

Hao (Charles) Chen

M.Sc.

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Research Interests

Modelling and Simulation
Phase Transitions
Machine Learning in Science

Education

Master in Materials Science and Engineering
Tongji University (985/211 national key univ, QS Ranking: 211)
Average Score: 84.48/100

2021
Shanghai, China

Bachelor in Materials Science and Engineering
Hebei University of Science & Technology
Average Score: 85.66/100

2017
Hebei, China

Research Experience

"First-principles investigation of the evolution mechanism of ω phase and carbides in Fe-C alloys" **Master Thesis**

Supervisor & Co-supervisor: Prof. Hongping Xiang (Tongji University), Prof. Dehai Ping (NIMS, Japan)

- Performed DFT calculations to study the phase transitions process in steel based on experimental discoveries of Prof. Ping.
- Provided theoretical evidence for the existence of ω -Fe phase which has been neglected for decades in carbon steel.
- Proposed the stability mechanism of ω -Fe phase and its relationships with α -Fe and γ -Fe.
- Suggested a new formation process of cementite (θ -Fe₃C) and pearlite which are key factors for steel properties.
- Submitted a paper to *Scripta Materialia*.

"Study on ω -Fe and its effect on microstructure formation of carbon steel" **NSFC Project (No.51971159)**

Project Leader & Collaborator: Prof. Hongping Xiang (Tongji University), Prof. Dehai Ping (NIMS, Japan)

- Studied the formation mechanism of metastable carbide ω -Fe(C) by combining experiments and theoretical calculations.
- Calculated electron diffraction patterns using the CrystalMaker software in comparison with experimental TEM data.
- Confirmed a new kind of metastable carbide θ' -Fe(C) existed in the quenched high carbon Fe-C alloys.
- Investigated the transformation mechanism θ' -Fe₃C \rightarrow θ -Fe₃C by TEM observations and DFT calculations.
- Proposed a transition route ($\omega \rightarrow \omega' \rightarrow \theta' \rightarrow \theta$) during the coarsening of ultra-fine ω -Fe₃C particles.
- Published a paper in *Scientific Reports* and another one in *Crystal Growth & Design*.

"First low-spin carbodiimide, Fe₂(NCN)₃, predicted from first-principles investigations" **Master Project**

Project Leader: Prof. Hongping Xiang (Tongji University)

- Investigated the crystal structure of the Fe (III) carbodiimide Fe₂(NCN)₃.
- Studied the structural stability and physical properties of Fe₂(NCN)₃ within GGA+U framework.
- Predicted Fe₂(NCN)₃ to be a ferromagnetic half-metal and an interesting compound as a spintronic material.
- Published a paper in *Zeitschrift für Naturforschung B* to celebrate Prof. Richard Dronskowski's (RWTH) 60th birthday.

"Microstructure analysis of Austenitic stainless steel during deformation" **Bachelor Thesis**

Supervisor: Prof. Jiangang Wang (Hebei University of Science & Technology)

- Prepared austenitic stainless-steel specimens for mechanical experiment (wire-electrode cutting, uncoil and acid pickling).
- Observed microstructure changes of the specimens under different conditions by metallurgical microscope and AFM.
- Characterized the relationship between microstructure change and corrosion resistance of austenitic stainless steel.

Teaching Experience

Thesis Mentor, School of Materials Science and Engineering, Tongji University

Spring 2021/2020

Mentored two undergraduates on their graduation theses.

- Provided topics and guide the design of calculation scheme.
- Taught calculation methods and software using.
- One was awarded with "outstanding graduates" title.

Teaching Assistant, School of Materials Science and Engineering, Tongji University
"Computational Materials Science" course for 87 undergraduate students.

Fall 2020

- Helped solve technical problems in software installation and using.
- Exercise.

Specialized Course Consultant, Remedial Classes of Postgraduate Entrance Examination

Fall 2020/2019

"Fundamentals of Materials Science" course for ~15 undergraduates who want to apply for Master program in Materials Science at Tongji University.

- Gave 20 hours of lectures including crystallography, phase transitions, materials properties etc.
- Exercise and test.

Professional Skills

Language: Chinese Mandarin (native), English (IELTS: overall 6.5/B2, CET: band 6/highest)
Scientific Software: VASP (VTST), Materials Studio (CASTEP), CrystalMaker, VESTA
Operate System: Windows, Linux
Characterization: XRD, TEM, SEM, AFM, OES
Computing: Machine Learning, Python (with Coursera certificates)

Publications

Chen H, Xiang H. P, First low-spin carbodiimide, $\text{Fe}_2(\text{NCN})_3$, predicted from first-principles investigations. *Zeitschrift für Naturforschung B* 76(10-12): 783-788 (2021). <https://doi.org/10.1515/znb-2021-0128>

Ping D. H, **Chen H**, Xiang H. P, Formation of $\theta\text{-Fe}_3\text{C}$ Cementite via $\theta'\text{-Fe}_3\text{C}$ ($\omega\text{-Fe}_3\text{C}$) in Fe-C Alloys. *Crystal Growth & Design* 21, 1683–1688 (2021). <https://dx.doi.org/10.1021/acs.cgd.0c01533>

Ping D. H, Xiang, H. P, **Chen H**, et al. A transition of $\omega\text{-Fe}_3\text{C} \rightarrow \omega'\text{-Fe}_3\text{C} \rightarrow \theta'\text{-Fe}_3\text{C}$ in Fe-C martensite. *Scientific Reports* 10, 6081 (2020). <https://doi.org/10.1038/s41598-020-63012-9>

Chen H, Xiang H. P, Ping D. H, Stability of C atoms in $\gamma\text{-Fe}$, $\alpha\text{-Fe}$, and $\omega\text{-Fe}$ in Fe-C alloys: A first-principles study. (In revision)

Contribute to:

Lu W. F, Wang Z. L, Xiang H. P, et al. Exploration of the atomic-level structures of the icosahedral clusters in Cu-Zr-Al ternary metallic glasses via first-principles theory. *Materials Research Express* 9, 065203 (2022) <https://doi.org/10.1088/2053-1591/ac7516>

Honors and Awards

Tongji University Full Scholarship	Oct. 2020
Tongji University Full Scholarship	Oct. 2019
The First Prize Scholarship, Hebei University of Science & Technology	Jun. 2017
The First Prize Scholarship, Hebei University of Science & Technology	Jun. 2016
The First Prize Scholarship, Hebei University of Science & Technology	Jun. 2015
The Second Prize Scholarship, Hebei University of Science & Technology	Jun. 2014

References

References available upon request