

Mgr. Maroš Halama, PhD.

Technická univerzita v Košiciach

Fakulta materiálov, metalurgie a recyklácie

Ústav materiálov a inžinierstva kvality

Podklady k habilitačnému konaniu

**ZOZNAM PÔVODNÝCH PUBLIKOVANÝCH VEDECKÝCH A ODBORNÝCH PRÁC,
UČEBNÍČ A UČEBNÝCH TEXTOV SO ZOZNAMOM EVIDOVANÝCH CITÁCIÍ
A OHLASOV**

Technická univerzita v Košiciach
Prehľad publikačnej činnosti vrátane ohlasov
Autor: HALAMA, Maroš
Rok vydania od: 2002 do: 2021
Rok vykazovania od: 2002 do: 2021
Dátum generovania výstupu: 18. 8. 2021, 9:52:25

Skupina A1 - Knižné publikácie charakteru vedeckej monografie (AAA, AAB, ABA, ABB, ABC, ABD)

Počet záznamov: 1

ABC - Kapitoly vo vedeckých monografiách vydané v zahraničných vydavateľstvách (1)

Skupina A2 - Ostatné knižné publikácie (ACA, ACB, BAA, BAB, BCB, BCI, EAI, CAA, CAB, EAJ, FAI)

Počet záznamov: 15

ACB - Vysokoškolské učebnice vydané v domácich vydavateľstvách (1)

BAB - Odborné monografie vydané v domácich vydavateľstvách (3)

BCI - Skriptá a učebné texty (1)

FAI - Redakčné a zostavovateľské práce knižného charakteru (bibliografie, encyklopédie, katalógy, slovníky, zborníky...) (10)

Skupina B - Publikácie v karentovaných vedeckých časopisoch a autorské osvedčenia, patenty a objavy (ADC, ADD, AEG, AEH, BDC, BDD, CDC, CDD, AGJ)

Počet záznamov: 9

ADC - Vedecké práce v zahraničných karentovaných časopisoch (8)

AGJ - Autorské osvedčenia, patenty, objavy (1)

Skupina C - Ostatné recenzované publikácie (ACC, ACD, ADE, ADF, AEC, AED, AFA, AFB, AFC, AFD, AFE, AFF, AFG, AFH, BBA, BBB, BCK, BDA, BDB, BDE, BDF, BEC, BED, BFA, BFB, BGH, CDE, CDF)

Počet záznamov: 98

ADE - Vedecké práce v zahraničných nekarentovaných časopisoch (9)

ADF - Vedecké práce v domácich nekarentovaných časopisoch (7)

AEC - Vedecké práce v zahraničných recenzovaných vedeckých zborníkoch, monografiách (2)

AED - Vedecké práce v domácich recenzovaných vedeckých zborníkoch, monografiách (1)

AFB - Publikované pozvané príspevky na domácich vedeckých konferenciách (1)

AFC - Publikované príspevky na zahraničných vedeckých konferenciách (21)

AFD - Publikované príspevky na domácich vedeckých konferenciách (17)

AFE - Abstrakty pozvaných príspevkov zo zahraničných konferencií (1)

AFF - Abstrakty pozvaných referátov z domácich konferencií (3)

AFG - Abstrakty príspevkov zo zahraničných konferencií (14)

AFH - Abstrakty príspevkov z domácich konferencií (12)

BDF - Odborné práce v domácich nekarentovaných časopisoch (4)

BFA - Abstrakty odborných prác zo zahraničných podujatí (konferencie...) (6)

Skupina N - Nové kategórie EPC v zmysle Vyhlášky č. 456/2012 (ADM, ADN, AEM, AEN, BDM, BDN, CBA, CBB)

Počet záznamov: 3

ADM - Vedecké práce v zahraničných časopisoch registrovaných v databázach Web of Science alebo SCOPUS (2)

ADN - Vedecké práce v domácich časopisoch registrovaných v databázach Web of Science alebo SCOPUS (1)

Počet záznamov spolu: 126

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Menný zoznam citovaných publikácií:

ADC - Vedecké práce v zahraničných karentovaných časopisoch(8)

ADC001 [59894] **Anodic oxidation of both particulate and compact iron in chloride-containing acetate buffer electrolytes** / Maroš Halama, Daniela Kladeková, Miriam Gálová - 2007. In: Particulate Science and Technology. Vol. 25, no. 3 (2007), p. 261-274. - ISSN 0272-6351 Spôsob prístupu: <http://www.informaworld.com/smpp/content?content=10.1080/02726350701375840>.

