6. International publications

6.1. Peer review papers

פרסומים 1-17 נכללו במסגרת הדרגה הקודמת. פרסומים 17-47 חדשים.

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6.1.2. S. Barzilai, A. Raveh, N. Frage, "Annealing of niobium coating deposited on graphite", *VACUM*, 79 (2005) 171-177.

6.1.3. S. Barzilai, N. Frage, A. Raveh, "Niobium layers on graphite: Growth parameters and thermal annealing effects", *Surface and coating technology*, 200-14,15 (2006) 4646-4653.

6.1.4. S. Barzilai, A. Raveh, N. Frage, "Inter-diffusion of carbon into niobium coatings deposited on graphite", *Thin solid film*, 496 (2006) 450-456.

6.1.5. S. Barzilai, M. Aizenshtein, N. Froumin, N. Frage, "Interface phenomena in the Y_2O_3/(Al-Cu) system", *Materials Science Engeeniring A*, 420 (2006) 291-295.

6.1.6. S. Barzilai, M. Aizenshtein, N. Froumin, N. Frage, "Y_2O_3/(Cu-Me) systems (Me=Ti,Al): Interface reactions and wetting", *Journal of Materials Science*, 41 (2006) 5108-5122.

6.1.7. S. Barzilai, M. Lomberg, N. Froumin, N. Frage, "Wetting /Dewetting Phenomena in the CaF_2/Ga and CaF_2/Ge Systems", *Advances in science and technology*, 45 (2006) 1532-1536.

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6.1.10. S. Barzilai, M. Aizenshtein, M. Lomberg, N. Froumin, N. Frage, "Interface reaction and wetting in the CaF_2/(Me) systems", *Journal of alloys and compounds*, 452 (2008) 154-160.

6.1.11. N. Froumin, S. Barzilai, M. Aizenshtein, M. Lomberg, N. Frage, "Wetting induced by near-surface Ti-enrichment in the CaF_2/In-Ti and CaF_2/Cu-Ti systems", *Materials Science and Engineering A*, 495 (2008) 181-186.

6.1.12. S. Barzilai, N. Argaman, N. Froumin, D. Fuks, N. Frage, "*ab-initio* modeling of Al adsorption on CaF_2 surfaces", *Materials Science and Engeeniring A*, 495 (2008) 36-42.

6.1.13. M. Aizenshtein, S. Barzilai, N. Froumin, N. Frage, "Interface interaction and wetting in the Er_2O_3/(Cu-Al) and Er_2O_3/(Cu-Ti) systems", *Journal of Materials Science*, 43 (2008) 1259-1264.

6.1.14. S. Barzilai, N. Argaman, N. Froumin, D. Fuks, N. Frage, "First-principles modeling of metal layer adsorption on CaF_2(111)", *Surface Science*, 602 (2008) 1517-1524.

6.1.15. S. Barzilai, N. Argaman, N. Froumin, D. Fuks, N. Frage, "The effect of Ti on the wetting of CaF_2 substrate by In-Ti and Ga-Ti alloys-*ab initio* consideration", *Applied. Physics A.*, 93 (2008) 379-385. **(Invited Paper).**

6.1.16. S. Barzilai, H. Nagar, M. Aizenshtein, N. Froumin, N. Frage, "Interface interaction and wetting of Sc_2O_3 exposed to Cu-Al and Cu-Ti melts", *Applied. Physics A.*, 95-2 (2009) 507-512.

6.1.17. S. Barzilai, N. Argaman, N. Froumin, D. Fuks, N. Frage, "The influence of the solvent on the wetting of CaF_2 by Me-Ti alloys - *ab initio* consideration", *Surface Science* 603 (2009) 2096-2101.

6.1.18. S. Barzilai, M. Aizenstein, N. Froumin, N. Frage, "The effect of thermodynamic properties of Me-Ti (Me=In, Sn, Ga, Au and Ge) melts on the wetting of the CaF_2 substrate", *Journal of Materials Science*, 45 (2010) 2085-2089.

