Linyuan Shi

100 Rhines Hall – 32611 GAINESVILLE – US
(352)283-9950 • linyuan.shi@outlook.com

Education

University of Florida **Gainesville, FL**
Doctor of Philosophy in Material Science and Engineering, Cumulative GPA:3.86 *Aug 2016–May 2021*

Central South University **ChangSha, CHINA**
Bachelor of Science in Powder Material Science and Engineering, GPA:88.20/100 Rank:5/88 Sep 2012–Jun 2016

Research Experience

Mesoscale Framework for multi-physics simulation of ablative thermal protection system **Gainesville, FL**
Ph.D. Candidate, Dr. Simon R Phillpot Research Group *Jan 2018–Present*
Objective: Develop a multiphysics tool to predict the structure on pyrolysis and ablation of phenolic impregnated carbon ablator(PICA) thermal protection system(TPS).
- Characterize the structure of carbon fiber and generate the high fidelity carbon fiber model at atomic scale.
- Measure the mechanical and thermal properties of carbon fiber including tensile strength, thermal conductivity etc.
- Simulate the pyrolysis and oxidation of carbon fiber under high temperature using accelerated reactive molecular dynamics.

Mechanical Properties of Zr-H system **Gainesville, FL**
Graduate Research Assistant, Dr. Simon R Phillpot Research Group *Feb 2017–Mar 2020*
Objective: Investigate the mechanical properties of Zr with H interstitial and ZrHx inclusions using nanoindentation.
- Verify the fidelity of COMB3 potential for ZrHx system.
- Compute mechanical properties of ZrHx
- Analyze load vs. indentation depth, hardness vs. indentation curve of ZrHx and investigate deformation mechanisms.

Molecular dynamics simulation of radiation damage on tungsten **ChangSha, CHINA**
Research assistant, State Key Laboratory of Powder Metallurgy *Nov 2015–Jun 2016*
Objective: Investigate the mechanical properties, crystal structure stability, thermodynamic performance and stimulate the cascade progress on tungsten.
- Studied the number and distribution of defects produced by displacement cascades.
- Analyzed relations between primary knock on atom(PKA) energy and the number of defects at stable state.
- Found the threshold energy of tungsten at different crystal orientations.

Evaluation of W–TiC interface cohesion **ChangSha, CHINA**
Research assistant, State Key Laboratory of Powder Metallurgy *Nov 2014–Mar 2015*
Objective: Reveal the fundamental mechanism in terms of electronic structures and provide a deep understanding to various interface properties of W-TiC.
- Optimized the bulk lattice constant and crystal structures of W and TiC.
- Found a proper number of surface layers with a vacuum layer.
- Calculated the work of separation (W_{sep}) of W–TiC interfaces.

Skills

Programming Languages
- *C/C++*: Familiar with Modern C++ and experienced in C++ STL, smart pointer and templates.
- *Python*: Skilled in Numpy, Scipy, Pandas and Matplotlib.
- *Matlab*: Proficient in writing scientific scripts and implementing scientific algorithms.
- *Fortran*: Implementing and amending scientific algorithms.

Specialty Software
- *VASP*: Skillful in computing mechanical and thermodynamics properties of materials and plotting band structures.
- *LAMMPS*: Familiar with modeling a dynamic process and calculating basic properties of materials.
- *OVITO*: Experienced with analyzing materials by developing customized plugin via Python interface.
- *VESTA*: Experienced with visualizing crystal structures and exporting specific format files.

Honors and Awards

- ICMEd summer school fellowship awarded by National Science Foundation, June 2017
- NBTM Outstanding Student Fellowship awarded by NBTM New Material Group Co., Ltd, Fall 2015
- National Endeavor Fellowship awarded by Ministry of Education of PRC, Fall 2014

Publication

- **Linyuan Shi**, Marina Sessim, Michael Tonks and Simon Phillpot, Generation and characterization of an improved carbon fiber model by molecular dynamics (Recently accepted by Journal of Carbon)
- **Linyuan Shi**, Shi, Linyuan, Michele L. Fullarton, and Simon R. Phillpot. "Nanoindentation of ZrH2 by molecular dynamics simulation." Journal of Nuclear Materials (2020): 152391.
- **Linyuan Shi**, Marina Sessim, Michael Tonks and Simon Phillpot, Modeling Carbon fiber oxidation under high temperature by ReaxFF based molecular dynamics simulation, "AIAA SciTech Forum, American Institute of Aeronautics and Astronautics, 2020, Chaps." https://doi.org/10.2514/6.2020-0484
- Phillpot, Simon R., Andrew C. Antony, **Linyuan Shi**, Michele L. Fullarton, Tao Liang, Susan B. Sinnott, Yongfeng Zhang, and S. Bulent Biner. "Charge Optimized Many Body (COMB) potentials for simulation of nuclear fuel and clad." Computational Materials Science 148 (2018): 231-241.
- D.Y. Dang, **L.Y. Shi**, J.L. Fan, H.R. Gong, First-principles study of W–TiC interface cohesion, Surface and Coatings Technology, 25 August 2015, ISSN 0257-8972