2nd RUSSIA-BRAZIL ONLINE SYMPOSIUM

NOVEL COMPLEX ALLOYS AND ADVANCED PROCESSES FOR OPTIMIZED FUNCTIONAL PROPERTIES

December 9-12, 2025

PROGRAM & BOOK of ABSTRACTS

SCOPE

This symposium focuses on the design, modeling, production and characterization of alloys with microstructural characteristics optimized for different applications. The following properties of the alloys are of particular interest:

corrosion and wear resistance;

mechanical strength and microstructure stability at high temperatures,

hydrogen storage in solids forming hydrides or solid solutions with hydrogen.

Presentations may include works on complex systems such as high-entropy alloys, metallic glasses, nanocrystalline alloys, and quasicrystals as well as results of the in-depth fundamental studies of conventional and well-established alloy systems processed by the advanced methods.

The symposium will promote collaboration between Russian and Brazilian researchers and strengthen scientific ties between the countries.

The participation of graduate and post-graduate students in the symposium is encouraged.

ORGANIZERS

Lavrentyev Institute of Hydrodynamics SB RAS, Novosibirsk, Russia Novosibirsk State Technical University, Russia Federal University of São Carlos, SP, Brazil

ORGANIZING COMMITTEE

Guilherme Y. Koga, Brazil (Chairman) Evgeny M. Rudoy, Russia Dina V. Dudina, Russia (Chairman) Alexander K. Khe, Russia

Tomila M. Vidyuk, Russia Alberto Moreira Jorge Jr., Brazil, France

Vyacheslav V. Krizhanovskiy, Russia Guilherme Zepon, Brazil

Alexandr A. Shtertser, Russia Francisco Gil Coury, Brazil

Igor S. Batraev, Russia Eric Marchezini Mazzer, Brazil
Ivan A. Bataev, Russia Lucas Barcelos Otani, Brazil

Alexander G. Anisimov, Russia Brenda Juliet Martins Freitas, Brazil

Vladimir Yu. Ulianitsky, Russia Alexander P. Chupakhin, Russia

SYMPOSIUM WEBPAGE

https://www.hydro.nsc.ru/science/events/russia-brasil-symposium.php

Program

Dec 9, 2025 Chair – Guilherme Koga

Date	Time	Time	Duration	Participant	Presentation
	(Russia)	(Brazil)	(min)		type
December 9	19h00	9h00	10	Guilherme Koga,	welcome
				Ivan Bataev &	speech
				Alexander Khe	
December 9	19h10	9h10	25 + 5	Witor Wolf	invited
December 9	19h40	9h40	15 + 5	Brenda Martins	oral
December 9	20h00	10h00	15 + 5	Tatiana Ogneva	oral
December 9	20h20	10h20	15 + 5	Luana Cristina	oral
December 9	20h40	10h40	20	Break	-
December 9	21h00	11h00	25 + 5	Alberto Moreira	invited
				Jorge Jr.	
				Krizhanovskii	oral
December 9	21h30	11h30	15 + 5	Vyacheslav	
December 9	21h50	11h50	15 + 5	Isabela Dainezi	oral

Dec 10, 2025 Chair – Tomila Vidyuk

Date	Time	Time	Duration	Participant	Presentation
	(Russia)	(Brazil)	(min)		type
December 10	19h00	9h00	25 + 5	Tales Ferreira	invited
December 10	19h30	9h30	15 + 5	Aylanna Priscila	oral
December 10	19h50	9h50	15 + 5	Natalia	oral
				Aleksandrova	
December 10	20h10	10h10	15 + 5	Denise De Sousa	oral
December 10	20h30	10h30	20	Break	-
December 10	20h50	10h50	25 + 5	Juliane Ribeiro da	invited
				Cruz Alves	
December 10	21h20	11h20	15 + 5	Elielson Alves	oral
December 10	21h40	11h40	15 + 5	Roman Khabirov	oral
December 10	22h00	12h00	25 + 5	Ivan Bataev	invited

Dec 11, 2025 Chair – Ivan Bataev

Date	Time	Time	Duration	Participant	Presentation
	(Russia)	(Brazil)	(min)		type
December 11	19h00	9h00	25 + 5	Ricardo Floriano	invited
December 11	19h30	9h30	15 + 5	Arthur de Bribean	oral
December 11	19h50	9h50	15 + 5	Tomila Vidyuk	oral
December 11	20h10	10h10	15 + 5	Victor Hugo Mafra	oral
December 11	20h30	10h30	20	Break	-
December 11	20h50	10h50	25 + 5	Daria Lazurenko	invited
December 11	21h20	11h20	15 + 5	André Vidilli	oral
December 11	21h40	11h40	15 + 5	Igor Vitoshkin	oral

Dec 12, 2025 Chair – Brenda Juliet Martins Freitas

Date	Time	Time	Duration	Participant	Presentation
	(Russia)	(Brazil)	(min)		type
December 12	19h00	9h00	25 + 5	Juliano Soyama	invited
December 12	19h30	9h30	25 + 5	Alexey Shutov	invited
December 12	20h00	10h00	15 + 5	Thiago Cavalcante	oral
December 12	20h20	10h20	15 + 5	Igor Nasennik	oral
December 12	20h40	10h40	20	Break	-
December 12	21h00	11h00	25 + 5	Eric Mazzer	invited
December 12	21h30	11h30	15 + 5	Arina Ukhina	oral
December 12	21h50	11h50	10	Guilherme Koga,	closing remarks
				Brenda Martins,	
				Ivan Bataev &	
				Alexander Khe	

Microstructure and thermal conductivity of Cu–Diamond composites prepared by Hot Pressing (HP) and Spark Plasma Sintering (SPS)

A.V. Ukhina¹, D.V. Dudina^{1,2}, B.B. Bokhonov¹, M.A. Esikov²

Diamond is well known for its high thermal conductivity (1200–2500 W m⁻¹ K⁻¹). In order to obtain heat sink materials from diamond powders, a metallic binder is required, as binder-free diamonds cannot be sintered, unless high pressures are applied. A suitable binder is copper owing to its high thermal conductivity and a relatively low cost. Unfortunately, copper has a poor wettability towards the diamond surface, which causes pore formation at the copper/diamond interface and reduced heat transfer. To overcome this problem, several approaches have been used: preliminary modification of the diamond surface prior to the sintering process, direct modification of the copper matrix with carbide-forming metals to react in situ, and optimization of the synthesis parameters of the composites.

In this work, two ways were used to enhance the wettability of diamond particles by copper: preliminary surface modification of the diamond and modification of the copper matrix. In the first case, tungsten- and molybdenum-containing coatings on diamond were obtained by rotary chemical vapor deposition (RCVD) or by treating the diamond microcrystals in a hot press (HP)/spark plasma sintering (SPS) facility. In RCVD, tungsten carbonyl W(CO)₆ was used as a precursor. In the case of HP and SPS, powders of tungsten, molybdenum and tungsten trioxide WO₃ were used as sources of the metal. It was found that the morphology and phase composition of the coatings depend on the deposition conditions and the metal source. In the second case, carbide-forming metallic additives (W, Mo, Cr, Ti) were introduced into the copper matrix to improve the wettability of diamond particles in the copper-diamond composites. The samples were prepared by SPS and HP. The phase composition, microstructure and thermal conductivity of the samples were investigated.

¹ Institute of Solid State Chemistry and Mechanochemistry, Siberian Branch of the Russian Academy of Sciences, Kutateladze str. 18, Novosibirsk, 630128 Russia

² Lavrentyev Institute of Hydrodynamics, Siberian Branch of the Russian Academy of Sciences, Lavrentyev Ave. 15, Novosibirsk, 630090 Russia

Deposition of metallic coatings on diamond crystals via treatment in a planetary mill

Boris B. Bokhonov¹, <u>Dina V. Dudina</u>^{1,2}, Alexander I. Gavrilov¹, Alberto Moreira Jorge Jr.³,
Witor Wolf⁴

During mechanical alloying, the powder often adheres severely to the surface of milling balls and walls of the vials. While this effect may be detrimental for the technology of powder preparation, there exists a possibility of using it to produce coatings on substrates of different geometries. For that, the object to be coated is placed into the vial and the material to form a coating is added in the powder state. This presentation will focus on the deposition of iron [1], silver [2] and Al-Cu-Fe quasicrystalline [3] coatings on diamond microcrystals via treatment in a planetary mill without adding milling balls. The morphology and composition of the coatings are described. The effect of the deposition selectivity of the {111} facets of diamond is addressed. A possible mechanism of the coating formation is discussed.

