

An Outline of My Activities

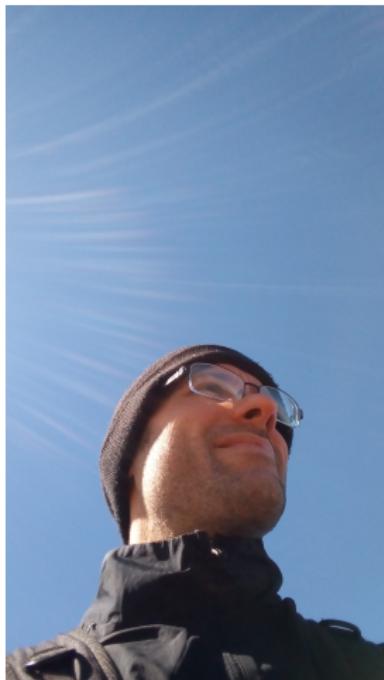
Mariano Forti

2019

Interview for a postdoctoral position at Helmholtz Centre Potsdam
Atomistic Modeling of (geo) Materials
Profesor Maribel Nuez Valdez

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

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:

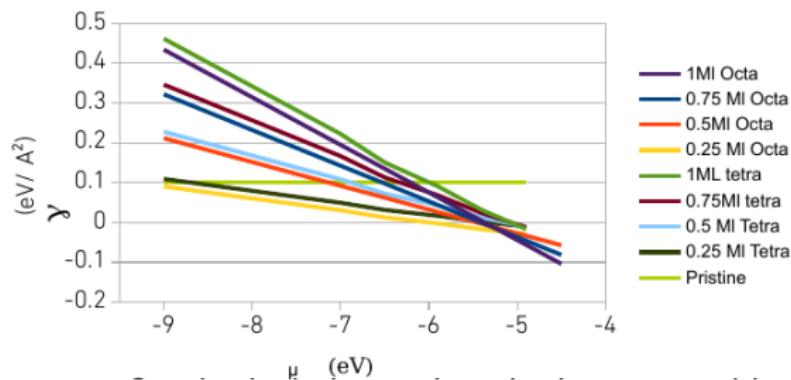
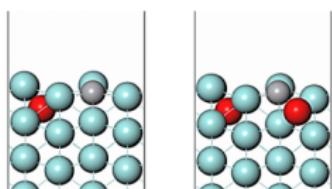
- documentation registries and archiving
- documentation codification

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

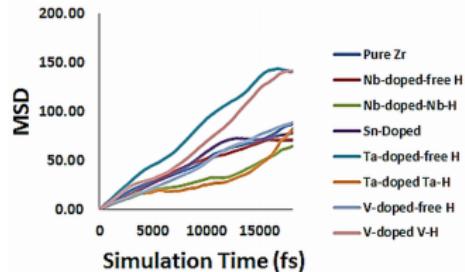
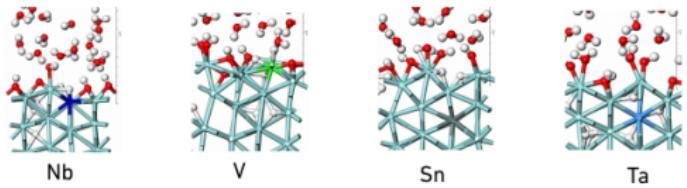


Zr(10̄10) surface, Oxygen and Hydrogen Absorption

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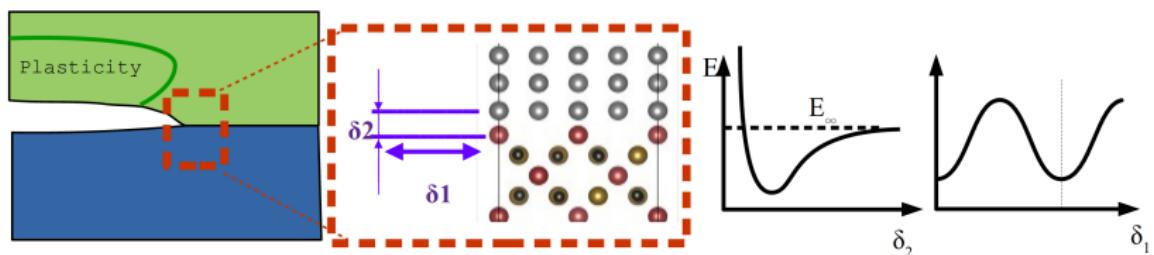
Progress so far

