Université de Lomé, Togo
FDS, Département de physique
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Kokou Gawonou N'TSOUAGLO

RESEARCH SKILLS

- Kinetic activation-relaxation technique (K-ART): An off-lattice self-learning kinetic Monte Carlo algorithm
- Kinetic Monte Carlo (KMC)
- Molecular Dynamics (Lammps)
- Materials modeling and Materials science
- ReaxFF, MEAM, EAM and Stillinger-Weber potential
- Debugging and modifying code (writing in Fortran (90/95), C/C++ and Python(in progress))
- MPI and OpenMP programming
- A background in solid state physics and semiconductor physics
- Familiar Unix/Lunix
- Study of defect in complexes materials
- Surface and interface diffusion
- Energy landscape exploration (Minima Hoping, Basin Hoping, Autonomous Basin Climbing, Tabu Search)

Education

2012-2015	**Master of Science in Computational Physics**, *Physics department, Condensed Matter Physics Theory Group* , University of Montreal, *(Canada)*.
2008-2009	**Master of Science in Theoretical Physics and Materials science**, *Faculty of Science, Theoretical Physics*, University of Lome, *(Togo)*.
2003-2007	**Bachelor of Science in Physics**, *Faculty of Science, Theoretical Physics*, University of Lome, Togo.
2003	**High School Diploma (BAC serie D)**, *Physics and biology*, Tsevie-Togo.

Experience

2015-	**Teaching Assistant**, *Physics department*, University of Montreal.
	explain undergraduate physics and tutorial
2010-2012	**Teaching Assistant**, *Ecole Supérieure d'Agronomie*, University of Lomé *(Togo)*.
	Working as Prof Mohou's Assistant; Teach undergraduate physics and tutorial
2010-2012	**Tutorial monitor**, *physics departement*, University of Lomé *(Togo)* .
	Teach undergraduate physics
2007-2012	**Teacher of physical sciences** , *Lycée Solidarité*, Lomé TOGO.
	Preparing student for High school diploma
2007-2012	**Teacher of physics and mathematics**, *Institut National de Formation Professionnelle et de Perfectionement (I.N.F.P.P)*, Lomé *(Togo)*.
	Preparing student for engineering physics and mathematics

2006-2009	**Framer of Advanced Women in science**, *Science of Faculty*, University of Lomé *(Togo)*.
	Teach physics and mathematics

Master Thesis in Montreal (Canada)2015

Title
: *Kinetics of the Si/SiO2 interface using Kinetic Monte Carlo and Molecular Dynamic simulation*

Supervisor
: **Prof. Normand Mousseau**

Description
: I am working with Kinetic ART, powerful transition-state searching method ART nouveau, coupled with a topological tool, NAUTY to offer an off-lattice kinetic Monte Carlo method with on-the-fly catalog building to study complex systems written in Fortran 90 full parallelized using MPI. Kinetic Art incorporates exactly all elastic effects at the minimums and the saddle points.

First, with this Kinetic Monte Carlo simulation, I have studied two systems, 50 vacancy aggregation in 2000 atoms of Fe with the EAM potential and energy relaxation in ion-bombarded of 27000 atoms of c-Si with the Stillinger-Weber potential. We compare a number of various algorithms used for sampling energy landscape of complex materials. The various algorithms chosen are those that use the Bell-Evans-Polanyi principle (well known in chemistry) to progress on the potential energy surface.This study allowed us to understand the steps needed to escape a local minimum to a another and controller research to quickly find the global minimum. This study also allowed us to understand the power of these methods on the kinetics of the structural evolution of complex materials.

In the second part, we have built a simulation tool (ReaxFF potential in Lammps code coupled with Kinetics-ART) able to study the first stages and oxidation process of silicon compare to the experimental time. To validate the system in place, we have tested the very first step of the silicon oxidation. The results obtained are in agreement with the literature. This tool will be used to understand the true oxidation process, the possible transitions of oxygen atoms at the silicon surface and the barrier associated with.

Diplome Etude Approfondie D.E.A (Equivalent master) in materials sciences in Lome (Togo) 2009

Title
: *Study of optical field inside and outside of a diode laser double heterostructure*

Supervisor
: **Prof. Mohou Messanh Agbeko**

Description
: We use the Maxwell, Hughens and fraunhofer equations to realize the electromagnetic theory of the double heterostructure (DH) $GaAs - Al_xGa_{1-x}As$ laser .This has permitted the establishment of an expression for the field interior the DH, of the equation of dispersion, of confinement factor and of DH far field in the orthogonal plane of the heterojunction. The knowledge of the properties of GaAs and $Al_xGa_{1-x}As$ alloys has permitted the calculation of index of different layers of DH lasers in order to represent the intensity of the electric field within and outside of DH lasers, the confinement factor and the variation of width in half height of the intensity of the field outside the DH lasers. The study of the progression of the electric field within and outside the DH lasers with characteristics parameters such as the thickness d of the active layer and the composition x in aluminum is the objective of this report .We show that a variation of the composition in aluminium and of thickness modify as well the electric field within and outside the DH.

Language

French	**Native**
English	**in progress** *Toefl iBT and GRE in preparation, I will sit for it soon*

Computer skills

Basic	Fortran 90, C/C++, Lunix/Unix, LaTeX, gnuplot, Work on High Performance Computing (HPC)
Intermediate	Python, Mathematica, Matlab, MPI, OpenMP
Tools	Modeling material simulation, Kinetic activation-relaxation technique (K-ART), Kinetic Monte Carlo, Molecular Dynamic (LAMMPS)
Miscellaneous	Windows, Office, Linux

Publications

[1] **Gawonou Kokou N'TSOUAGLO and al. ,** "Probing Potential energy surface exploration strategies for complex systems," **Accepted in J. Chem. Theory Comput.**

[2] N. Mousseau, P. Brommer, J.F. Joly, F. El-Mellouhi, L. K. Béland, **G. K N'TSOUAGLO** and al. , "Following atomistic kinetics on experimental timescales with the kinetic Activation-Relaxation Technique" **Computational Materials Science (2014) Elsevier**

[3] **Gawonou Kokou N'TSOUAGLO** and Normand Mousseau "Kinetic of Silicon Oxidataion using ReaxFF potential" **In preparation and it will be submitted soon**

Conference participation

March 2013	**APS March Meeting**, *Characterization of the relation between energy landscape and the time evolution of complex materials using kinetic ART*, **Maryland (USA)**, Oral presentation given in English.
May 2013	**CAP Congress**, *The time evolution of complex materials using kinetic ART*, **Montreal (Canada)**, Oral presentation given in English.
Nov 2009	**Sixth International Workshop on Contemporary Problems in Physics**, *Study of optical field inside and outside of a diode laser double heterostructure*, **Cotonou (Benin)**, Oral presentation given in French.
2012-2014	**Several seminars on Condensed Matter**, *DFT, Material Modeling, Kinetic Monte Carlo simulation ...* , **Montreal (CANADA)**.

Award and scholarship

2012	**Scholarship from IDB**, *covering the studies towards the MSc in physics and Condensed Matter Theory*, **at the university of Montreal**.
2014	**Scholarship from University of Montreal Physics department**, *completing the studies towards the MSc in physics and Condensed Matter Theory*, **at the university of Montreal**.

Contact of References

References upon request