[1] B.B. Bokhonov, D.V. Dudina, A.I. Gavrilov, An unexpected effect of selective deposition of metallic particles on the {111} facets during mechanical treatment of diamond crystals in a planetary mill, Diamond & Related Mater. 138 (2023) 110259. https://doi.org/10.1016/j.diamond.2023.110259
[2] B.B. Bokhonov, A.I. Gavrilov, D.V. Dudina, Selective deposition of silver particles on {111} or {100} diamond facets, CrystEngComm 26 (2024) 666–672. https://doi.org/10.1039/d3ce01137b
[3] B.B. Bokhonov, D.V. Dudina, A.I. Gavrilov, A. Moreira Jorge Jr., W. Wolf, Deposition of a quasicrystalline Al-Cu-Fe alloy on diamond via mechanical treatment in a planetary mill, Mater. Lett. 402 (2026) 139361. https://doi.org/10.1016/j.matlet.2025.139361

¹ Institute of Solid State Chemistry and Mechanochemistry SB RAS, Kutateldadze str. 18, Novosibirsk, 630090, Russia

² Lavrentyev Institute of Hydrodynamics SB RAS, Lavrentyev Ave. 15, Novosibirsk, 630090, Russia; e-mail: dina1807@gmail.com

³ Federal University of São Carlos, Via Washington Luiz, km 235, São Carlos 13565-905, SP, Brazil

⁴ University of São Paulo (USP), São Carlos School of Engineering, Department of Materials Engineering, Avenida João Dagnone 1100, 13563120, São Carlos, SP, Brazil

Design, processability and characterization of a Fe-based bulk metallic glass composite via laser powder bed fusion

A.P.M. De Araujo^{1,2}, P. Ramasamy³, J. Eckert^{3,4}, and P. Gargarella^{1,2,5}

e-mail: aylannapriscila@hotmail.com

Fe-based bulk metallic glass composites (BMGCs) combine excellent magnetic, corrosion, and mechanical properties with low cost, but their poor glass-forming ability limits casting. Laser Powder Bed Fusion (LPBF), an additive manufacturing technique, can overcome these limitations by enabling rapid cooling rates in bulk parts with complex geometries. Selecting suitable Fe-based alloys for LPBF remains challenging, as compositions adapted from casting or melt spinning often exhibit poor processability. This work designed, produced, and characterized a Fe-Mo-P-C-B BMGC for LPBF. The glass-forming ability, liquidus temperature, and phase formation were first evaluated using a glass-forming ability parameter and CALPHAD calculations. The selected alloy was gas-atomized, processed by LPBF under varying laser powers, scan speeds, scanning strategies, hatching distances, layer thicknesses, and remelting conditions, and then fully characterized. Processing parameters were optimized to obtain intact samples containing the glassy phase. The best LPBF samples were selected, and their processing conditions were correlated with microstructure, and mechanical behavior. Optimal parameters were 50-80 W and 100-700 mm/s, with the chessboard strategy enhancing glassy phase formation. Low laser power and high scan speed increased both porosity and glassy phase content; within the explored parameters range, pore and crack fractions as low as 1% and glassy phase fractions up to 24% were achieved, though not simultaneously. Both powders and LPBF samples exhibited a glassy-crystalline composite microstructure consisting of Fe(Si)-α (bcc), B₅₀-Fe_{1.04} ((tetragonal), and Fe_{0.75}Mo_{0.122}C_{0.128} (bcc) phases embedded in a glassy matrix. While Vickers microhardness remained around 1100 HV, compression resistance was strongly parameter-dependent, ranging from 110 to 900 MPa. These results highlight the importance of alloy design and provide guidelines for LPBF's potential to overcome the traditional glassforming limitations of Fe-based BMGCs.

¹ Graduate Program in Materials Science and Engineering, Federal University of São Carlos, Rod. Washington Luis Km 235, 13565-905, São Carlos, Brazil;

² Department of Materials Engineering, Federal University of São Carlos, Rod. Washington Luis Km 235, 13565-905, São Carlos, Brazil.

³ Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, 8700 Leoben, Austria.

⁴ Montanuniversitat Leoben, Franz Josef-Strasse 18, 8700 Leoben, Austria.

⁵ Center for Characterization and Development of Materials (CCDM), Federal University of São Carlos (UFSCar), Rod. Washington Luiz, Km 235, CEP: 13.565-905 - São Carlos – SP, Brazil.

Grain Refinement of Stainless Steels Produced by Additive Manufacturing

Dr. Brenda Juliet Martins Freitas*, Dr. Guilherme Yuuki Koga, Dr. Claudemiro Bolfarini

Federal University of São Carlos (Materials Engineering Department)

*e-mail: brenda@ppgem.ufscar.br

Alloys produced by additive manufacturing often exhibit undesired features such as cracking, anisotropy, brittleness, and coarse columnar grains. In this study, we report the successful fabrication of boron-containing stainless steel composites by Laser Powder Bed Fusion (L-PBF). The addition of boron effectively transforms coarse columnar grains (~200 µm) into equiaxed ultrafine grains (~1 µm). In addition to outstanding grain refinement, the high boron content promotes the in-situ formation of nanometric Cr₂B particles decorating grain boundaries. This remarkable refinement is attributed to extended thermal undercooling during solidification, driven by boron segregation at the solid-liquid interface. The boron-enriched boundary layer suppresses grain growth and enhances the nucleation rate on the underlying layer, effectively preventing the development of columnar grain structures of the primary phase. These findings provide a mechanistic understanding of boron-induced grain refinement and establish a framework for the design of next-generation stainless steel composites with tailored microstructures and multifunctional properties through strategic alloying and advanced additive manufacturing.

Fundação de Amparo à Pesquisa do Estado de São Paulo/FAPESP (scholarship nº 2019/05885-7, 2021/10735-4).

Evaluation of cermets composed of NbC bonded with 316L stainless steel and

Denise De Sousa e Silva

zirconia

Federal University of São Carlos, Rua Antônio Fisher dos Santos, 254 CEP 13.564-390 e-mail: denisesousa@estudante.ufscar.br

This study evaluated the behavior of composites based on niobium carbide (NbC) and 316L stainless steel (SS316L), with the addition of partially stabilized tetragonal zirconia polycrystals (3Y-TZP), as a corrosion inhibitor for steel. The composites were developed with different zirconia contents (0.65 vol.% and 2.57 vol.%) and processed using two sintering methods: conventional sintering and spark plasma sintering (SPS). Three distinct compositions were produced: 100N, N-95S5Z, and N-80S20Z. Densification was determined using the Archimedes method, while surface and microstructure analysis was carried out using optical microscopy and scanning electron microscopy (SEM). Mechanical properties were investigated using microhardness and indentation toughness tests. The results indicated that higher 3Y.ZrO₂ contents reduced densification and induced the formation of porosity. Immersion tests and electrochemical impedance spectroscopy (EIS) revealed that 0.65%.vol of 3Y.ZrO₂ improved corrosion resistance. Furthermore, the behavior of NbC/SS316L/3Y.ZrO₂ composites during sintering, as well as their mechanical properties and feasibility for application in cutting tools, was investigated. The results demonstrated that the SPS technique was more efficient than conventional sintering, promoting greater densification and better mechanical properties, especially in the N-95S5Z composition, which achieved a relative density of 98%, almost nonexistent apparent porosity ($\sim 0\%$), hardness of 1750 HV, fracture toughness of 7.98 MPa·m^{1/2}, and an average grain size of 2.22 ± 0.20 µm. The sintered samples achieved hardness values between 1550 and 1850 HV and an average fracture toughness of approximately 8.0 MPa·m^{1/2}, surpassing values reported in the literature for different binder contents, indicating potential for application in cutting tools. A reduction in zirconia concentration resulted in composites with higher densities.