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

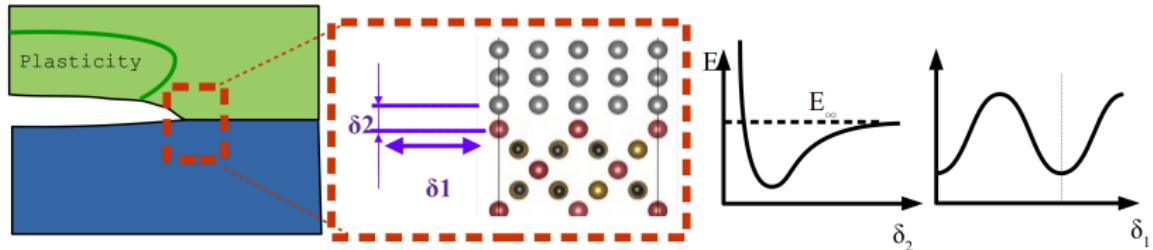


Adhesion in FeBCC/Fe₃O₄ interface

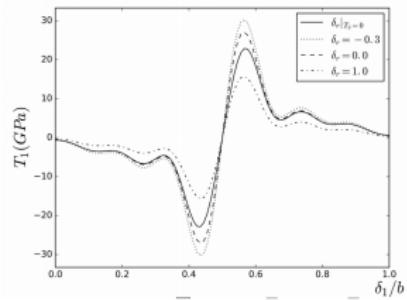
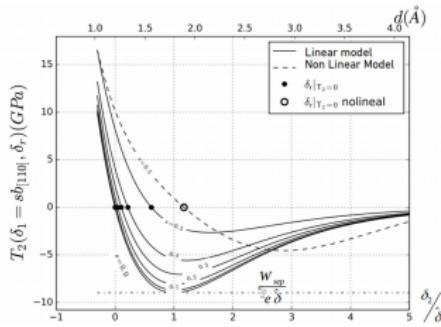
Separating the parts of the interface it is possible to obtain energy vs separation curves from DFT calculations. Then the forces can be obtained from interface potential models!



Adhesion in FeBCC/Fe₃O₄ interface



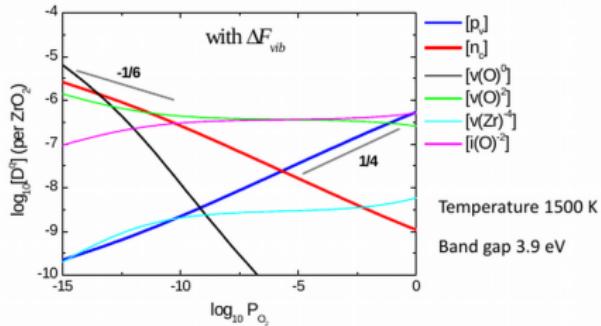
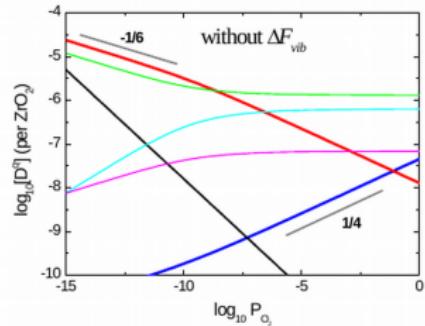
$$\tilde{L}_{\delta_1} = \frac{E_{\text{ad}}}{W_{\text{sep}}} = \exp\left(\frac{\delta_2}{\delta}\right) \sum_{i=0}^{i_{\max}} (1+\beta)^i \left[-1 + f(\delta_1)(1+\beta)^i \right] \alpha_i \left(\frac{\delta_2}{\delta} \right)^i \quad T_1(\delta_1, \delta_2) = -\frac{\partial W}{\partial \delta_1} \quad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



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.