[HALAMA, Maroš (34%) - KLADEKOVÁ, Daniela (33%) - GÁLOVÁ, Miriam (33%)]

Ohlasy:

2013 [1] PIKNA, L. et al. Anodic dissolution of iron microparticles in chloride-containing acetate buffer electrolytes studied by elimination voltammetry In: Journal of solid state electrochemistry Vol. 17, no. 10 (2013), p. 2687-2696 ISSN: 1432-8488

ADC002 [109521] **Prediction of Atmospheric Corrosion of Carbon Steel Using Artificial Neural Network Model in Local Geographical Regions** / M. Halama, K. Kreislova, J. Van Lysebettens - 2011. In: Corrosion : The Journal of Science and Engineering. Vol. 67, no. 6 (2011), p. 1-6. - ISSN 0010-9312 Spôsob prístupu: <http://dx.doi.org/10.5006/1.3595099>.

[HALAMA, Maroš (80%) - KREISLOVA, Katerina (10%) - LYSEBETTENS, Jeroen Van (10%)]

Ohlasy:

2015 [1] SHI, Jiangbo, WANG, Jihui, MCDONALD, Digby Donald Prediction of primary water stress corrosion crack growth rates in Alloy 600 using artificial neural networks In: Corrosion Science Vol. 92 (2015), p. 217-227 ISSN: 0010-938X

2019 [1] CHEN, Bo et al. Performance evaluation of veticulated shell with atmospheric corrosion damage In: Advances in Structural Engineering Vol. 22, no. 4 (2019), p. 850-867 ISSN: 1369-4332

2019 [3] ZHENHUA, Li, YONGHAO, Lu, XINYU, Wang Modeling of stress corrosion cracking growth rates for key structural materials of nuclear power plant In: Journal of Materials Science Dostupné na internete: <https://doi.org/10.1007/s10853-019-03968-w> ISSN: 0022-2461

2018 [1] HAVEROVÁ, L. et al. An in vitro corrosion study of open cell Iron structures with PEG coating for bone replacement applications In: Metals Vol. 8, no. 7 (2018), p. art. num. 499 ISSN: 2075-4701

2017 [1] LO, Chih-Min, CHIU, Yen-Ming, LIN, M.D. Predicting atmospheric corrosion rates of copper in Taiwan industrial zones using artificial neural network In: IEEE International Conference on Industrial Engineering and Engineering Management (IEEM) : Singapore, Hong Kong, 10-13 December 2017 P. 1276-1280 ISSN: 2157-3611

ADC004 [111648] **Quality Evaluation of Resistance Spot Welds of Hot-Dip Galvanized Sheets In Corrosive Environment** / Ľuboš Kaščák ... [et al.] - 2011. In: Chemické listy. Vol. 105, no. S (2011), p. 709-712. - ISSN 0009-2770 Spôsob prístupu: http://www.chemicke-listy.cz/docs/full/2011_17_s705-s716.pdf.

[KAŠČÁK, Ľuboš (25%) - BREZINOVÁ, Janette (25%) - HALAMA, Maroš (25%) - VIŇÁŠ, Ján (25%)]

Ohlasy:

2017 [1] SEJČ, P. et al. Stability of Ni / TiB₂ coating on CuCrZr electrodes for resistance spot welding galvanized steel sheet In: Manufacturing Technology Vol. 17, no. 4 (2017), p. 570-576 ISSN: 1213-2489

2020 [3] REYAD, Masud Mohammad Numerical Analysis of Resistance Spot Welded Joints Under Static Load In: International Journal of Innovative Science and Research Technology Vol. 5, no. 3 (2020), p.