Degradation Mechanisms of TiNbCr RMPEA under Oxidizing and Sulfur-

Rich Environments

Isabela Dainezia*, Brian Gleesonb, Carlos Alberto Della Roverea

Refractory multi-principal element alloys (RMPEAs) have attracted increasing interest due to

Federal University of Sao Carlos, Department of Materials Engineering, Rodovia Washington

Luiz, km 235 SP-310, 13565-905, São Carlos, São Paulo, Brazil

Department of Mechanical Engineering and Materials Science, University of Pittsburgh,

Pittsburgh, PA 15261, USA

conditions.

*e-mail: isabeladainezi@estudante.ufscar.br

their mechanical strength and potential for high-temperature applications. However, their environmental degradation behavior remains a challenge. While most studies focus on oxidation resistance, the effect of sulfur-containing atmospheres is still an open issue, despite being a critical factor in material selection, as sulfidation rates are typically orders of magnitude higher than oxidation rates. This study investigates the influence of sulfur in the atmosphere on the high-temperature degradation of the TiNbCr RMPEA, comparing its performance with the Cobased alloy 188, which is widely used in sulfur-rich environments. Isothermal tests were conducted between 600°C and 1100°C for up to 100 h, followed by characterization via SEM/EDS and XRD analyses. Under oxidation conditions, TiNbCr exhibited linear kinetics between 800°C and 1000°C due to the formation of non-protective oxides. However, at 1000°C, a Cr₂O₃-rich layer developed, leading to a tendency toward parabolic behavior. In a sulfidizing atmosphere, TiNbCr exhibited parabolic kinetics with the internal formation of NbS2, though with reduced protection compared to pure Nb due to Cr and Ti cation intercalation. In contrast, alloy 188 formed non-protective reaction products (i.e., liquid eutectics), whereas TiNbCr demonstrated superior performance, suggesting its potential for applications in sulfur-containing

environments. This study advances the understanding of high-temperature degradation

mechanisms in RMPEAs, providing insights into their behavior under oxidation and sulfidation

Keywords: Multi-principal element alloy, refractory elements, high-temperature oxidation

10

In situ Synthesis of WC-W₂C-Cu-Graphite Composites by Spark Plasma Sintering

Tomila Vidyuk

Khristianovich Institute of Theoretical and Applied Mechanics, Siberian Branch of Russian Academy of Sciences, Institutskaya str., 4/1, Novosibirsk, 630090, Russia e-mail: vidyuk@itam.nsc.ru

In situ synthesized metal matrix composites possess a fine reinforcing particle size, uniform particle distribution, and clean particle-matrix interfaces with good bonding. These advantages allow in situ composites to have high mechanical properties. Spark Plasma Sintering (SPS) of reactive powder mixtures is a way of obtaining nanostructured composites by the synthesis of new phases in a metallic matrix. Before SPS, mechanical milling of a mixture of starting powders is usually conducted in order to facilitate their interactions. In the W-C-Cu system, the WC and W₂C phases can be synthesized through exothermic reactions during SPS. In this study, the components in the reaction W-C(graphite)-Cu mixtures were taken in three different molar ratios of elements of 1:1:3, 1:1.3:3 and 1:1.7:3. The excess of graphite remained unreacted in the sintered materials. The present study focuses on the structure formation of the material during SPS and the properties of the sintered materials. The structure of the sintered composites is unconventional: Cu-rich regions are located between the composite W-rich areas, in which the WC and W₂C particles are distributed uniformly. The formation of this structure is related to inter-particle melting during SPS induced by high electrical current densities. Increasing the concentration of graphite reduced both electrical conductivity and hardness of the composites. The WC-W₂C-Cu-graphite composite (processing conditions: W-C(graphite)-3Cu mixture, 15 min of milling, SPS at 980°C) shows an attractive combination of properties: a hardness of 250 HV, an electrical conductivity of 25% of the International Annealed Copper Standard, a residual porosity less than 5%, a coefficient of friction in a pair with a WC-6Co ball of 0.58, and a specific wear rate of 0.6×10^{-5} mm³ N⁻¹ m⁻¹.

The work has been funded by the Russian Science Foundation, grant number № 25-79-00253, https://rscf.ru/en/project/25-79-00253/.

Probing Engineering Materials at the SKIF Synchrotron Facility

Ivan Bataev

Novosibirsk State Technical University, K. Marks 20, Novosibirsk, Russian Federation, 630073 e-mail: i.bataev@corp.nstu.ru

The talk will be split into two parts. The first part is devoted to our previous studies of engineering materials at the ESRF, DESY, and other synchrotron sources. Examples of phase transformations and the evolution of dislocation structure in steels, Ti alloys, high-entropy alloys, and other engineering materials will be discussed. These detailed studies were previously published in [1-3]. The second part of the talk is devoted to the presentation of a concept for a new beamline for engineering materials at the SKIF synchrotron facility, which has been developed by our group.

- [1] Thoemmes, A., et al. Microstructure and lattice parameters of suction-cast Ti–Nb alloys in a wide range of Nb concentrations. *Materials Science and Engineering: A*, 2021, 818: 141378.
- [2] Ivanov, I., et al. Anomalous growth of dislocation density in titanium during recovery. *Materials Today Communications*, 2023, 35: 106298.
- [3] Bataev, I. A., et al. A novel operando approach to analyze the structural evolution of metallic materials during friction with application of synchrotron radiation. *Acta Materialia*, 2020, 196: 355-369.

The influence of heat treatment on the structure and mechanical properties

high-entropy bulk metallic glass Zr₃₅Hf_{17.5}Ti_{5.5}Al_{12.5}Co_{7.5}Ni₁₂Cu₁₀

Nasennik Igor^{1,2}

¹ Novosibirsk State Technical University, Novosibirsk, Russia

² Siberian Circular Photon Source (SKIF), Boreskov Institute of Catalysis SB RAS, Kol'tsovo,

Russia

e-mail: nasennik.2017@corp.nstu.ru

The unique combination of high strength and plasticity in high-entropy bulk metallic glasses (HE-BMGs) makes them promising for advanced applications. However, their metastable nature leads to structural changes under thermal exposure, significantly affecting properties. This study investigates the effect of isothermal annealing below the glass transition temperature (Tg) on the structure and mechanical behavior of the Zr₃₅Hf_{17.5}Ti_{5.5}Al_{12.5}Co_{7.5}Ni₁₂Cu₁₀ HE-BMG.

The HE-BMG alloy was prepared by arc-melting and copper mold suction casting. Amorphous structure was confirmed by X-ray diffraction (XRD). Samples were subjected to isothermal annealing at temperatures 370, 400, 430, 460°C for 3 hours. Structural evolution was analyzed using XRD, transmission electron microscopy (TEM). Mechanical properties were assessed via Vickers microhardness measurements and uniaxial compressive testing at room temperature.

The initial relaxation stage caused a 10-15% increase in microhardness and compressive strength, attributed to the densification of the glassy structure. However, this was accompanied by a drastic embrittlement, with plastic strain reducing to near zero. The subsequent nanocrystallization further increased hardness but led to catastrophic failure without macroscopic plasticity due to the loss of the homogeneous deformation mechanism and the nucleation of cracks at crystal-amorphous interfaces.

Heat treatment of the Zr-based HE-BMG allows for tailoring its mechanical properties but presents a trade-off between strength and plasticity. Structural relaxation, while increasing strength, causes severe embrittlement. The controlled formation of nanocrystals can enhance hardness but requires precise optimization to avoid a complete loss of ductility. These findings are crucial for developing thermal processing routes for HE-BMGs intended for use in loadbearing conditions.

The study was supported by the Ministry of Science and Higher Education of the Russian Federation as a part of the state task FSUN-2024-0005 "Structural transformations in surface layers of metal alloys under extreme thermal and deformation impacts".