6.1.19. S. Barzilai, M. Aizenstein, N. Froumin, N. Frage, "Mechanisim of interfacial interactions between thermodynamically stable oxides and Al containing melts", *Advances in Applied Ceramics*, 110 (2011) 15-19.

6.1.20. S. Barzilai, H. Nagar, N. Froumin, N. Frage,"Wetting and infiltration of volatile fluorides by In-Ti melt", *Journal of Materials Science*, 46-17 (2011) 5698-5701.

6.1.21. S. Barzilai, I. Halevi, O. Yehaskel, "Bulk modulos of scandia, Ab initio calculations and experimental results", *Journal of applied Physics,* 10 (2011) 43532-43533.

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6.1.26. S. Barzilai, F. Tavazza, L.E. Levine, "The effect of internal impurities on the mechanical and conductance properties of gold nanowires during elongation", *Modeling and simulation in material science and engineering,* 21 (2013) 25004: 1-8.

6.1.27. S. Barzilai, F. Tavazza, L.E. Levine, "First-principles modeling of gold adsorption on BeO (0001)", *Suface Science 609* (2013) 39-43.

6.1.28. F. Tavazza, S. Barzilai, D. M. Smith, L.E. Levine, "The increase in conductance of a gold single atom chain during elastic elongation", *Journal of Applied Physics* 113 (2013) 054316:1-5.

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6.1.30. S. Barzilai, F. Tavazza, L.E. Levine, "Sensitivity of gold nano conductors to common contaminations- *ab initio results" Journal of Materials Science,*48 (2013) 6619-6624.

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6.1.35. S. Barzilai, S. Hayun, "Mechanical alloying and thermal analysis of Ta-Ti alloys", *Journal of Materials Science* 50 (2015) 6833-3838.

6.1.36. S. Barzilai, C. Toher, S. Curtarolo and O. Levy, "Evaluation of the tantalum-titanium phase diagram from *ab-initio* calculations", *Acta Materialia* 120 (2016) 255-263.

6.1.37. A. Abramovich, S. Barzilai, S. Cohen, N. Shamir, Y. Eisen, M.H. Mintz, S. Zalkind, "Effect of ion irradiation damage on the initial interactions of oxygen with polycrystalline gadolinium" *Solid States Ionics 3009* (2017) 130-136.

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6.1.41. S. Barzilai, M. H. Mintz "The effect of vacancies and surface hydroxyls on the interaction of hydrogen with rare earth oxides – DFT calculations on gadolinium oxide", *Journal of Alloys and Compounds*, 740 (2018) 926-934.

6.1.42. L. Shelly, D. Schweke, S. Zalkind, N. Shamir, S. Barzilai, T. Gouder, S. Hayun, "The effect of U content on the activation of H_2O on $Ce_{1-x}U_xO_{2+\delta}$" Chemistry of materials 30 (2018) 8650-8660.

6.1.43. E. Struma, S. Hayun, S. Barzilai, Y. Finkelstein, R. Ben-David, O. Yehaskel, "In situ detection of thermally induced porosity in additively manufactured and sintered objects", *Journal of Materials Science* 54 (2019) 8665-8674.

6.1.44. E. Edelshtein, S. Barzilai, S. Curtarolo, O. Levy, "First principle investigation of cold curves of metals", *Isr. J. Chem.* 60 (2020) 1-9.

6.1.45. S. Barzilai, M. Aizenshtein, M. H. Mintz, S. Hayun " Effect of oxygen adsorbent on the dissociation of H_2O over gadolinium oxide surfaces – DFT calculations and experimenta results", *J. of Physical Chemistry C*, 124-27 (2020) 14613-14621.

6.1.46. Y. Mordekovitz, S. Sagi, S. Barzilai, S. Hayun "Effect of Nd content on the energetic of H_2O adsorption and defect structure in the $Ce_{1-x}Nd_xO_{2-0.5x}$ system", *J. of Materials Chemistry A*, 8 (2020) 21842-21851.