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444-449 ISSN: 2456-2165

ADC005 [112724] **Analýza Fe-Al medzifázovej vrstvy v Zn-povlaku ocele HX180YD** / Gejza Rosenberg ... [et al.] - 2011. In: Chemické listy. Vol. 105, no. Symposia (2011), p. 568-570. - ISSN 0009-2770

[ROSENBERG, Gejza (40%) - GAŠKO, Marek (20%) - SINAIOVÁ, Iveta (20%) - HALAMA, Maroš (20%)]
Ohlasy:

2012 [3] WESSELY, E., EVIN, E., TOMAS, M. Prediction of deformation properties of steel sheets by numerical simulation In: DAAAM International Scientific Book 2012 Vol. 11 (2012), p. 019-026 ISSN: 1726-9687 ISBN: 978-3-901509-86-5

ADC006 [147041] **Hall Effect in ZnO Extrinsic Structure** / B. Dolník ... [et al.] - 2014. In: Acta Physica Polonica A. Vol. 126, no. 1 (2014), p. 76-77. - ISSN 1898-794X Spôsob prístupu:

<http://przrybwn.icm.edu.pl/APP/PDF/126/a126z1p034.pdf>.

[DOLNÍK, Bystrík (65%) - KURIMSKÝ, Juraj (20%) - MARTON, Karol (1%) - KOLCUN, Michal (1%) - TOMČO, Ladislav (1%) - BRIANČIN, J. (4%) - FABIÁN, M. (1%) - HALAMA, Maroš (1%) - VOJTKO, Marek (4%) - RAJNÁK, Michal (2%)]

Ohlasy:

2014 [4] TKÁČ, Ján, HVIŽDOŠ, Marek Meranie vlastností nelineárnych dielektrík na báze titánu In: Starnutie elektroizolačných systémov Roč. 9, č. 2 (2014), s. 16-18 ISSN: 1337-0103

ADC007 [207918] **Anti-corrosive surface effect of ascorbic acid caused on the ZnO nanoparticles - Experimental and theoretical investigations** / Lucia Mydlova ... [et al.] - 2019. In: Applied Surface Science : A Journal Devoted to Applied Physics and Chemistry of Surfaces and Interfaces. - Amsterdam (Holandsko) : Elsevier, 1985 č. 483 (2019), s. 562-571 [print]. - ISSN 0169-4332 Spôsob prístupu:

<https://doi.org/10.1016/j.apsusc.2019.03.324>.

[MYDLOVA, Lucia (30%) - KLUZA, Kamil (15%) - HALAMA, Maroš (30%) - MAKOWSKA-JANUSIK, Malgorzata (25%)]

Ohlasy:

2021 [1] Radkowska, Ilona, Bragieli, Piotr 1-Naphthols as components for multifunctional material systems (MFMS): the molecular modeling approach In: Structural Chemistry : an international journal concerned with energy, structure, and their relationships to chemical, physical, and biological properties : Computational and Experimental Studies of Chemical and Biological Systems Roč. 32, č. 1 (2021), 259-273 [print] ISSN: 1040-0400

ADC008 [219299] **Mechanical surface smoothing of micron-sized iron powder for improved silica coating performance as soft magnetic composites** / Peter Slovenský ... [et al.] - 2020. In: Applied Surface Science : A Journal Devoted to Applied Physics and Chemistry of Surfaces and Interfaces. - Amsterdam (Holandsko) : Elsevier, 1985 č. 531 (2020), s. 1-8 [print, online]. - ISSN 0169-4332

[SLOVENSKÝ, Peter (40%) - KOLLÁR, Peter (10%) - NANXUAN, Mei (5%) - JAKUBČIN, Miloš (5%) - ZELENÁKOVÁ, Adriana (5%) - HALAMA, Maroš (10%) - ODNEVALL WALLINDER, Inger (5%) - HEDBERG, Yolanda S. (20%)]