13

Investigation of L1₂ homogeneity range by TiAl₃-Me diffusion couples, where

Me = Cr, Mn, Fe, Ni, Cu

Natalia Aleksandrova^{1,2}

¹ Novosibirsk State Technical University, Novosibirsk, Russia

² Siberian Circular Photon Source (SKIF), Boreskov Institute of Catalysis SB RAS, Kol'tsovo,

Russia

e-mail: aleksandrovanatalie99@gmail.com

The application of titanium trialuminide is limited by high brittleness, which is inherent to its tetragonal D022 crystal structure. Alloying with transition metals enables the transformation of the D0₂₂ structure into the cubic L1₂ phase, thereby enhancing the compound's ductility [1]. Nevertheless, the formation of brittle secondary phases is often observed in alloys, which counterbalances the effect of stabilization of the L1₂ structure [2].

To solve the problem of secondary phase precipitation in alloys, TiAl₃-Me diffusion couples were obtained, where Me is Cr, Mn, Fe, Ni, Cu. The purpose of this investigation was to evaluate the L1₂ homogeneity range. Samples were obtained by spark plasma sintering. Then samples were heat-treated for 100 hours at 800 °C.

The presence of an L12 layer in TiAl3-Me diffusion couples was confirmed using synchrotron Xray diffraction. The L1₂ homogeneity range was determined using elemental analysis on a Carl Zeiss EVO50 XVP scanning electron microscope equipped with an X-Act energy dispersion Xray detector. The results indicate that single-phase alloys should contain more titanium (~ 25-26 at. %) compared to the literature data.

Acknowledgments

The study was supported by the Ministry of Science and Higher Education of the Russian Federation as a part of the state task FSUN-2024-0005 "Structural transformations in surface layers of metal alloys under extreme thermal and deformation impacts".

The structural research was carried out at core facility "Structure, mechanical and physical properties of materials", NSTU.

References

[1] Stoloff N. S., Sikka V. K. Physical metallurgy and processing of intermetallic compounds. – Berlin/Heidelberg: Springer Science & Business Media, 2012.

[2] Mabuchi H. et al. Formation of ternary L12 intermetallic compound and phase relation in the Al-Ti-Fe system. Mater. Trans. JIM. 41 (2000) 733–738.

Effect of ZrO_2 additive on structure and magnetic properties of Mn-Zn ferrites

Roman R. Khabirov*, Anna V. Mass, Mikhail Yu. Agafonov, Alexander. A. Miller Novosibirsk State Technical University, K. Marx Ave. 20, Novosibirsk, 630073, Russia *e-mail: xabirov.2016@stud.nstu.ru

Mn–Zn ferrites are employed in magnetic cores for electronic components. The drive to higher operating frequencies to improve device efficiency necessitates the development of a fine-grained ferrite microstructure, which ensures reduced eddy-current losses. At the same time, Mn–Zn ferrites are prone to abnormal grain growth arising from trace impurities. To inhibit the growth of oversized grains, insoluble additives such as ZrO₂ are introduced into the ferrite composition. In this study we investigate the effect of a 500 ppm ZrO₂ additive on sintered Mn–Zn ferrites and examine its interaction with trace impurities in the starting oxide powders.

Ferrite cores were fabricated from oxide mixtures with varying impurity levels: batch A contained 250 ppm Ba and 600 ppm Ca; batch B contained no Ba and 200 ppm Ca. The ZrO₂ additive was introduced during the milling stage after mixing and calcination of the precursor oxides. Sintering was performed at 1300 °C, followed by cooling under reduced oxygen partial pressure.

Ferrites derived from batch A without ZrO_2 exhibited a fine-grained structure (average grain size $\sim 2.5~\mu m$) but included abnormal large grains ($\sim 25~\mu m$). The addition of 500 ppm ZrO_2 suppressed abnormal grain growth and yielded a 40 % reduction in eddy-current losses. The increase in density from 4.60 to 4.93 g/cm³ facilitated higher maximum induction and lower hysteresis losses. In the case of batch B, the average grain size decreased from 9.5 to 8.3 μm with ZrO_2 addition, although the density declined from 4.80 to 4.68 g/cm³. No abnormally large grains were detected, and the additive promoted increased initial permeability and reduced hysteresis losses. The lowest total losses at 400 kHz were observed for the fine-grained ferrite from batch A with 500 ppm ZrO_2 .

Research were conducted at core facility "Structure, mechanical and physical properties of materials".

Application of computer simulation to exlpain the experimental data and predict the structure and properties of intermetallic coatings

Daria V. Lazurenko

Novosibirsk State Technical University, Karl Marks av., 20, Novosibirsk, 630073, Russia e-mail: Pavlyukova_87@mail.ru

In this study, titanium aluminide-based coatings formed by the method of non-vacuum electron beam cladding were examined. Formation of the structure by this method can be quite complex. Often, heterogeneity in chemical composition is observed in coatings and the appearance of metastable phases occurs. Computer modeling methods can be used to analyze the composition of local coating zones and assess the influence of structural and phase heterogeneity on the properties of cladding layers. It was shown that calculation of phase diagrams and modeling within the framework of density functional theory can be effective tools for confirming and explaining experimental results and predicting the properties of the materials under study.

Microstructural influence on stress corrosion cracking of the carbon steel in

ethanol environment

Elielson Alves dos Santos

Federal University of São Carlos, Rua Rotary Clube 144, Vila Celina, São Carlos – SP, Brazil

e-mail: elielson.alves@ufscar.br

API X70 steel has been widely used in Brazil for the manufacture of ethanol transport pipelines,

however, a recognized problem in carbon steel pipes exposed to ethanol is stress corrosion

cracking (SCC). The goal of this work was to evaluate the SCC for X70 steel exposed to a

ethanol environment, with a view to the microstructure/environment interaction. Quench

treatment in synthetic mineral oil was developed to modification of as-received microstructure.

Mechanical tests were performed to analyze SCC susceptibility. Results on notched specimens

with as-received microstructure (AR) and heat treated as-received microstructure (HTRA)

revealed a important strain reduction after slow strain rate tests in ethanol solution. Under

constant load (CL), the AR microstructure steel appears no be sensitive to SCC at stress levels

below the yield strength, however, under staggered constant load (SCL) the phenomenon was

observed in both types of microstructure. The interaction between HTRA microstructure and

ethanol solution revealed better performance for steel evaluated.

Keywords: API X70 steel, Stress corrosion cracking, Ethanol environment.

17

Assessment of Air Carbon Arc Gouging Effects on Corrosion and Mechanical

Behavior of Stainless Steels

Arthur de Bribean Guerra

Department of Materials Engineering, Federal University of São Carlos (DEMa–UFSCar), Rodovia Washington Luís, km 235 – São Carlos, SP, 13565-905, Brazil e-mail: aguerra@ufscar.br, arthurdbguerra@gmail.com

Air carbon arc gouging (ACAG) is a widely used technique for defect removal and surface preparation prior to repair welding. However, its application to stainless steels remains controversial due to concerns over sensitization, carbon contamination, and localized corrosion. This work integrates findings from recent studies on austenitic (AISI 304, 316L, 321, 347H) and duplex (AISI 2205) stainless steels subjected to ACAG followed by submerged arc welding (SAW), providing a comprehensive understanding of the metallurgical and electrochemical effects of the process. Experimental assessments included microstructural characterization, double-loop electrochemical potentiokinetic reactivation (DL-EPR) tests, and oxalic acid etching in accordance with ASTM A262 and ISO 12732 standards. Mechanical performance was evaluated through tensile and Charpy impact testing. The results demonstrate that the influence of ACAG strongly depends on alloy composition and surface preparation. For low-carbon and stabilized austenitic grades (316L, 321, 347H), no increase in sensitization or intergranular corrosion susceptibility was detected, even in as-gouged conditions, validating ACAG as a safe and efficient method for field repairs. Conversely, AISI 304/ER308L welds exhibited significant sensitization, primarily due to the thermal cycle of SAW rather than the gouging process itself. In duplex stainless steel (2205), as-gouged surfaces showed higher DL-EPR activation ratios, but rewelded joints retained excellent mechanical integrity (UTS > 750 MPa) and resistance to localized corrosion when proper cleaning and joint geometry were employed. Overall, these results clarify the conditions under which ACAG can be confidently applied to stainless steels, ensuring defect removal and mechanical reliability without compromising corrosion resistance an outcome of particular relevance for petrochemical, offshore, and nuclear industries.

