

An Outline of My Activities

Mariano Forti

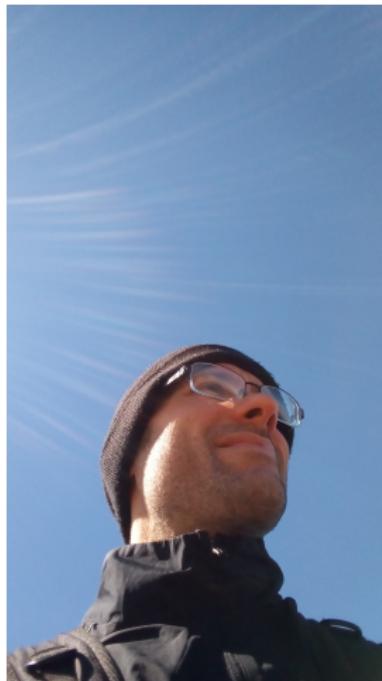
2019

Interview details here

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Who am I

Who am I?



Current positions



Comisión Nacional
de Energía Atómica



- Materials Engineer (2010), PhD Materials Science (2017)
- Wide Experience in DFT Calculations
- based at Argentina, Ciudad de Buenos Aires

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Current Research

Scientific support to Special Alloys Foundry

taking a small part since August 2018, but special challenge because this is strictly related to production of security related components of the CAREM reactor.

Standard and Technical documentation interpretation.

comparation of chemical analysis methods.

Quality assurance related stuff:

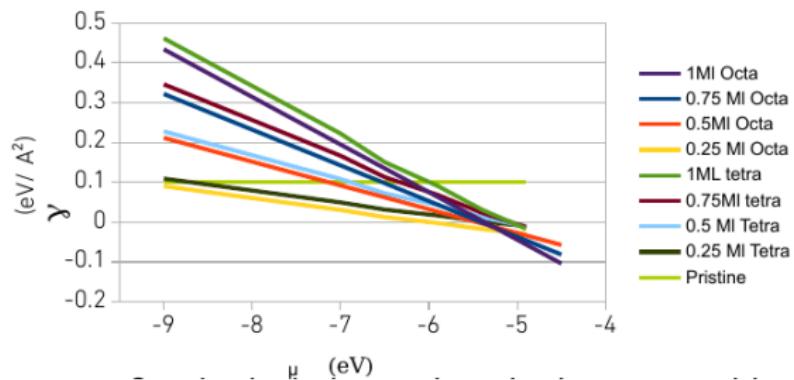
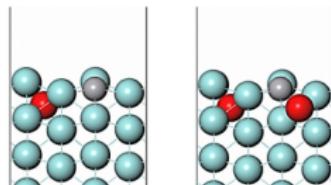
- documentation registries and archiving
- documentation codification

Zr(10̄10) surface, Oxygen and Hydrogen Absorption

This project is carried on in collaboration with Fernando Soto, a Postdoc at Perla Balbuena's group in Texas A&M University, USA.

Progress so far

- Oxygen Coverage with alloy elements

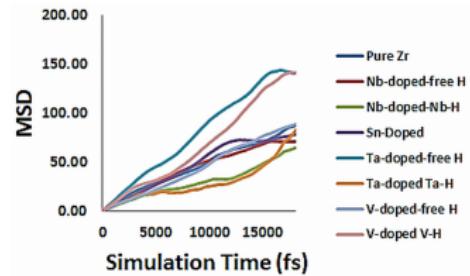
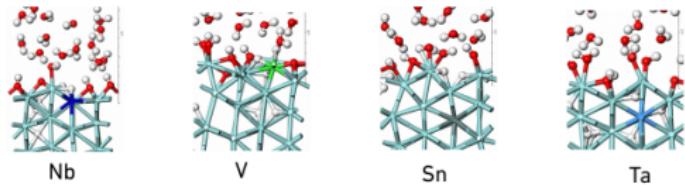


Zr(10̄10) surface, Oxygen and Hydrogen Absorption

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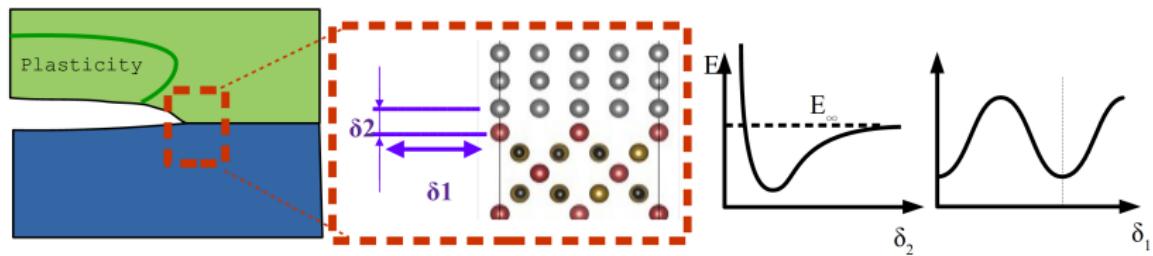
Progress so far