Ohlasy:

2021 [1] Yi, Xuwu et al. Microstructure and magnetic properties of FeSiAl soft magnetic composites prepared by chemical in-situ coprecipitation with NaOH In: Materials Chemistry and Physics : including materials science communications : an international interdisciplinary journal on science, characterization and processing of advanced materials : The International Journal of the Materials Research Society-Taiwan (MRS-T) Roč. 267 (2021) ISSN: 0254-0584

2021 [1] Nie, Wen et al. High-performance core-shell-type FeSiCr@MnZn soft magnetic composites for

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high-frequency applications In: Journal of Alloys and Compounds : an interdisciplinary journal of materials science and solid-state chemistry and physics Roč. 864 (2021)[print, online] ISSN: 0925-8388

2021 [1] Wang, Jinghui et al. Improvement of magnetic properties for FeSi/FeSiAl compound soft magnetic composites by introducing impact of powder size matching In: Journal of Materials Science : Materials in Electronics Roč. 32, č. 7 (2021), 8545-8556 [print, online] ISSN: 0957-4522

2021 [1] Dolmatov, Arthur V. et al. Deposition of a SiO₂ Shell of Variable Thickness and Chemical Composition to Carbonyl Iron: Synthesis and Microwave Measurements In: Sensors Roč. 21, č. 14 (2021) ISSN: 1424-3210

ADE - Vedecké práce v zahraničných nekarentovaných časopisoch(9)

ADE001 [56772] **Korózna odolnosť TiAlN povlakov** / Mária Hagarová, Maroš Halama - 2006.In: Koroze a ochrana materiálu. Vol. 50, no. 4 (2006), p. 78-83. - ISSN 0452-599X [HAGAROVÁ, Mária (50%) - HALAMA, Maroš (50%)]

Ohlasy:

2007 [4] DRAGANOVSKÁ, D.: Stanovenie spotreby povlakovacieho materiálu v nadväznosti na mikrogeometriu otryskaného povrchu. In: Acta Mechanica Slovaca. Roč. 11, č. 4-C (2007), s. 41-46. ISSN 1335-2393.

ADF - Vedecké práce v domácich nekarentovaných časopisoch(7)

ADF001 [63053] **Preparation mode of Fe nanoparticles** / O. Milkovič ... [et al.] - 2007.In: Acta Metallurgica Slovaca. Roč. 13, mimoriadne č. 1 (2007), s. 694-697. - ISSN 1335-1532 [MILKOVIČ, Ondrej (25%) - HALAMA, Maroš (25%) - LONGAUER, Svätoboj (25%) - NIŽNÍK, Štefan (25%)]

Ohlasy:

2008 [4] SOPKO, Martin Význam magnetických nanodrôtov Fe a ich príprava In: Metalurgia Junior 2008 : zborník prednášok z konferencie : 27.-28. máj 2008, Košice S. 147-150 ISBN: 978-80-553-0037-5

2010 [4] PEĽÁK, Slavomír, SOPKO, Martin Použitie nanočastíc železa v medicíne In: Metalurgia Junior 2010 : zborník prednášok z konferencie : Košice, 2010 S. 135-138 ISBN: 978-80-553-0430-4

ADM - Vedecké práce v zahraničných časopisoch registrovaných v databázach Web of Science alebo SCOPUS(2)

ADM001 [156957] **Mechanical and corrosion properties of aluminium alloy EN AW 6082 after severe plastic deformation (SPD)** / Petra Lacková ... [et al.] - 2015.In: Metalurgija. Vol. 54, no. 1 (2015), p. 181-183. - ISSN 0543-5846 Spôsob prístupu: http://hrcak.srce.hr/index.php?show=clanak&id_clanak_jezik=187222. [LACKOVÁ, Petra (40%) - BURŠÁK, Marián (30%) - KVAČKAJ, Tibor (20%) - HALAMA, Maroš (10%)]