Electrochemical Characterization of Cr40Co40Ni20 Multi-Principal Element

Alloy: Corrosion Resistance and Passivation in Chloride Rich Environments

<u>Victor Hugo Mafra Monfredo Ferreira</u>^{a,b,d,z}, Virginie Roche^d, Margarita Diaz-Ramos^b,

Gustavo Bertoli^{a,b}, Alberto Moreira Jorge Junior^{a,d}, Jean-Claude Leprêtred Walter José Botta^{a,b},

Francisco Gil Coury^{a,b}, Guilherme Yuuki Koga^{a,b,c}

The corrosion resistance of the Cr40Co40Ni20 multi-principal element alloy was evaluated in chloride-rich electrolyte. The alloy was synthesized via vacuum induction melting and subjected to thermomechanical processing, including homogenization at 1100 °C, rolling to a final thickness of \sim 1 mm, and recrystallization heat treatment at 1050 °C for 30 minutes. Structural characterization using x-ray diffraction, scanning electron microscopy, and electron backscatter diffraction confirmed a refined and homogeneous single-phase microstructure with an average grain size of \sim 20 μ m.

The corrosion behavior was analyzed through cyclic potentiodynamic polarization and electrochemical impedance spectroscopy in 0.6M and 0.1M NaCl solutions. The results revealed that Cr40Co40Ni20 alloy is corrosion-resistant, forming a highly protective and stable passive film. The polarization resistance was measured at 200 k Ω ·cm² in 0.6M NaCl, significantly higher than the ~120 k Ω ·cm² observed for Inconel 625, indicating superior passivation. Electrochemical impedance spectroscopy analyses demonstrated a capacitive-like response with phase angles close to -85° and a resistivity at metal/oxide interface profile suggesting an insulator-like passive layer with a resistivity of 109 Ω ·cm, outperforming Inconel 625.

Keywords: High-entropy alloys, EIS, Passivation, Marine corrosion.

^a Federal University of São Carlos, Graduate Program in Materials Science and Engineering, Rod. Washington Luis, km 235, CEP 13565-905, São Carlos, SP, Brazil

^b Federal University of São Carlos, Department of Materials Science and Engineering, Rod. Washington Luis, São Carlos, SP, CEP 13565–905, Brazil

^c Federal University of São Carlos, Center for Characterization and Development of Materials (CCDM), Rod. Washington Luis, São Carlos, SP, CEP 13565–905, Brazil Washington Luis, São Carlos, SP, CEP 13565–905, Brazil

^d Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS, Grenoble INP, Institute of Engineering and Management Univ. Grenoble Alpes, LEPMI, Grenoble 38000, France ^zCorresponding author: victormonfredo@estudante.ufscar.br; *phone* +55 9198900-4152

Plasma Transferred Arc Deposition of Fe-Cr-Mo-Nb-B Coatings: Influence of

Processing Parameters on Wear Resistance

<u>L.C.M. Rodrigues</u>^{a,b,*}, G.Y. Koga^{b,c}, Ferreira, T^{a,b}, C. Bolfarini^b, C.S. Kiminami^b, Gustavo S. Prass^d, A. S. C. M. d' Oliveira^d e W.J. Botta^b

An innovative approach to process protective coatings used gas-atomized Fe₆₈Cr₈Mo₄Nb₄B₁₆ powders, deposited by Plasma Transferred Arc (PTA) process, with four distinct processing conditions, varying feeding rate (6 g/min and 10 g/min), particle size distribution (fine: 53-106 μm, coarse:106–180 μm, and a mix: 53-180 μm) and current intensity (120 A and 180 A). The coatings exhibited thicknesses of $\sim 2-3$ mm, porosity ranging from 0.11 ± 0.05 vol.% to 0.32 \pm 0.17 vol.%, strong metallurgical bonding, and dilution levels between 7% and 19%. Inspite of the challenges associated with processing crack free boron-rich alloys sound coatings were processing under the tested conditions. The best-performing coating, produced with 106-180 µm powders, feeding rate of 10 g/min, and current of 120 A, exhibited the lowest specific wear rate $(\sim 5.0 \times 10^{-5} \text{ mm}^3 \cdot \text{N}^{-1} \cdot \text{m}^{-1})$. The microstructure consisted of a dense matrix of crystalline α -Fe, M₂B, and M₃B₂ phases, with a dendritic α-Fe matrix and interdendritic borides, achieving Vickers microhardness values between 309 and 436 HV_{0.5}. The wear mechanisms observed included abrasive, oxidative, and adhesive processes, with hard debris incorporation and oxygen enrichment on worn surfaces. Compared to coatings produced by the L-PBF and HVAF it shows a high effectiveness both for refurbishing worn parts and to enhance steel components operating under severe wear conditions. The innovations focus on the relevance of processing parameters, which are decisive for the coating efficiency and the final properties of the material.

^a Federal University of São Carlos, Graduate Program in Materials Science and Engineering, Rod. Washington Luis, km 235, CEP 13565-905 São Carlos, SP, Brazil

^b Federal University of São Carlos, Department of Materials Science and Engineering, Rod. Washington Luis, km 235, CEP 13565-905 São Carlos, SP, Brazil

^c Federal University of São Carlos, Center for Development and Characterization of Materials (CCDM), Department of Materials Science and Engineering, Rod. Washington Luis, km 235, CEP 13565-905 São Carlos, SP, Brazil

^d Federal University of Paraná, Department of Mechanical Engineering, Curitiba – PR, Brazil Corresponding author: gykoga@ufscar.br (GYK) and luanacmiguel@gmail.com (LCMR)

Segregation-induced microstructural refinement in a FeMnAlC-TiB metal matrix composite by laser powder bed fusion

André L. Vidilli^{1,2,*}, Leonardo F. Gomes³, Adriel P. de Oliveira^{1,3}, Mainak Saha⁴, Taisuke Sasaki⁴, Lucas B. Otani², Ilva Okulov³, Claudemiro Bolfarini^{1,2}

Introducing titanium (Ti) and boron (B) into ferrous alloys has emerged as a promising strategy

to improve the mechanical performance of lightweight steels, such as Fe-Mn-Al-C systems, by

generating in-situ reinforcements and reducing overall density [1,2]. However, conventional

casting routes often involve slow cooling rates, which lead to coarse morphologies of the reinforcing particles and limit the potential of these composites. Additive manufacturing, particularly Laser Powder Bed Fusion (LPBF), provides a novel pathway for designing metal matrix composites with refined microstructures by leveraging rapid solidification and steep thermal gradients [3]. Despite these advantages, the role of solute segregation in grain refinement during LPBF processing remains not fully established, especially in complex ferrous systems. This work investigates the solidification behavior and microstructural development of a FeMnAlC-TiB composite fabricated via LPBF. The resulting material featured a δ -Fe matrix with nanometric equiaxed grains and no crystallographic texture, reinforced by in-situ formed carbide nanoprecipitates and an M₂B-type boride network. A combination of EBSD, TEM-ASTAR, and 3D Atom Probe analyses revealed significant boron segregation to grain boundaries during solidification, which led to the formation of a thermal undercooling zone ahead of the solid-liquid interface. This condition promoted heterogeneous nucleation and induced a columnar-to-equiaxed grain transition. The combined effect of grain refinement and reinforcing phases resulted in a 150% increase in hardness compared to the base alloy and enhanced mechanical strength relative to arc-melted and spray-formed counterparts. However, the presence of a brittle boride network contributed to reduced ductility. These results demonstrate the ability of LPBF to tailor solidification pathways and engineer high-performance ferrous composites through solute-driven microstructural control.

¹ Graduate Program in Materials Science and Engineering, Federal University of São Carlos, Rod. Washington Luiz, Km 235, 13564-905, São Carlos, SP, Brazil.