- Oxygen Coverage with alloy elements
- AIMD: Hydrogen moves differently in the presence of Ta and V,

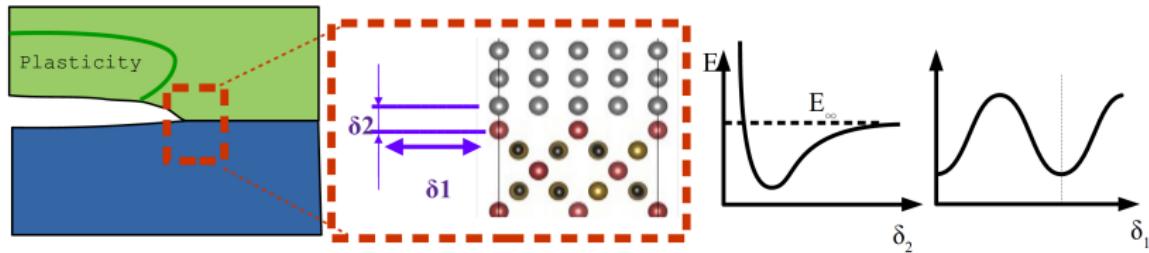


Adhesion in FeBCC/Fe₃O₄ interface

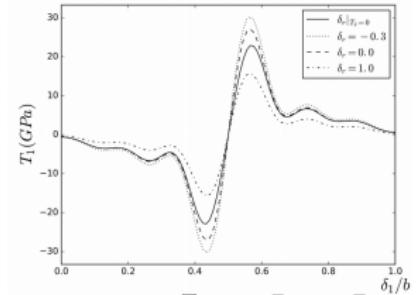
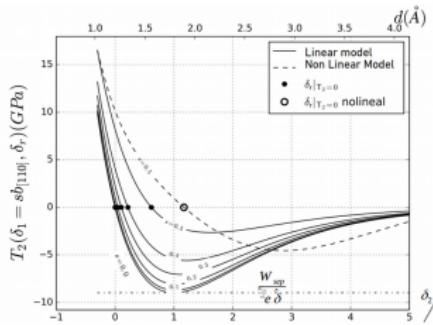
Separating the parts of the interface it is possible to obtain energy vs separation curves from DFT calculations. Then the forces can be obtained from interface potential models!



Adhesion in FeBCC/Fe₃O₄ interface



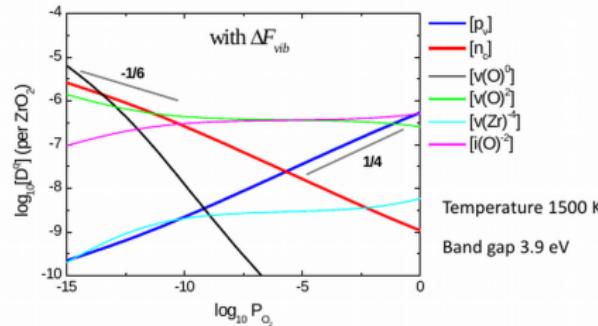
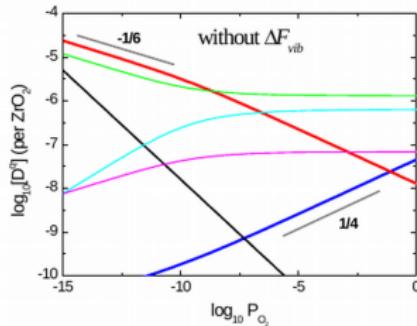
$$\tilde{L}_{\delta_1} = \frac{E_{\text{ad}}}{W_{\text{sep}}} = \exp\left(\frac{\delta_2}{\delta}\right) \sum_{i=0}^{i_{\max}} (1+\beta)^i \left[-1 + f(\delta_1)(1+\beta)^i \right] \alpha_i \left(\frac{\delta_2}{\delta} \right)^i \quad T_1(\delta_1, \delta_2) = -\frac{\partial W}{\partial \delta_1} \quad T_2(\delta_1, \delta_2) = -\frac{\partial W}{\partial \delta_2}$$



Point Defect Equilibria in tetragonal ZrO₂

This Project is carried on in collaboration with Pablo Gargano and Gerardo Rubiolo from DAE. We performed DFT of Vibrational energies using a Debye Model.

$$\Delta E_{D,q}^f = E_{tot}^{DFT}(D^q) - E_{tot}^{DFT}(\text{perfect}) - \Delta n_D \mu_D + q(E_{VBM} + \mu_F)$$