6.1.47. J. Barrio, S. Barzilai, N. Karjule, P. Amo-Ochoa, F. Zamora, M. Shlom,"Synergistic doping and surface decoration of carbon nitride macrostructure by single crystal design" Applied energy materials (2021) doi.org/10.1021/acsaem.0c02964

6.2. Conferences (Proceedings, Oral presentations, Posters)

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6.2.1. S. Barzilai, M. Lomberg, N. Froumin, M. Aizenshtein, N. Frage, "Interaction in the Al-CaF_2 system, *ab-initio* calculations and experimental verification", Proceeding of the 6th Israeli-Russian Bi-National Workshop on the optimization of composition, structure and properties of metals, oxides, composites, nano and amorphous materials. Edit by M. Zinigrade and E.A. Pastukhov, Israeli Academy of Science and Humanites, pp. 246-255, 24-28/6/07, Jerusalem, Israel.

6.2.2. S. Barzilai, M. Aizenshtein, N. Froumin, and N. Frage, "Wetting and interface interaction between thermodynamically stable oxides and Al containing melt", Proceeding of the 5th international conference on mathematical modeling and computer simulation of material technologies, MMT-2008, Ed. By M. Zinigrad, Ariel, 22/8/2008, Vol. 1, pp. 3.26-3.33.

6.2.3. S. Barzilai, M. Lomberg, N. Froumin, and N. Frage, "The effect of substrate volotility on the wetting kinetics", Proceeding of the 5th international conference on mathematical modeling and computer simulation of material technologies, MMT-2008, Ed. By M. Zinigrad, Ariel, 22/8/2008, Vol. 2, pp. 5.28-5.32.

6.2.4. S. Barzilai, M. Aizenshtein, N. Froumin, N. Frage, "Wettability in the Y_2O_3/(Cu–Al) system", Euromat 2005, European Congress on Advanced Materials and Processes, 5-8 September 2005, Prague, Czech Republic.

6.2.5. S. Barzilai, M. Aizenshtein, N. Froumin, and N. Farge, "Chemical interaction in Y_2O_3/(Cu-Al) system", International Conference on Modern Materials Science: Achievements and Problems, Kiev-Ukraine, Sep., 26-30, 2005.

6.2.6. S. Barzilai, M. Lomberg, M. Aizenshtein, N. Froumin, and N. Farge, "Examination of brazing material for thermodynamically stable Y_2O_3 and Er_2O_3 oxides", the Israel welding conference 16/1/2007 Israel.

6.2.7. S. Barzilai, M. Lomberg, M. Aizenshtein, N. Froumin, and N. Farge, "Developing of brazing alloyes based on wetting experiment in the CaF_2/Me systems", the Israel welding conference 16/1/2007 Israel.

6.2.8. N. Froumin, S. Barzilai, M. Aizenshtein, M. Lomberg, and N. Farge, "Wetting phenomena in halide/metal systems", the 5th High Temperature Capilarity Conference, HTC-2007, Alicante (Spain), 21-24 March 2007, p. 47.

6.2.9. M. Lomberg, S. Barzilai, M. Aizenshtein,N. Froumin, N. Frage, "Evaluation of compatibility of CaF_2 with reactive melts using the sessile drop method", CAMPI: Corrosion, advanced materials and processes in industry, Sami Shamoon College of Engineering, 29-31/5/07, Beer-Sheva, Israel.

6.2.10. S. Barzilai, M. Lomberg, N. Froumin, M. Aizenshtein, N. Frage, "Interaction in the Al-CaF_2 system, *ab-initio* calculations and experimental verification", the 6th Israeli-Russian Bi-National Workshop 2007 on the optimization of composition, structure and properties of metals, oxides, composites, nano and amorphous materials, Israeli Academy of Science and Humanites, 24-28/6/07, Jerusalem, Israel.

6.2.11. S. Barzilai, M. Aizenshtein, M. Lomberg, N. Argaman, N. Froumin, D. Fuks and N. Farge, "The effect of Ti addition on the wetting behavior of the CaF_2/In and CaF_2/Cu systems", the 13th Israel materials engineering conference, IMEC, Israel, 9-10 december 2007, p 74.