Ohlasy:

2020 [1] PEDDAVARAPU, Sreehari, VEERAPPAN, A. Muthu, RAGHURAMAN, S. Tribological study of Graphene reinforced AA6082 surface composite processed through Friction Stir Processing In: Materials Today-Proceedings : MMM 2020 : International Conference on Materials and Manufacturing Methods : Tiruchirappalli, 5-7 Jul, 2019 Vol. 27, no. 3 (2020) p. 2225-2229 ISSN: 2214-7853

AEC - Vedecké práce v zahraničných recenzovaných vedeckých zborníkoch, monografiách(2)

AEC001 [156173] **Non-destructive technique for evaluation of degradation on solar cells** / Maroš

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Halama ... [et al.] - 2015. In: Materials Science Forum volume 811 : Corrosion in Power Industry. - Switzerland : TTP, 2015 P. 3-10. - ISSN 0255-5476 Spôsob prístupu:

<https://www.scientific.net/MSF.811.3>

[HALAMA, Maroš (70%) - TKÁČ, Ján (10%) - MONBALIU, Ornella (10%) - ZHU, Ying (10%)]

Ohlasy:

2018 [1] HAVEROVÁ, Lucia et al. An in vitro corrosion study of open cell Iron structures with PEG coating for bone replacement applications In: Metals Vol. 8, no. 7 (2018) ISSN: 2075-4701

AFC - Publikované príspevky na zahraničných vedeckých konferenciách(21)

AFC016 [90675] **Active corrosion management in automotive industry: Hyphenation of electrochemical noise analysis with artificial neural networks - feasibility study. Part 1** / Maroš Halama ... [et al.] - 2009. In: EUROCORR 2009. - Frankfurt am Main : Dechema, 2009 P. 1-8.

[HALAMA, Maroš (40%) - JEROLITSCH, David (20%) - LINHARDT, Paul (20%) - FAFILEK, Guenter (20%)]

Ohlasy:

2010 [3] MILLS, D. J.: Eurocorr 2009: "Corrosion from the nanoscale to the plant" - part 2. In: Corrosion Engineering, Science and Technology. Vol. 45, no. 1 (2010), p. 3-9. ISSN 1478-422X.

AFC017 [100843] **Improvement of ENA-NOCS technique using artificial neural networks approach for the detection of corrosion** / M. Halama ... [et al.] - 2010. - 1 elektronický optický disk (CD-ROM). In: EUROCORR 2010 : the European Corrosion Congress : From the Earth's Depths to Space Heights : 13-17 September 2010, Moscow, Russia. - Moskva : MAK Press, 2010 P. 1-8. - ISBN 978-5-317-03383-5 [HALAMA, Maroš (40%) - JEROLITSCH, David (20%) - ŽILKOVÁ, Jaroslava (10%) - DZEDZINA, Rastislav (10%) - LINHARDT, Paul (20%)]

Ohlasy:

2016 [1] MASOUMI, M. et al. Texture and grain boundary study in high strength Fe-18Ni-Co steel related to hydrogen embrittlement In: Materials and Design Vol. 91 (2016), p. 90-97. ISSN: 0264-1275

2016 [1] MASOUMI, M. et al. Texture Study Across Thickness of API X70 Steel After Hot Deformation and Different Posttreatments In: JOM Vol. 68, no. 1 (2016), p. 401-409 ISSN: 1047-4838

2016 [1] MASOUMI, M, SILVA, C.C., DE ABREU, H.F.G Effect of crystallographic orientations on the hydrogen-induced cracking resistance improvement of API 5L X70 pipeline steel under various thermomechanical processing In: Corrosion Science Vol. 111 (2016), p. 121-131 ISSN: 0010-938X

2017 [1] MASOUMI, M. et al. Role of crystallographic texture on the improvement of hydrogen-induced crack resistance in API 5L X70 pipeline steel In: International Journal of Hydrogen Energy Vol. 42, no. 2 (2017), p. 1318-1326 ISSN: 0360-3199

