Aditya Sundar, Ph.D student, University of Michigan

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Education

2017 – 2022 **Ph.D., University of Michigan** in Materials Science and Enginering CGPA: 3.93/4.00
Thesis title: *Modelling the structural and chemical stability of materials in extreme environments*
Certificate: Computational Discovery and Engineering
Advisor: Liang Qi

2017 – 2015 **M.S., Cornell University** in Materials Science and Engineering CGPA: 3.90/4.00
Thesis title: *The Structure and Chemistry of Epitaxial 2D Chalcogenides*
Advisor: Huili Grace Xing

2011 – 2015 **B.Tech., Indian Institute of Technology Madras**
in Metallurgical and Materials Engineering CGPA: 8.66/10.00
Thesis title: *Printed Silver Lines in MIS Solar Cells*
Advisor: Parasuraman Swaminathan
Minor degree: Management studies

Experience

Summer 2021 **Idaho National Laboratory,** Idaho Falls, USA
Research Internship, Computational Mechanics and Materials organisation

- Worked with experimental and computational researchers to guide materials selection for high temperature solid hydride nuclear moderators and metal/oxide claddings by
- Designing multiscale models to quantify hydrogen stability, transport and retention mechanisms using
- Density functional and density functional perturbation theory calculations, ab initio molecular dynamics and kinetic monte carlo simulations
- Learning the application of neural networks to solve materials problems.

Summer 2013 **Larsen & Toubro,** Mumbai, India
Engineering Internship, Heavy Engineering division

- Used non destructive evaluation techniques such as liquid dye penetrant testing and ultrasonic testing to identify surface and internal defects (cracks and porosity) in weld components

Skills

Methods	Electronic structure, molecular dynamics, monte carlo, potential energy landscape, computational thermodynamics, spectroscopy
Atomic Simulation	VASP, Quantum ESPRESSO, LAMMPS, ART Nouveau (Activation Relaxation Technique)
Materials Simulation	Thermo-Calc, Abaqus FEA.
Computation & design	Mathematica, Python (NumPy, Scikit), LaTeX, Linux, HPC
Image Processing	openCV
Experiments	XRD, XPS, EXAFS, Raman, SEM, Conductive-AFM

Research Publications

Manuscripts in Preparation

1. **Sundar**, **A.**, Kinzer, B., & Bala Chandran, R. (n.d.). Thermodynamic and kinetic modeling to evaluate co2 induced oxidation and carburization in fe and ni alloys.
2. **Sundar**, **A.**, Yu, J., & Cinbiz, M. (n.d.). Hydrogen stability and transport in al203 claddings.

Journal Articles

1. Hu, Y., **Sundar**, **A.**, Ogata, S., & Qi, L. (2021). Screening of generalized stacking fault energies, surface energies and intrinsic ductile potency of refractory multicomponent alloys. *Acta Materialia*, *116800*. link.
2. **Sundar**, **A.**, Chen, G., & Qi, L. (2021b). Substitutional adsorptions of chloride at grain boundary sites on hydroxylated alumina surfaces initialize localized corrosion. *npj Materials Degradation*, *5*. link.
3. **Sundar**, **A.**, & Qi, L. (2021). Stability of native point defects in al203 under aqueous electrochemical conditions. *Journal of Applied Electrochemistry*. link.
4. Lu, H., Reese, C., Jeon, S., **Sundar**, **A.**, Fan, Y., Rizzi, E., … Goldman, R. (2020). Mechanisms of gan quantum dot formation during nitridation of ga droplets. *Applied Physics Letters*, *116*(6), 062107. link.
5. Li, W., Nomoto, K., **Sundar**, **A.**, Lee, K., Zhu, M., Hu, Z., … Gao, X. et al. (2019). Realization of gan polarmos using selective-area regrowth by mbe and its breakdown mechanisms. *Japanese Journal of Applied Physics*, *58*(SC), SCCD15. link.
6. Vishwanath, S., **Sundar**, **A.**, Liu, X., Azcatl, A., Lochocki, E., Woll, A. R., … Peng, X. et al. (2018). Mbe growth of few-layer 2h-mote2 on 3d substrates. *Journal of Crystal Growth*, *482*, 61–69. link.

Conference Proceedings

1. Hu, Y.-J., **Sundar**, **A.**, Chen, G., & Qi, L. (2021). Title: Screening of generalized stacking fault energies, surface energies and intrinsic ductile potency of refractory multicomponent alloys. In *The minerals, metals & materials society 2021 annual meeting & exhibition*, Orlando, USA.
2. Kinzer, B., **Sundar**, **A.**, & Bala Chandran, R. (2021). Oxide dispersion particle clustering using phase field modelling in nickel-based superalloys. In *2021 mrs spring meeting & exhibit*, Phoenix, USA.
3. **Sundar**, **A.**, Chen, G., & Qi, L. (2021a). Electronic structure mechanisms to explain the onset of cl-induced localised corrosion in al203. In *The minerals, metals & materials society 2021 annual meeting & exhibition*, Orlando, USA.
4. **Sundar**, **A.**, Kinzer, B., & Bala Chandran, R. (2021). Oxidation and carburization behavior of iron- and nickel-based alloys in supercritical co2 environments. In *2021 mrs spring meeting & exhibit*, Phoenix, USA.
5. **Sundar**, **A.**, & Qi, L. (2019). Electric field dependent ionic transport in passive corundum al203 from dftapplication to localized corrosion. In *2019 mrs fall meeting & exhibit*, Boston, USA.