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



Teaching

Teaching FEM basics

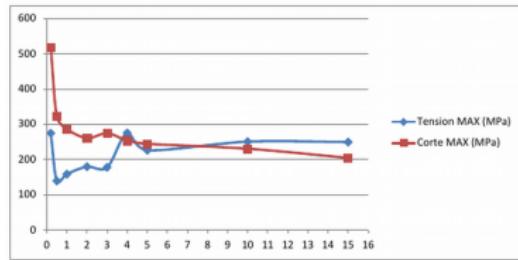
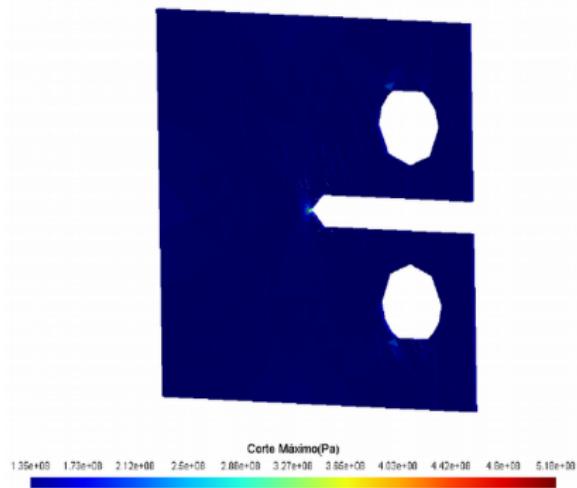
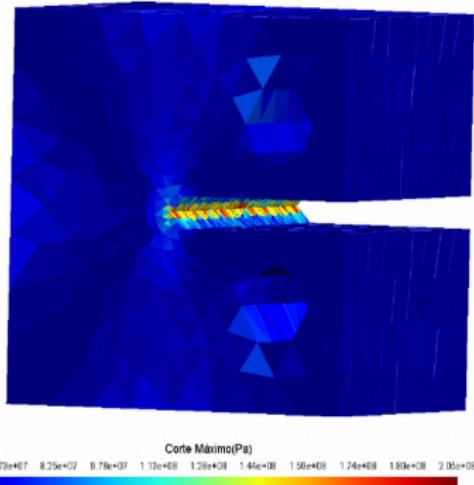


Fig. 11: Ordenadas: tensiones en MPa. Abscisas: espesor en cm.



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

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 image shows a composite of three windows. On the left is a terminal window with a command-line interface. In the center is a file browser showing a directory tree with various files and folders. On the right is a status bar or footer with some system information.

Terminal content:

```
sftp: Listado completo.  
marinomhoff@Bitacoras: ~$ ls  
ayuda  .Menú  Ver  ☰Editor  ☰Copiar  ☰RenMov  ☰Mdir  ☰Borrar  ☰Menú  ☰Salir  (*)  
50 51 cd $TD  
52 53 54 FEIXPAR>1  
55 CASE<HG  
56 USEPOTCAR=$SLURM_SUBMIT_DIR/submit  
57 cd $SLURM_SUBMIT_DIR/>.sh  
58 USEINCAR=$SLURM_SUBMIT_DIR/INCAR/INCAR-8CASE  
59 USEPOTCAR=$SLURM_SUBMIT_DIR/INPUTS/POTCAR  
60 USEKPOINTS=$SLURM_SUBMIT_DIR/INPUTS/KPOINTS-TOTEN  
61 62 runmysave  
63 64 65 cd $SLURM_SUBMIT_DIR  
66
```

File Browser content:

Ordenador	Archivo	Opciones	Derecho	Nombre	Ordenador	Archivo	Opciones	Derecho	Nombre
..	Nombre			DIR-ANT	Tamaño	Fecha Modif			DIR-ANT
/					4096	sep 11 19:04			
/Bitacoras				/INCARS	4096	sep 20 23:22			
/compromitesPago				/INPUTS	4096	sep 20 23:22			
/CSC				(22).atd1	4096	sep 30 05:49			
/cuadernoTrabajo					4096	oct 1 17:15			
/desktop					4096	ago 16 16:37			
/devs					20480	jun 26 19:59			
/Documents					4096	sep 7 09:46			
									/z1_atd1
				DIR-ANT					

Status Bar:

50,0-1 73% 07/07/2017 10:00:00

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



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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