² Department of Materials Engineering, Federal University of São Carlos, Rod. Washington Luiz, Km 235, 13564-905, São Carlos, SP, Brazil.

³ Leibniz Institute for Materials Engineering – IWT, Badgasteinerstraße 3, 28359 Bremen, Germany.

⁴ Nanostructure Analysis Group, Research Center for Magnetic and Spintronic Materials, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan *e-mail: andre.vidilli@ufscar.br

Thermomechanical Fatigue Performance of DED-LB processed IN718

Thiago Cavalcante

Federal University of São Carlos, Rod. Washington Luis, km 235 - São Carlos - SP - BR CEP:

13565-905

e-mail: thiagorfc@ufscar.br

Additively manufactured IN718 produced by Directed Energy Deposition-Laser Beam (DED-LB) requires a clear understanding of how processing parameters and post-deposition heat treatments influence microstructural stability and high-temperature mechanical performance. In this work, a processing window was first established to minimize lack-of-fusion defects and porosity, yielding as-built conditions with a density exceeding 99.6% and a cellular-dendritic microstructure containing Laves and δ phases. Six heat-treatment routes were then applied, generating distinct microstructural states: homogenization promoted recrystallization and enhanced ductility, whereas aging treatments increased strength and hardness through γ'/γ' precipitation but reduced uniform elongation due to grain-boundary precipitation and coarsening. Tensile testing at 650 °C showed that the DED-LB as-built condition exhibited higher ultimate tensile strength than reported for forged IN718, while presenting greater ductility than the HSDA condition, though with lower strength relative to the aged states. Fractography revealed predominantly intergranular features in both forged and heat-treated DED-LB specimens. Outof-phase thermomechanical fatigue (TMF-OP) tests under 100% mechanical strain restriction demonstrated strong sensitivity to heat treatment: the as-built sample failed at ~2200 cycles, whereas the HSDA condition achieved ~4200 cycles, reflecting the beneficial distribution of coherent γ'/γ'' precipitates. Literature for conventionally processed IN718 indicate higher TMF lives, emphasizing the influence of residual porosity, segregated phases, and microstructural heterogeneity inherent to DED-LB. Overall, the findings elucidate the interplay between processing, microstructure, and high-temperature cyclic performance, providing essential guidance for optimizing DED-LB IN718 for service in thermomechanically demanding environments.

Porous Metallic High-Entropy Alloy Electrodes: Dealloyed Microstructure, Composition, and OER Proof-of-Concept

Yannick Champion^{a*}, Marian Chatenet^b, Virginie Roche^b, Remi Daudin^a, Gregory Berthomé^a,

Alberto Moreira Jorge Junior b,c

High-entropy alloys (HEAs) offer unique opportunities for tailoring microstructure and functionality through the design of multicomponent systems. In this work, a nanoporous HEA was created from the precursor composition (Ti₃₁V₂₆Zr₁₂Nb₂₆Co₅)₅₀Fe₅₀ via selective Fe dealloying. The resulting material exhibits a hierarchical porous morphology and retains mechanical integrity, rendering it a self-supporting electrode. Surface analysis showed compositional redistribution and the formation of Co- and V-based oxides/hydroxides, indicating dynamic surface reconstruction under alkaline conditions. Electrochemical measurements in 1 M NaOH confirmed the material's functional viability, with an overpotential of approximately 370 mV at 10 mA cm⁻² and stable cycling behaviour. For context, conventional NiFe hydroxides and noble-metal oxides achieve lower overpotentials but require either very costly powder processing or very costly precursors or are limited in scalability. In contrast, the present HEA is produced through metallurgical routes, is binder-free, and exhibits activity comparable to that of current HEA catalysts. This proof-of-concept study highlights nanoporous HEAs as a versatile material platform combining structural robustness with potential in energy-related electrochemical systems.

Keywords: high-entropy alloys, nanoporous structures, dealloying, microstructural characterisation, binder-free electrodes, alkaline electrolysis

^a Univ. Grenoble Alpes, CNRS, Grenoble INP, SIMaP, 38000 Grenoble, France

^b Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS, Grenoble INP (Institute of Engineering, Univ. Grenoble Alpes), LEPMI, 38000 Grenoble, France

^c Federal University of São Carlos, Graduate Program of Materials Science and Engineering, DEMa, São Carlos 13565-905, Brazil

Formation of Decagonal and Icosahedral Quasicrystals in the Al-Cu-Fe-Cr

System Under Diverse Processing Conditions

Adilson Vitor Rodrigues¹ & Witor Wolf^{2,*}

¹ Federal Institute of Education, Science and Technology of São Paulo

² University of São Paulo

*corresponding author: witorw@usp.br

Quasicrystals exhibit a remarkable range of physical and chemical properties, including low friction coefficients during sliding, low surface energy, low thermal conductivity, high hardness, high elastic modulus, and excellent wear resistance. However, their intrinsic brittleness at room temperature motivates the development of composite microstructures in which quasicrystalline phases are embedded within ductile matrices such as Al-FCC. Owing to this combination of characteristics, aluminum-based quasicrystalline alloys and composites show strong potential for tribological protection applications. In this work, we present recent advances in our studies of quasicrystal-forming alloys within the Al-Cu-Fe-Cr system. We demonstrate that a variety of manufacturing techniques, such as conventional casting, spray forming, gas atomization, laser remelting, and laser cladding, enable the production of microstructures containing quasicrystals and complex intermetallic phases. Our results indicate that the Al-Cu-Fe-Cr system is among the most flexible and cost-effective systems capable of forming quasicrystals under diverse processing conditions. Both decagonal and icosahedral quasicrystals can be obtained depending on alloy composition and solidification rate. Furthermore, these phases can be embedded in an Al-FCC matrix using either rapid or slow solidification routes, reinforcing the versatility of this system for designing advanced tribological materials.

In situ observation of phase transformations in Al-Cu-Li-Ag alloy

Igor Vitoshkin*, Alexander Malikov

Khristianovich Institute of Theoretical and Applied Mechanics SB RAS, Institutskaya str., 4/1,

Novosibirsk, 630090, Russia

*e-mail: vitoshkin@itam.nsc.ru

Al-Li alloys are known for their high strength to density ratio which is achieved by the formation

several strengthening phases. In case of the Al-Cu-Li-Ag alloy V-1469 alloy (developed by All-

Russian scientific research institute of aviation materials, VIAM) these phases are T₁ (Al₂CuLi)

and Ω (Al₂Cu) precipitated in form of 1-10 nm thin particles in result of heat treatment. Since

they both contain Cu atoms their formation is a competitive process. However, the Ω phase

formation provides better strengthening effect. Thus, heat treatment parameters optimization is

required.

In this work the behavior of these phases during heating is studied. To do this in situ synchrotron

diffraction study was conducted. In result, it was found that both T_1 and Ω decompose at

~520 °C and ~580 °C respectively. However, the Ω phase forms again at ~570 °C during the T₁

phase decomposition and stays stable when heating up to 600 °C (5 °C/min) and cooling down to

room temperature (~20 °C/min).

Thus, it was shown that Ω phase stabilizes after T₁ phase decomposition at ~580 °C. Holding the

material at this temperature before quenching may allow to precipitate higher amount of Ω phase

instead of T_1 phase, thereby achieve stronger hardening effect.

Funding sources

This research was funded by Russian Science Foundation, grant number 23-79-00037

(https://rscf.ru/project/23-79-00037/).

Acknowledgements

The work included the use of the equipment of the Equipment Sharing Center "Mechanics" of

ITAM SB RAS, the equipment of Sharing Center "Nanostructures" of ISP SB RAS and the

shared research center SSTRC on the basis of the VEPP-4 - VEPP-2000 complex at BINP SB

RAS.