2017 [1] BERES, M. et al. Role of lattice strain and texture in hydrogen embrittlement of 18Ni (300) maraging steel In: International Journal of Hydrogen Energy Vol. 42, no. 21 (2017), p. 14786-14793 ISSN: 0360-3199

2017 [1] MASOUMI, M. et al. Texture evolution and phase transformation of 25Cr-6Mo-5Ni experimental duplex stainless steel during hot and cold rolling In: Journal of Materials Research and Technology-JMR and T Vol. 6, no. 3 (2017), p. 232-240 ISSN: 2238-7854

AFD - Publikované príspevky na domácich vedeckých konferenciách(17)

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Podklady k habilitačnému konaniu

AGJ - Autorské osvedčenia, patenty, objavy(1)

AGJ001 [87142] **Spôsob izolácie Fe nanočastíc elektrochemickou separáciou** patent č. 286895/
Ondrej Milkovič ... [et al.] - Banská Bystrica : ÚPV SR - 2009. - S. 3.
[MILKOVIČ, Ondrej (50%) - HALAMA, Maroš (10%) - NIŽNÍK, Štefan (20%) - LONGAUER, Svätoboj (20%)]

Ohlasy:

2008 [4] SOPKO, Martin Význam magnetických nanodrôtov Fe a ich príprava In: Metalurgia Junior 2008 : Košice S. 147-150 ISBN: 978-80-553-0037-5

2009 [4] SOPKO, Martin Dôležité vlastnosti a charakteristiky nanočastíc na báze železa In: Metalurgia Junior '09 : Deň doktorandov Hutníckej fakulty : zborník prednášok z konferencie : 17.-18. september 2009, Košice S. 47-50 ISBN: 978-80-553-0250-8

2011 [4] PEĽÁK, Slavomír Superparamagnetické nanočastice železa pre biomedicínske použitie In: Metalurgia Junior 2011 : zborník prednášok z konferencie : Košice S. 207-210 ISBN: 978-80-553-0625-4

2009 [4] PEĽÁK, Slavomír Možnosti využitia nanočastíc železa pre medicínske účely In: Metalurgia Junior 2009 : zborník prednášok z konferencie : Košice S. 35-38 ISBN: 978-80-553-0250-8

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Citácie autora M. Halamu, zdroj Web of Science Core Collection, Publons (stav k augustu 2021)

Web of Science ResearcherID
C-6529-2011

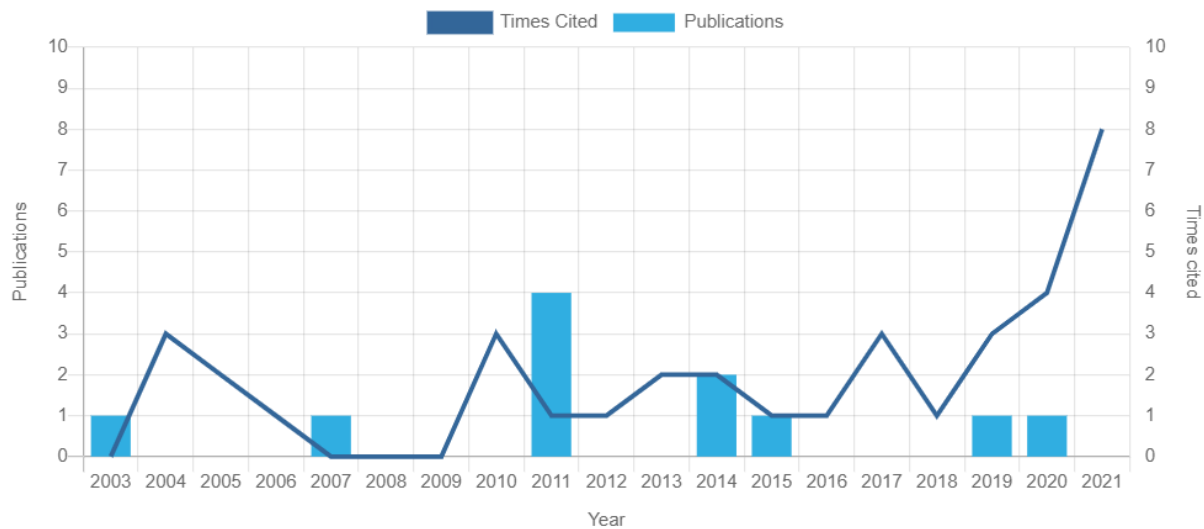
Researcher (Academic) - Technical University of Košice

