Mariano Daniel Forti

Contact: mariano.forti@icams.rub.de mforti@cnea.gov.ar marianodforti@gmail.com

Introduction

I have recently started a postdoctoral position at the Interdisciplinary Center of Advanced Materials Simulations (ICMAS), under the supervision of Dr. Prof. Ralph Drautz and Dr. habil. Thomas Hammerschmidt. There, I will carry on investigations about Niquel based Superalloys using Datascience and Machine learning techinques.

Since 2017 I have been a researcher at Comisión Nacional de Energía Atómica, Argentina. My activities are carried on at División Aleaciones Especiales (Special Alloys Division) where I started working as a specialist in DFT calculations in 2017. My research is about mechanical stability of interfacial systems, mainly in the Iron/Magnetite interface and more recently the Zr / ZrO_2 system as well. I also participate actively in other activities carried on in the group, where we study point defects in ZrO_2.

My responsibilities at DAE also included the maintenance of two private (though rather small) Linux computing clusters owned by DAE. Hence, during my professional career, I have acquired a wide experience in Linux System Administration for deskop and High Performance Computing Clusters. My programming skills include a variety of languages including Bash, Fortran, Python, php and javascript, and I also have wide experience in Matlab and Octave environments. I make a daily use of other tools as vim, OriginLab and gnuplot. In particular, I am an user and enthusiast of open source tools as the KDE desktop and the LibreOffice suite.

I also work as a teaching assistant in an advanced course about the Finite Element Method for the Materials Engineering program at Instituto Sabato.

Current Positions

Postdoctoral Resercher at Interdisciplinary Centre for Advanced Materials Simulation http://www.icams.de, Ruhr University Bochum, Germany. **Adviser**: Dr. Prof. Ralf Drautz (ralf.drautz@rub.de), Dr. habil. Thomas Hammerschmidt (thomas.hammerschmidt@rub.de). Machine Learning and Datascience applied to Ni and Fe based superalloys.

Researcher at Comisión Nacional de Energía Atómica, Gerencia Materiales. División Aleaciones Especiales. **Adviser**: Dr. Paula Alonso (pralonso@cnea.gov.ar). Position: Researcher. Density Functional Theory calculations in interfacial systems: Fe / Fe_3O_4, Zr/ZrO_2. Electronic properties of ZrO_2. Linux System Administration in Desktop and Cluster Computers for High Performance Calculations. Daily use of Bash, Fortran and Python. This position is on a long term licence until postdoctoral studies were finished in 2022.

Teaching assistant at Instituto Sabato (UNSaM-CNEA), Ayudante de 1ra. "Computer Simulation of Processes and Materials". Professor: Ruben Weht (ruweht@cnea.gov.ar). In this course students make their own implementation of several numerical methods for solving differential equations including Finite Differences and Finite Elements.

Main Publications

"Shear Behavior of Fe/Fe_3O_4 interfaces". Revista Materia V23-N2 (2018). Mariano Forti, Paula Alonso, Pablo Gargano, Gerardo Rubiolo.

"Properties of hexagonal Zr and tetragonal ZrO_2 low index surfaces from DFT calculations". Revista Materia V23-N2 (2018). Paula Alonso, Pablo Gargano, Laura Kniznik, Gerardo Rubiolo.

"A DFT study of atomic structure and adhesion at the Fe(BCC)/Fe_3 O_4 interfaces". Surface Science 647 (2016) 55–65. Mariano Forti, Paula Alonso, Pablo Gargano,Perla Balbuena, Gerardo Rubiolo.

"Charge difference calculation in Fe/Fe_3O_4 interfaces from DFT results". Procedia Materials Science 8 (2015) pp 1066 – 1072. Diego Tozini, Mariano Forti, Paula Alonso, Pablo Gargano, Gerardo Rubiolo.

"Ab-initio studies on carburization of Fe_3 Al based alloys". Procedia Materials Science 1 (2012) 191 – 198. Mariano Forti, Perla Balbuena, Paula Alonso.

Last Congress Participations

2020 Express Conference on the Physics of Materials and its application in Energy and Environment, 17-19 August 2020 , https://sites.google.com/view/e-cpm2020/. "Control of the valence band maximum state in tetragonal ZrO2 with pressure". Poster Presentation.

5th Nuclear Materials Conference, Elsevier – IAEA, 14-18 October 2018 Seattle, USA. Poster Presentations: *1) "First-principles thermodynamic study of point-defect structure and electrical conductivity in tetragonal non-stoichiometric zirconia including lattice vibrations"* , Gargano, Kniznik, Alonso, Forti, Rubuiolo. *2) "DFT Study of the Early Stages of Oxidation of the*

Zr(1010) Surface" , F. Soto, M. Forti, P. Alonso, P. Gargano, L. Kniznik, G. Rubiolo, P. Balbuena. *3) "A DFT study of the resistance to traction and shear loads of the Fe(BCC) / Fe_3O_4 interface"*, M.Forti, P. Alonso, P. Gargano, L. Kniznik, G. Rubiolo. https://elsevier.conference-services.net/programme.asp?conferenceID=4229&action=prog_list&session=45340

16º SAM-CONAMET, November 2016 Córdoba, Argentina. *"Shear stress in Fe/Fe 3 O4 interfaces".* Sociedad Argentina de Materiales. http://sam-conamet2016.congresos.unc.edu.ar/

Ongoing projects

Simulación y ensayo de una aleación propuesta para reactores nucleares de alto quemado , PICT-2018-01671. Comisión Nacional de Energía Atómica, Agencia Nacional de Promoción Científica y Tecnológica, Ministerio de Ciencia, Técnica e innovación Productiva.

In the search for anewalloy for fuel ements of the CAREM-25 Power Plant, Project 80020160500046SM. InstitutoSabato, Universidad de San Martin, Comisión Nacional de Energía Atómica, Ministerio de Ciencia, Técnica e Innovación Productiva.

Education

Doctor in Materials Science and Technology (PhD), September 2017. Instituto de Tecnología Prof. Jorge Sabato, Universidad Nacional de General San Martín.

Adviser: Gerardo Rubiolo (rubiolo@cnea.gov.ar).

PhD Thesis title: Pasivating film in steel pipes used in nuclear power plants steam generators.

Abstract: The main objective of this work was to calculate the fracture toughness of the α-Fe /(magnetite)Fe_3O_4 interface using Density Functional Theory (DFT). Traction and shear mode strains are introduced to the system to separate the parts, and total energy calculations are used to investigate the behavior of the interface and the influence of atomic arrangement.

Materlials Engineer, August 2010. Instituto de Tecnología Prof. Jorge Sabato, Universidad Nacional de General San Martín.

Title of the Engineering dissertation: "Ab-Initio Studies about Carburization of Fe_3Al Based Alloys".

Advisers: Perla Balbuena (balbuena@tamu.edu), Paula Alonso (pralonso@cnea.gov.ar)

Abstract: Fe-Al based alloys exhibit excellent properties but suffer metal dusting in carburizing atmospheres. Surface composition can be a determinant factor in the solution of this problem. We calculate in this work the C adsorption energies in the $L2_1$ Fe_2AlX (X=Ti,V,Nb) structures and we study the influence of surface covering. Our results show the beneficial effect of Ti, suggesting that there could exist an activation energy to promote the incorporation of C in the subsurface layers when the surface is covered enough.