

# Linyuan Shi

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## Education

### University of Florida

*Master of Science in Material Science and Engineering, Cumulative GPA:3.77*

**Gainesville, FL**

*Aug 2016–May 2018*

### Central South University

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

**ChangSha, CHINA**

## 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 at high temperature using accelerated reactive molecular dynamics.

### Mechanical Properties of Zr-H system

*MS student, Dr. Simon R Phillpot Research Group*

**Gainesville, FL**

*Feb 2017–Present*

Objective: Investigate the mechanical properties of Zr with H interstitials and ZrH<sub>x</sub> inclusions using nanoindentation.

- Verify the fidelity of COMB3 potential for ZrH<sub>x</sub> system.
- Compute mechanical properties of ZrH<sub>x</sub>
- Analyze load vs. indentation depth, hardness vs. indentation curve of ZrH<sub>x</sub> and investigate deformation mechanisms.

### Molecular dynamics simulation of radiation damage on tungsten

*Research assistant, State Key Laboratory of Powder Metallurgy*

**ChangSha, CHINA**

*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

*Research assistant, State Key Laboratory of Powder Metallurgy*

**ChangSha, CHINA**

*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

### Laboratory Apparatus

- Skillful operation with electronic universal testing machine, electronic tensile testing machine, powder forming press, CVD furnace, mechanical testing machine, etc
- Familiar with microhardness tester, SEM, TEM, Rockwell hardness tester, vacuum sintering furnace, etc.

### Programming Languages

- *Python*: Skilled in scientific libraries, plotting and using Asyncio to create asynchronous programs.
- *Matlab*: Proficient in writing scientific scripts and implementing scientific algorithms.
- *C/C++*: Familiar with C/C++ concepts and modifying scientific programs.
- *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

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- ICME 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

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- 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
- 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.