PUBLICATIONS

11

TOTAL TIMES CITED

36



Mgr. Maroš Halama, PhD.

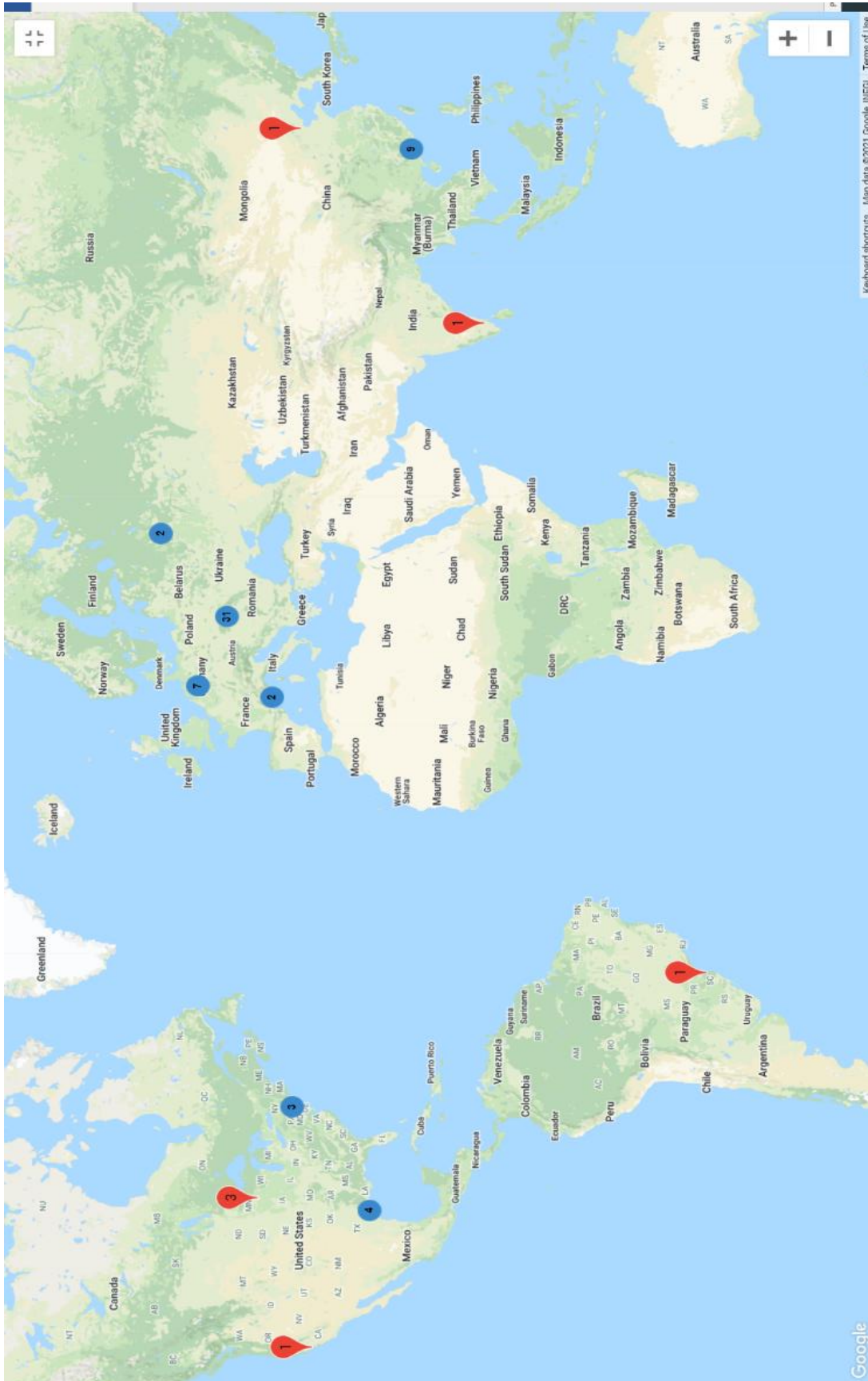
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Distribúcia citácií autora M. Halama, zdroj Web of Science Core Collection, (stav k augustu 2021)