25

Engineering Cavitation- and Corrosion-Resistant FeCrMnSiB Coatings

Processed by Thermal-Spray Techniques

Juliane Ribeiro da Cruz Alves

Department of Mechanical Engineering, University of São Paulo, Av. Prof. Mello Moraes, 2231, São Paulo, SP, 05508-030, BR

e-mail: juliane.rcruz@usp.br

Boron-containing austenitic stainless steels with low stacking-fault energy have been developed as cost-effective alloys for improved wear and cavitation resistance. In this work, the cavitation and corrosion resistance of FeCrMnSiB austenitic stainless-steel coatings processed by PTA were evaluated. The effects of boron content (0, 0.2, 0.5, and 1 wt%), powder chemicalcomposition homogeneity (atomized versus mechanically mixed powders), surface cold-work hardening (polished and machined), and different manufacturing techniques were investigated. Corrosion in 3.5 wt.% NaCl and cavitation erosion in deionized water were analyzed considering microstructural integrity, chemical partitioning, phase formation, and susceptibility to straininduced martensitic transformation, with comparisons to commercial reference materials. PTAprocessed B-containing coatings consisted of austenitic dendrites and an interdendritic eutectic of austenite plus needle-like Cr-rich borides. Cr partitioning depleted the adjacent austenite, making this region prone to cavitation and pitting corrosion. Despite developing more negative corrosion potentials, PTA coatings maintained competitive low corrosion current densities. Coatings produced with atomized powders exhibited an incubation period about three times longer than those made with mechanically mixed powders, attributed to cavitation strain-induced martensitic transformation. Increasing boron promoted microstructural refinement and higher FeCrB eutectic fractions, raising microhardness and reducing maximum cavitation-erosion rates. Cold working further improved performance, increasing hardness from 353 to 462 HV and lowering the cavitation maximum erosion rate. Due to strong metallurgical bonding, FeCrMnSiB coatings processed by PTA showed the lowest cavitation-erosion rates compared with coatings produced by arc plasma spray, cold spray, HVOF, and HVAF, which failed mainly by splat detachment and/or splat fracture. These findings support the design and processing of costeffective alloys and coatings for combined wear and corrosion resistance in hydraulic machinery.

Powder metallurgy processing of TiAl: counteracting their challenging densification through sintering

Juliano Soyama

School of Mechanical Engineering, University of Campinas, Rua Mendeleyev, 200, Campinas, 13083-860, Brazil

e-mail: jsoyama@unicamp.br

TiAl alloys are a class of intermetallics that are quite attractive for aerospace applications, considering their low density and good mechanical properties at high temperatures. Typical processing routes include casting and thermomechanical treatments, which are extremely costly. Consequently, as an alternative method, powder metallurgy is a strong candidate for small to medium-sized parts. Nonetheless, the powder routes in which sintering is required for densification have a serious drawback, considering the need for high sintering temperatures and the typical residual porosity. One of the greatest challenges of powder metallurgy processing of titanium aluminides is to deal with their high sintering temperatures (>1400 °C). In this work, processing of ternary Ti-45Al with Co or Ni additions was conducted to facilitate sintering through liquid phase formation. The specimens were cylinders with 8 mm diameter prepared using blended elemental powders, followed by cold uniaxial pressing. Sintering was carried out under argon atmosphere at different temperatures ranging from 1100 to 1400 °C for 2 hours in an alumina tube furnace. Microstructural investigation was conducted by Scanning Electron Microscopy and X-Ray Diffraction. Porosity and densification were determined by image analysis using Light Optical Microscopy and the software ImageJ. The mechanical properties were evaluated through Vickers microhardness tests and compression creep. The results indicated that there was an increase in densification with Co and Ni additions. Due to the exothermic formation of intermetallics, the relative density of the reference material Ti-45Al was approximately 53%. Nevertheless, Co and Ni additions led to a relative density in the order of 80%. An increase in hardness was also observed in comparison to the reference alloy Ti-45Al, as well as an improved compression creep resistance.

Multicomponent Alloys for Hydrogen Storage: From Design to Performance

Ricardo Floriano*

School of Applied Sciences, University of Campinas (FCA-UNICAMP), Pedro Zaccaria, 1300,

13484-350, Limeira, Brazil

e-mail: rflorian@unicamp.br

Multicomponent alloys (MAs) are emerging as promising materials for solid-state hydrogen storage due to their broad compositional range and tunable properties. This presentation explores recent advancements in the design, synthesis, and characterization of new MAs as metal hydrides for hydrogen storage at room temperature. Our focus is on AB₂-type intermetallic hydrides with a high amount of C14-Laves phase. We employ a systematic MAs design strategy integrating semi-empirical parameters - atomic radius ratio (rA/rB \approx 1.116), mixing enthalpy (Δ Hmix), atomic size mismatch (δ), electronegativity difference ($\Delta \chi$), and valence electron concentration (VEC) - along with CALPHAD thermodynamic simulations and machine learning approach. MAs are synthesized via arc melting and characterized using SEM, TEM, and XRD. Their hydrogen storage properties are assessed through kinetic measurements and pressurecomposition-temperature (PCT) isotherms. Our results indicate that several MAs predominantly

form the C14 Laves phase with minor BCC (<5 wt%) content. Reversible hydrogen capacities

range from 1.70 to 1.90 wt% with rapid absorption kinetics at room temperature. Notably, MAs

derived from the TiZrCrMnFeNi, TiZrMnFeCo and TiZrNbFeNi begin hydrogen absorption

immediately, while others require mild activation (Zr33(CrMnFeNi)67, Zr33Cr22Mn15Fe25Ni5, and TiZrFeNiV). These findings highlight MAs as the potential for efficient hydrogen storage

applications.

Keywords: High-entropy Alloys, Hydrogen Storage, CALPHAD, C14-Laves Phase

28

Influence of magnetic pulse welding parameters on phase composition and structure of nickel-aluminum joints

Tatiana Ogneva

Novosibirsk State Technical University, Karl Marks ave. 20, Novosibirsk, Russia e-mail: pandorra.06@mail.ru

This work presents a comprehensive experimental and numerical study on magnetic pulse welded (MPW) joints of nickel and aluminum. The welding was performed using a unique flatsheet inductor setup at impact angles of 10° and 13°. The joint interface was characterized using scanning electron microscopy (SEM), transmission electron microscopy (TEM), energydispersive X-ray spectroscopy (EDX), and nanoindentation. Numerical modeling combined Smoothed Particle Hydrodynamics (SPH) to simulate the macro-scale process (temperature, pressure, interface morphology) with molecular dynamics (MD) to investigate atomic-scale interdiffusion. Key findings reveal that the interface morphology transitions from flat at the weld start to wavy at the end, with the 13° sample exhibiting more pronounced waves and vortex mixing. SPH results showed higher interface temperatures in the 10° sample (1370–1910 K) compared to the 13° sample (1320–1580 K). Elevated temperatures promoted the formation of NiAl₃ and NiAl intermetallics. The 13° sample's interface consisted mainly of a nickel-inaluminum solid solution. At the end of the 10° sample weld, a smooth, continuous layer formed due to temperatures exceeding nickel's melting point. The increased nanohardness suggests the presence of hard intermetallics like Ni₂Al₃ in these areas. MD simulations confirmed intensified interdiffusion at 1910 K, with interdiffusion coefficients $7 \times 10-8 \text{ m}^2/\text{s}$. The study demonstrates that phase composition in Ni-Al MPW joints can be controlled via welding parameters. The combined SPH, MD and experimental approach provides a pathway for optimizing MPW processes for dissimilar materials.

The study was supported by the Ministry of Science and Higher Education of the Russian Federation as a part of the state task FSUN-2024-0005 "Structural transformations in surface layers of metal alloys under extreme thermal and deformation impacts".