Research Projects

2020 – 2022 **Screening the chemomechanical properties of multicomponent BCC refractories**

- Developing DFT-based regression models for the prediction of intrinsic ductility/brittleness of BCC refractory alloys.
- Models parametrised using binary and ternary alloy data predict Re/Ru containing non-equimolar alloys with superior intrinsic ductility.

Research Projects (continued)

2018 – 2021 **Ab initio modelling of chloride induced localised corrosion in passive oxides**

- Validated the Point Defect Model by completely sampling the energy landscape of point defects in $\alpha-Al_2O_3$ using ab initio calculations
- Designed and implemented kinetic monte carlo simulations to model electromigration; by calculating electrical field dependent ionic migration barriers
- Identified the electronic origins of Cl adsorption at weak surface sites; from static and dynamic molecular simulations in standard aqueous conditions
- Lower adsorption energy of Cl at grain boundary sites accelerates and sustains a catalytic Al_2O_3 dissolution reaction, compared to single crystal surfaces.

2020 – 2021 **Alloy selection for high temperature heat exchanger materials, in supercritial CO_2**

- Developing CALPHAD based thermokinetic models to study oxidation-carburisation of Fe and Ni alloys in supercritical CO_2
- Recommended the use of Ni based Haynes 214 due to better carburisation resistance, compared to Fe based Incoloy MA 956
- 1D reaction-diffusion simulations show larger amounts of brittle carbide precipitation and carburisation depths in Incoloy MA 956

2019 – 2019 **Thermodynamic model for GaN quantum dot formation**

- Provided ab initio results to explain surface coverage dependent GaN quantum dot formation on Si. Results used to interpret morphological characteristics of MBE grown GaN quantum dots.
- Designed and calculated adsorption thermodynamics of Ga atoms to explain QD size distribution on oxidised and nitrided Si(100)-2×2 reconstructed surfaces.

2015 – 2017 **Structural, chemical and electronic properties of MBE grown 2D materials**

- Confirmed up to 44% Te alloying in MBE $MoSe_xTe_{2-x}$ on CaF_2 and GaAs substrates; by XRD, Raman, XPS, TEM and EXAFS examinations. Compositional variation of bandgap and excitonic states shown by absorption spectroscopy.
- Imaged crystallographic orientation, twinning and mosaicity in ultrathin 2D heterostructures (graphene-transition metal dichalcogenides) by synchrotron measurements.
- Developed Mathematica scripts to parse, analyze and visualize large datasets obtained from synchrotron based diffraction and spectroscopy experiments.
- Identified highly conductive leakage paths along MBE regrown interfaces by correlating topography and current area maps, to explain limited reverse breakdown voltage.

Coursework Projects

Fall 2020 **Computer Vision**
Implemented a OpenCV and scikit based fruit-sorting algorithm using blob detection and superpixel image segmentation methods; to sort fresh and rotten fruits.

Winter 2020 **Data-Driven Materials Design and Genomics**
Used python API to retrieve data from the Materials Project; used the Pymatgen library to analyse Li ion conductivity in solid state electrolytes

Coursework Projects (continued)

Fall 2018
- Integrated Computational Materials Engineering
  Developed an Abaqus finite element model to simulate uniaxial compression of an Al-Li cylinder. Calibrated multiscale strength model with experiment to study precipitate evolution, texture and mechanical behaviour under compression.

Winter 2018
- Kinetic Monte Carlo simulations of crystal growth
  Developed a 2D code and Mathematica visualisations to simulate the epitaxial growth of zinc blende GaAs. Surface diffusion energies from molecular dynamics calculations were used to evaluate temperature dependent point defects and surface morphologies.

Mentoring and Leadership

2019 – 2021
- Guided and trained Master's degree student in the design and implementation of first principles calculations using VASP. Research topics included (1) surface stability of passive oxides and (2) electronic structure origin of Cl-induced depassivation.
- Mentored research projects for 3 undergraduate students in the (1) design of ab-initio calculations, (2) implementation of ab-initio calculations using Quantum Espresso and (3) analysis of results. Topics covered included (1) thermodynamic stability of semiconductor polymorphs and (2) electronic stability of point defects in crystal semiconductors.
- Lab group server & website operations: http://cms.engin.umich.edu/
- Vice President, SPIC MACAY (Society for the Promotion of Indian Classical Music And Culture Amongst Youth), University of Michigan chapter. Led a team of 10-15 students in the organisation of biannual musical concerts in the university. Responsible for securing grants and event logistics.

2021
- Graduate Student Instructor for senior materials science course. Familiarised students with atomic modelling and visualisation software (VESTA).

2018
- Graduate Student Instructor for undergraduate materials science course. Led weekly discussions and office hours, and designed problem sets and demonstrations for a class of 30 undergraduate students.