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Teaching

Teaching FEM basics

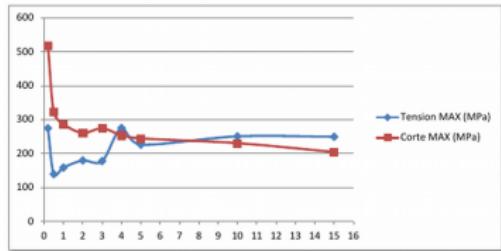
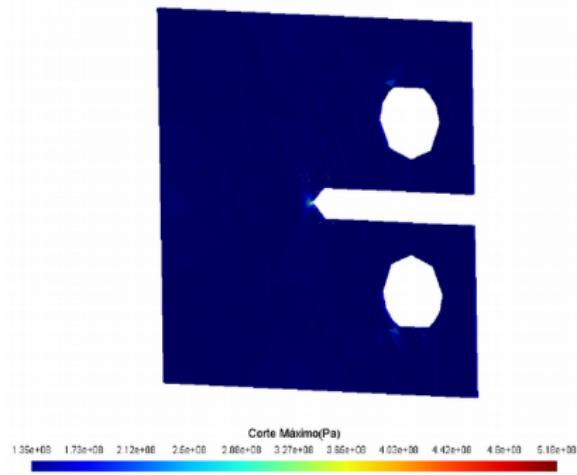
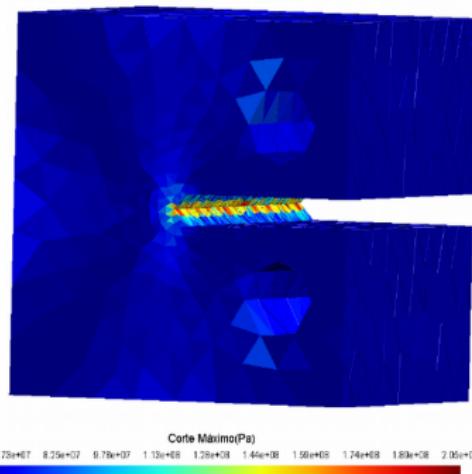


Fig. 11: Ordenadas: tensiones en MPa. Abscisas: espesor en cm.



We guide students make while they build their own implementation of the Finite Element Method in any language they choose.

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Other Skills

Workflow and Programming

■ Programming, Mainly scripting

- Mainly Bash,
- FORTRAN
- Python
- matlab
- Couple Markup Languages (HTML, L^AT_EX, Markdown)

■ Worflow Solutions, allways evolving

- bash, tmux and vim
- KDE
- local git repositories for versioning and history
- ssh, sftp
- Libreoffice and MSOffice

The screenshot shows a terminal window with two panes. The left pane displays a file browser with a tree view of a directory structure. The right pane shows a script editor with a portion of a shell script. The script includes commands for navigating directories, running jobs, and managing files.

```

ls -l
Nombre Tamaño Fecha Modifi
DIR-ANT may 23 15:00
/Bitacoras 4996 jun 26 2017
/corponentesPago 4996 ago 23 16:59
/crack 4996 ago 23 16:59
/CuadernoTrabajo 4996 oct 1 17:15
/Dropbox 4996 ago 23 16:59
/Devel 20480 jun 26 2017
/Documents 4996 sep 7 09:46

DIR-ANT
59440U/79G (7%) → /z1_atd1

sftp: Listado completo.
mariano@Office:Bitacoras $ ls
Ayuda Menú Ver Editar Copiar Renov NDir Borrar Menú Salir
50
51 cd $TD
52
53
54 #!/bin/bash
55 #!/bin/bash
56 #!/bin/bash
57 cd $SLURM_SUBMIT_DIR/*
58 USEINCAR=$SLURM_SUBMIT_DIR/ENCARD/ENCAR-USEINCAR
59 USEKPOINT=$SLURM_SUBMIT_DIR/INPUTS/POTCAR
60 USEKPOINTS=$SLURM_SUBMIT_DIR/INPUTS/KPOINTS-TOTEN
61
62 rm mysave
63
64
65 cd $SLURM_SUBMIT_DIR
66
67 lsch* lschh*

```

Disclaimer: Image is only an illustration, does not represent my real workflow

Linux Sysadmin

- Installation and maintenance of small Rocks Clusters
- Compilation and maintenance of VASP and other programs in this and other clusters.
- some basic file recovery with testdisk and scalpel



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Conclusions

Such Experience, Much promise

- Wide DFT experience gives me the tools to face all kind of difficult computational materials science problems
- Experience in programming and linux system administration can give me a good insight in everyday work
- experience in interacting in multidisciplinary workgroups.

Any Questions?

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