Zoznam citácií autora M. Halamu z databázy SCOPUS (stav k augustu 2021)

1. Yi, X., Peng, Y., Yao, Z., Xia, C., Zhu, S.: Microstructure and magnetic properties of FeSiAl soft magnetic composites prepared by chemical in-situ coprecipitation with NaOH,(2021) *Materials Chemistry and Physics*, 267, art. no. 124626

Cit.: Slovenský, P., Kollár, P., Mei, N.X., Jakubčín, M., Zeleňáková, A., Halama, M., Wallinder, I.O., Hedberg, Y.S., Mechanical surface smoothing of micron-sized iron powder for improved silica coating performance as soft magnetic composites (2020) *Appl. Surf. Sci.*, 531, p. 147340

2. Dolmatov, A.V., Maklakov, S.S., Zezyulina, P.A., Osipov, A.V., Petrov, D.A., Naboko, A.S., Polozov, V.I., Maklakov, S.A., Starostenko, S.N., Lagarkov, A.N.: Deposition of a SiO_2 shell of variable thickness and chemical composition to carbonyl iron: Synthesis and microwave measurements,(2021) *Sensors*, 21 (14), art. no. 4624

Cit.: Slovenský, P., Kollár, P., Mei, N., Jakubčín, M., Zeleňáková, A., Halama, M., Odnevall Wallinder, I., Hedberg, Y.S., Mechanical surface smoothing of micron-sized iron powder for improved silica coating performance as soft magnetic composites (2020) *Appl. Surf. Sci.*, 531, p. 147340.

3. Cai, Y., Xu, Y., Zhao, Y., Ma, X.: Extrapolating short-term corrosion test results to field exposures in different environments,(2021) *Corrosion Science*, 186, art. no. 109455

Cit: Halama, M., Kreislova, K., Van Lysebettens, J.: Prediction of atmospheric corrosion of carbon steel using artificial neural network model in local geographical regions (2011) *Corrosion*, 67., 065004.1-065004.6

4. Nie, W., Yu, T., Wang, Z., Wei, X.: High-performance core-shell-type FeSiCr@MnZn soft magnetic composites for high-frequency applications 2021) *Journal of Alloys and Compounds*, 864, art. no. 158215.

Cit.: Slovenský, P., Kollára, P., Mei, N.X., Jakubčín, M., Zeleňáková, A., Halam, M., Wallinder, I., Hedberg, Y.S., Mechanical surface smoothing of micron-sized iron powder for improved silica coating performance as soft magnetic composites (2020) *Appl. Surf. Sci.*, 531

5. Wang, J., Song, S., Sun, H., Xue, Z.: Improvement of magnetic properties for FeSi/FeSiAl compound soft magnetic composites by introducing impact of powder size matching 2021) *Journal of Materials Science: Materials in Electronics*, 32 (7), pp. 8545-8556.

Cit.: Slovensky, P., Kollar, P., Mei, N., Jakubcin, M., Zelenakova, A., Halama, M., Wallinder, I.O., Hedberg, Y.S., (2020) *Appl. Surf. Sci.*, 531, p. 147340

6. Radkowska, I., Bragieli, P.: 1-Naphthols as components for multifunctional material systems (MFMS): the molecular modeling approach 2021) *Structural Chemistry*, 32 (1), pp. 259-273.

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