6.2.12. M. Lomberg, N. Froumin, S. Barzilai, M. Aizenshtein, N. Farge, "How does thermodynamic activity of Ti affect the wetting of CaF_2 by noble metals?", the 13th Israel materials engineering conference, IMEC, Israel, 9-10 december 2007, p 78.

6.2.13. M. Lomberg, N. Froumin, S. Barzilai, M. Aizenshtein, and N. Farge, "The effect of thermodynamic activity of Ti on the wetting of CaF_2 substrate by nobel metals-Ti alloys", the Israel welding conference 15/1/2008 Israel.

6.2.14. M. Aizenshtein, N. Froumin, S. Barzilai and N. Farge, "The wetting behavior of thermodynamically stable oxides exposed to liquid Cu alloyed by Al and Ti", the Israel welding conference 15/1/2008, Israel.

6.2.15. S. Barzilai, N. Argaman, M. Lomberg and D. Fuks, "The influence of the interatomic interaction on the wetting of CaF_2 by Me-Ti melts. *Ab-initio* consideration", The 6th High Temperature Capilarity Conference, HTC-2009, Athens (Greece), 6-9 May 2009.

6.2.16. S. Barzilai, M. Aizenshtein, N. Froumin, and N. Farge, "Wetting and interface interaction between thermodynamically stable oxides and Al containing melt, Euromat 2009, Glasgow (U.K.), 6-11/9/2009.

6.2.17. S. Barzilai, I. Hakevi, O. Yehezkel, "The bulk modulus of scandia: ab-initio calculations and experimental verifications", the 14th Israel materials engineering conference, IMEC, Israel, 13-14 december 2009, p. 118.

6.2.18. S. Barzilai, A. Raveh and N. Frage, "Deposition of niobium Films by Radio-Frequency Magnetron Sputtering", 21st IVS General Conference Incorporating: Crystal Growth and Epitaxy, Nanohappening, Semiconductor Industry Application, minisymposium, Space Technology Session, Israel, sep 2002, p. P-CG14.

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6.2.22. S. Barzilai, M. Aizenshtein, N. Froumin, N. Frage, "Y_2O_3/Cu alloys System: Interface Reaction and Wetting", 6th international Workshop on Interfaces: Interfaces by Design, Santiago de compostela, June 26-30, 2005, p.66.

6.2.23. S. Barzilai, A. Raveh and N. Frage, "Diffusion of carbon into thin niobium films", the 12th Israel materials engineering conference, IMEC, Israel, march 2006, p. 229.

6.2.24. S. Barzilai, M. Aizenshtein, N. Froumin, and N. Frage, "Interface reaction of Y_2O_3 with reactive melts, the 12th Israel materials engineering conference, IMEC, Israel, march 2006, p 252.

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6.2.26. S. Barzilai, N. Argaman, N. Froumin, D. Fuks and N. Frage, "*ab-initio* modeling for Al adsorption on CaF_2 surfaces", The 5th High Temperature Capilarity Conference, HTC-2007, Alicante (Spain), 21-24 March 2007, p. 139.

6.2.27. M. Lomberg, S. Barzilai, M. Aizenshtein, N. Froumin and N. Frage, "Effect of Ti additions on interface interactions and wetting in the CaF_2/Cu and CaF_2/In systems", The 5th High Temperature Capillarity Conference, HTC-2007, Alicante (Spain), 21-24 March 2007, p. 140.

6.2.28. S. Barzilai, N. Argaman, N. Froumin, D. Fuks and N. Frage, "ab-initio modeling for Al adsorption on CaF_2 surfaces", Safed Summer School on Density Functional Theory: formalism, implementation, and Novel applications, 2-6/9/2007.

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6.2.30. M. Lomberg, M. Aizenshtein, S. Barzilai, N. Foumin, N. Frage, "The effect of thermodynamic properties of Me-Ti melts (Me=In, Ga, Au and Sn) on the wetting nature in the CaF_2/Me-Ti systems", the 9th international conference on the structure of surface (ICOSOS-9), 3-8 august 2008 Salvador-Brazil, p. 27.

