}AX_n$ describes the composition with M as an early transition metal (Ti, Zr, Cr,...), A as an A-group element (Si, Al,...) and X as carbon or nitrogen. For possible applications, particularly Al-, or Cr-based MAX-phases are claimed to guarantee good oxidation protection up to temperatures of more than 1100°C.

Operating with liquid phase deposition, usual thermal spray processes result in oxidation of the MAX-phase material and the decomposition into less protective compounds. In contrast, kinetic spray methods as cold spraying (CS) or aerosol deposition (AD) have the potential to retain the original MAX-phase structure in the coating without oxidation.

For the present study on aerosol deposition, the Ti_3SiC_2 MAX-phase was chosen as model system due to the availability of commercial powder and property data. The as received powder was milled to different nominal sizes. For revealing details on coating formation and possible bonding mechanisms, aerosol deposition experiments were performed for different particle size batches and varied process gas pressures. Microstructural analyses reveal, that coating formation preferably occurs for particle sizes smaller two microns. Using small particle sizes, crack-free, dense layers can be obtained. The individual deposition efficiencies for the particle different sizes, particularly the critical size below which deposition gets prominent, vary with process gas pressure. Detailed microstructural analyses of coatings and single impact phenomena by high resolution scanning electron microscopy reveal plastic deformation and fracture, both attributing to shape adaption to previous spray layers and probably bonding.

Thermal characterization of thin films

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Thermal properties of bulk and thin film materials are of great interest not only from a fundamental perspective but also from an industrial point of view. Thermal conductivity combined with a good knowledge of the material usually informs on transport mechanisms. On a more practical point of view, optimal thermal and thermo-mechanical properties are necessary specifications for materials functioning in harsh environments. Therefore, knowing the limitations related to a measurement set-up along with the specifications of a material is important in order to conclude on a material's behavior at high temperatures and consequently its potential.

Several techniques for thermal characterization of thin films will be presented and discussed. These include time and frequency domain thermoreflectance, the flash method, modulated photothermal radiometry and 3ω . Furthermore, parameters to consider, such as the interfacial thermal resistance that arises between film and substrate, but also between film and native oxide layer, grain size, roughness and physical properties of the substrate play an important role in data analysis.

Finally, scanning thermal microscopy will be briefly introduced to demonstrate the possibility of looking locally into the transport properties of multimaterials.

Textured growth of polycrystalline MAX phase carbide coatings and their oxidation resistance in steam

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Alumina-forming MAX phases reveal great potential for accident tolerant fuel (ATF) cladding application because of their favorable physical and mechanical properties plus excellent high-temperature oxidation resistance. As a family of high-ordered ternary compounds, synthesis of high purity, particularly phase-pure and textured polycrystalline MAX phase coatings on technically relevant substrates often remains a challenge. However, the presence of impurities, regardless of in bulk or in coating, degrades their oxidation performance and irradiation resistance. To overcome this issue, a two-step approach, i.e. magnetron-sputtering of nanoscale elemental multilayer stacks with subsequent ex-situ heat treatment in argon, is elaborated for potential synthesizing phase-pure MAX phase carbide coatings. The unique multilayer architecture within the as-deposited coatings has a nano-layered structure similar to the layered structure of MAX phase and guarantees a short diffusion length during subsequent annealing (to initiate the growth of MAX phase via elemental multilayer interdiffusion and reaction). This approach also reduces the crystallization temperature of the MAX phase due to chemical energy stored in such reactive multilayers. Ternary carbide coatings in three systems (Ti-, Zr-, Cr- C-Al) are fabricated on both researching substrates (alumina, SiO₂/Si) as well as on the Zircaloy-4 substrates, and their high-temperature oxidation mechanisms in steam have been examined. Basal-plane textured MAX phase coatings were realized in the Ti- and Cr- C-Al systems, while no MAX phase formation in the Zr-C-Al system. The phase formation paths and fundamental mechanisms contributing to growth of the textured MAX phase coatings are explored. Oxidation performances of the coatings presented herein can give some insights into utilization of these MAX phases as potential oxidation-resistant and protective coatings in a wide range of applications.