Mechanics-based surrogate models for accurate multiscale numerical analysis

of advanced materials

Alexey Shutov^{1,2,*}, Kirill Ufimzev^{1,2}

The multiscale finite element method (FEM²) is based on modeling of representative volume elements (RVEs) of the materials under study [1]. This general approach allows automatic generation of microstructure-based elasto-plastic constitutive relations covering a wide range of loading scenarios. To improve the computational efficiency of the FEM² approach, we suggest a novel type of surrogate models for RVEs, termed Ersatz Models (EMs). EMs are abstract mechanical devices characterized by generalized external and internal degrees of freedom [2]. Importantly, EMs inherently capture geometrical and material nonlinearities while strictly adhering to fundamental principles of constitutive modeling, including power balance, objectivity, and thermodynamic consistency. Due to their built-in non-affine kinematics, EMs can accurately represent the behavior of a broad spectrum of complex materials. Moreover, EMs involve relatively few adjustable parameters, allowing constitutive relations based on EMs to be calibrated using small synthetic datasets. Additionally, EMs have significantly fewer degrees of freedom than the original finite element models of RVEs, substantially enhancing computational efficiency in FEM² simulations. This presentation discusses the key principles behind EM construction and introduces an algorithm for their sequential refinement. Two application examples are provided, involving RVEs of porous metallic materials and alloys with distributed damage.

This study was supported by the Russian Science Foundation, project number 23-19-00514.

References:

- [1] Smit R.J.M., Brekelmans W.A.M., Meijer H.E.H., Prediction of the mechanical behavior of nonlinear heterogeneous systems by multi-level finite element modeling, Computer Methods in Applied Mechanics and Engineering, 1998, Vol. 155, No. 1-2, pp. 181–192.
- [2] Shutov A., Ufimzev K., Computationally efficient ersatz models for mechanical structures and refined material modeling, SSRN 4826630.

¹Lavrentyev Institute of Hydrodynamics, Novosibirsk, Russia

²Novosibirsk State University, Novosibirsk, Russia

^{*}e-mail: alexey.v.shutov@gmail.com

Modeling and Experimental Study of Electric Heating and Consolidation Mechanics of Material Granules under Spark Plasma Sintering Conditions

Krizhanovskii V.V.^{1,2,*}, Anisimov A.G.¹, Esikov M.A.¹, Dudina D.V.¹, Pruuel E.R.¹

Lavrentyev Institute of Hydrodynamics SB RAS, Novosibirsk, Russia¹

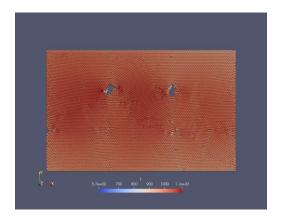
Novosibirsk State University (NSU), Novosibirsk, Russia²

*e-mail: FehtunKrizh@gmail.com; FehtunKrizh@mail.ru; krizhanovskij.v.v@hydro.nsc.ru

This work presents the development of a numerical method for simulating complex physical processes occurring during **Spark Plasma Sintering (SPS)** — one of the most promising techniques in powder metallurgy, combining rapid electric heating, mechanical pressing, and consolidation of granular materials. The main result of the study is the development and implementation of the Method of Movable Control Volumes (**MMCVM**) — a novel approach that unites the advantages of discrete and continuum modeling methods.

The essence of the method lies in representing the material as an ensemble of nodes, each associated with a control volume and interacting with its neighbors via elastic bonds. Unlike classical approaches (FEM, DEM), in **MMCVM** a node is not treated as a point mass, but as a small continuous volume defined by a characteristic length scale L_0 — the distance at which inter-nodal interaction forces vanish. This allows for a natural description of both mechanical deformation and consolidation, as well as heat and electric current transfer under strong gradients and bond breakage. A key feature of **MMCVM** is the **birth and death of inter-nodal bonds**, governed by distance thresholds: bonds are born when nodes approach within $L \le 0.95L_0$ and die when $L \ge 1.1L_0$. This approach enables modeling not only elastic and plastic deformations, but also fracture and consolidation processes **without the need for mesh regeneration** — a significant advantage over the Finite Element Method.

The method is applied to simulate spark plasma sintering of an ensemble of 9 granules (8379 nodes) with a diameter of $800 \mu m$. It is shown that under pulsed current conditions, localized overheating zones arise at inter-granular contacts — in agreement with experimental observations. Figure 1 demonstrates the final stage of pressing, when the consolidated material is fully formed.



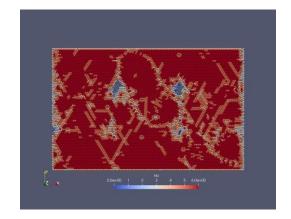


Figure 1. Final consolidated material obtained under pulsed current. Left: temperature field; right: distribution of the number of bonds.

Novelty of the work:

- A new numerical method (MMCVM) is proposed, fundamentally different from existing ones, combining discrete medium description with the ability to model continuous fields.
- For the first time within a single framework, electric heating, mechanical consolidation,
 and thermomechanical properties of the final material including its behavior under strength testing are modeled simultaneously.
- The method enables a natural description of **fracture and consolidation** without introducing additional criteria or requiring mesh reconstruction.
- Scientific and Practical Significance:
- MMCVM opens new opportunities for deep understanding of SPS mechanisms, including the nature of localized overheating, contact zone formation, and strength development.
- The method can be used to **optimize sintering regimes** without costly experimental campaigns.
- The ability to simulate mechanical tests (compression, tension, Poisson's ratio determination)
 on the final material makes MMCVM a powerful tool for predicting operational properties
 of engineered materials.

Thus, the developed **Method of Movable Control Volumes** represents a universal computational platform for studying complex multiphysical processes in granular media.

Characterization of hydrogen in alloys using Atom Probe Tomography

Eric Mazzer

Federal University of São Carlos, Rod. Washington Luís, s/n - Monjolinho, São Carlos - SP,

13565-905, Brazil

mechanisms.

e-mail: eric.mazzer@ufscar.br

This work presents a cryogenic atom probe tomography (cryo-APT) methodology developed to directly characterize hydrogen and deuterium in metallic alloys, with emphasis on Ti-6Al-4V. Conventional APT suffers from artefactual hydrogen contamination and specimen damage during preparation. To overcome these challenges, a series of workflows were developed integrating electrochemical deuterium charging, cryogenic transfer, and cryo-focused ion beam (cryo-FIB) specimen preparation. The optimized procedure enabled reliable isotope incorporation, preservation, and nanoscale detection. APT reconstructions revealed clear deuterium enrichment in the α phase, while uncharged baselines confirmed that hydrogen peaks originate from chamber background. Additional APT studies on Ni- and Fe-based alloys provided complementary insight into solute partitioning and defect segregation. Together, these results demonstrate that cryo-APT is a powerful and reproducible approach for studying hydrogen behavior in alloys and advancing the understanding of hydrogen-induced degradation

Development of Multifilamentary NbTi Superconducting Wires in Brazil at

CNPEM: Processing, Microstructure, and Performance

Dr. Tales Ferreira

Brazilian Center for Research in Energy and Materials – CNPEM

Technological Development Specialist – Adjunct Division of Technology (DAT-CNPEM)

Av. Giuseppe Máximo Scolfaro, 10.000 - Campinas - SP, 13083-970

e-mail: tales.ferreira@cnpem.br / tferreira.tales@gmail.com

The national production of NbTi superconducting wires requires overcoming critical challenges in alloy purity, billet sealing, thermo-mechanical processing, and microstructural control. This work presents a two-year effort to establish a complete manufacturing route for multifilamentary NbTi wires at CNPEM, addressing these challenges through an integrated processing and characterization approach. The NbTi alloy was produced using an in-house arc-melting furnace, designed to meet rigorous atmospheric requirements and minimize impurity incorporation. Billets were assembled with NbTi rods, Nb diffusion barriers, and oxygen-free copper stabilizer. TIG welding was adopted for billet sealing, replacing conventional electron-beam welding while ensuring vacuum integrity and reducing manufacturing costs. The sealed billets were processed by rotary forging and multi-step cold drawing with intermediate annealing to promote grain refinement, uniform filament deformation, and controlled α-Ti precipitation. Microstructural evolution was examined by SEM/EDS, TEM, and XRD, confirming filament homogeneity and NbTi-Nb-Cu interfaces. Cryogenic transport measurements superconducting behavior and a critical current density of 1500 A/mm² at 6 K in CNPEM's first multifilament prototype. These results demonstrate the feasibility of a national NbTi wiremanufacturing route and represent a significant step toward establishing Brazil's technological capability in superconducting materials.