6.2.31. S. Barzilai, M. Aizenshtein, N. Froumin, and N. Frage, "Wetting and interface interaction between thermodynamically stable oxides and Al containing melt", the 5th international conference on mathematical modeling and computer simulation of material technologies, MMT-2008, 22/8 /2008 Ariel-Israel.

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6.2.35. H. Nagar, S. Barzilai, N. Foumin, N. Frage, "Wetting phenomena and infiltration in the ceramic/In-Ti alloy systems", the 14th Israel materials engineering conference, IMEC, Israel, december 2009, p. 294.

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6.2.36. N. Frage, S. Barzilai, H. Nagar, N. Froumin, "Does good wtting is sufficint for infiltration?", Proceeding of the 6th international conference on mathematical modeling and computer simulation of material technologies, MMT-2008, Ed. By M. Zinigrad, Ariel, 22/8/2010, Vol. 2, pp. 5.28-5.32.

6.2.37. N. Froumin, S. Barzilai, M. Aizenshtein, H. Nagar and N. Farge, "Brazing of thermodynamically stable oxides", the Israel welding conference 26/1/2010, Israel.

6.2.38. D. Fuks, S. Barzilai, N. Froumina, N. Frage, E. Glickman, "Link of micro and macro in wetting phenomena: DFT modeling, bindung at the interface and contact angle", the 12th International Ceramics Congress, 6-11/6/ 2010, Montecatini terme, Tuscany, Italy.

6.2.39. N. Froumin, S. Barzilai, M. Aizenshtein, N Frage, "Mechanisim of interfacial interactions between thermodynamic stable oxides and Al containing melt", TOFA 2010, Discution meeting on thermodynamics of alloys", Porto, Portogal, 12-16/9/2010.

6.2.40. S. Salhov, M. Aizenshtein, N. Froumin, S. Barzilai, N. Frage, "Dissolution Kinetics and Solubility Limit of CaF_2 in molten KCl-NaCl Salt", P.62, IMEC-15, Dead Sea, Israel, 28.2-1.3.2012.

6.2.41. E. Glickman, D. Fuks, S. Barzilai, N. Froumin, N. Frage, "Thermodynamics and Kinetics of Non-Reactive Wetting: CaF_2/(In-Ti) system", 7th International Conference on High Temperature Capillarity, Eilat Israel ,18-22 March, 2012.

6.2.42. N. Froumin, M. Piness, S. Barzilai, M. Aizenshtein, N. Frage, "Interface interactions and wetting in quasi-binary oxides-Al melt systems", P. 14, 7th International Conference on High Temperature Capillarity, Eilat Israel, 18-22 March, 2012.

6.2.43. M. Aizenshtein, O. Kish, N. Froumin, S. Salhov, S. Barzilai, M. Gelbstein, N. Frage, "Wetting and interface interaction in the Ta2O5/Cu-Al system", P. 7, 7th International Conference on High Temperature Capillarity, Eilat Israel, 18-22 March, 2012.

6.2.44. M. Aizenshtein, S. Barzilai, N. Froumin, N. Frage, "Wetting and interface interaction in the Carbides, Borides, Oxides and Flourides – Metal systems" (Invited), P.27, IMEC-16, Haifa, Israel, 23-25.2.2014.

6.3. Thesis

6.3.1. S. Barzilai, "Niobium coating and formation of niobium carbide on graphite", Thesis for M.Sc. degree, Supervised by Prof. N. Frage and Dr. A. Raveh, Ben-Gurion university, faculty of engineering science, materials science and engineering department, april 2005.

6.3.2. S. Barzilai, "Chemical interactions and wetting of thermodynamically stable compounds exposed to liquid metals. Macroscopic and Microscopic Consideration", Thesis for Ph.D. degree, Supervised by Prof. N. Frage, Ben-Gurion university, materials science and engineering department, Mar. 2010.