Materials Informatics using Data from Calphad, ab initio and Machine Learning

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Abstract:

It has been argued that all sciences exhibit a transformation of the scientific paradigms from (1st) empirical, (2nd) theoretical, (3rd) computational to (4th) data science [Jim Gray on eScience: A Transformed Scientific Method, in: Kristin Tolle; Tony Hey; Stewart Tansley (2009). *The Fourth Paradigm: Data-Intensive Scientific Discovery (Volume 1)*. Microsoft Research. ISBN 978-0-9825442-0-4]. In materials science, the fourth paradigm is called materials informatics and uses big data approaches for materials discovery, materials design, process simulation and to advance understanding.

In this talk, data sources that can be used for materials informatics on phase stability are discussed and evaluated. It will be shown how the largest available data sources can be combined using human and machine learning: At 0 Kelvin, the largest available data sources are open quantum mechanical databases, such as materialsproject.org, oqmd.org or aflowlib.org. At elevated temperatures, the largest available databases are Calphad type databases that allow calculation of phase diagrams of metallic, oxidic or salt systems up to extremely high temperatures. The aiMP (ab initio Materials Project) database has recently been developed by GTT-Technologies to extrapolate the 0 K-phase stability from materialsproject.org to relevant temperatures using human and machine learning, making the data largely compatible with existing Calphad databases. It is shown how the different data sources can be combined in materials informatics approaches to materials selection and design for surface technology applications.

Ion irradiation of materials – an in situ observation perspective

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Material modification is produced by any radiation with sufficient energy large enough to cause atomic displacements. High energy ion damage and neutron damage in many respects produce similar microscopic and macroscopic material modifications. The use of ion irradiation allows the production of damage similar to that induced by neutrons but with significantly shorter timescales. Displaced atoms and created vacancies have complicated evolution in a material. This evolution is defined by the material itself, temperature and, in many cases, ambient conditions. Dynamic, in situ, evolution observation allows to obtain more accurate understanding of the processes of damage accumulation and annealing over time. The presentation will summarise the nuclear reactor relevant material data obtained at the MIAMI facility at the University of Huddersfield.

***In-situ* ion irradiation of MAX phase ceramics in the TEM: the importance of material design on radiation response**

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The approach followed in H2020 IL TROVATORE towards the accelerated development of innovative nuclear materials targeting specific applications in advanced nuclear systems requests the constant communication between application-driven material design, material synthesis, and material performance assessment in application-relevant conditions. Successfully implementing such an approach relies on the use of high-throughput material screening tools that are capable of reliably assessing material performance prior to in-pile testing; one such tool relies on the judicious use of ion/proton irradiation to assess material radiation tolerance. The MIAMI (Microscope & Ion Accelerator for Materials Investigations) facilities used in this work for the *in-situ* ion irradiation of MAX phase-based ceramics in the transmission electron microscope (TEM) offer unique insights into the dynamic evolution of radiation-induced damage in candidate nuclear materials. The MAX phases are nanolaminated ternary carbides/nitrides described by the $M_{n+1}AX_n$ general formula, where 'M' is an early transition metal, 'A' is an A-group element, 'X' is C or N, and $n = 1, 2$ or 3 . The properties of the MAX phases are compound-specific and can be tailored to meet the needs of the end applications by making solid solutions on the M, A and/or X sites. Due to their remarkable properties, select MAX phase compounds are considered as candidate materials for specific applications in Gen-II/III Light Water Reactors (LWRs) and Gen-IV Lead-Fast Reactors (LFRs), hence, it is important to assess their radiation tolerance. In this work, various ternary MAX phase compounds and solid solutions thereof in the (Zr,Nb,Ti,Cr)-(Al,Sn)-C system have been irradiated using 6 keV He⁺ in the 350-800°C temperature range. The thin foils (produced by focused ion beam, FIB) that have been irradiated in the MIAMI facilities were lifted out of MAX phase-based single crystals, polycrystalline ceramics, or PVD (physically vapour deposited) coatings deposited on commercial fuel cladding substrates. The performed ion irradiations revealed differences in the radiation response of MAX phase compounds with different microstructures, pointing out the importance of material design in order to optimize the radiation tolerance of MAX phase-based ceramics intended for specific nuclear applications.