7th IEA FM TCP workshop on theory and modelling of nuclear fusion materials
Yonsei University Global Campus, Songdo in Incheon, Korea – Jan 29-31, 2024

Meeting @ Room 105, Veritas Hall A (Building 401) (Lunch @ Room B102, Y-Plaza)

(https://ukaeaevents.com/7th-fusion-materials-theory-modeling-workshop/)

Registered Participants (If presenter, oral number in brackets)

Seoyeon Bak Seoul National University	Chaeyeong Kim Seoul National University	Luca Reali (O2.2) UK Atomic Energy Authority
David Cereceda (O3.2) Villanova University	Jae-Hyuk Kim Seoul National University	Ho Jin Ryu Korea Advanced Institute of Science and Technology
Krishna Chaitanya Pitike (O4.4) Pacific Northwest National Laboratory	Jae-Min Kwon (O5.3) Korea Institute of Fusion Energy	Wahyu Setyawan (O2.3) Pacific Northwest National Laboratory
Kunok Chang Kyung Hee University	Donggyu Lee Seoul National University	Michael Short (O1.3) MIT
Huiqiu Deng (O4.2) Hunan University, China	Byeongchan Lee Kyung Hee University	Sophia von Tiedemann (O3.1) University of Birmingham
Sergei Dudarev UK Atomic Energy Authority	Xiangyan Li (O4.5) Hefei Institutes of Physical Science, China	Chenxu Wang (O1.9) Peking University
Philip Edmondson (O1.8) University of Manchester	Jaime Marian (O2.6, O5.1) University of California, Los Angeles	Yugang Wang Peking University
Kim Gibum Seoul National University	Daniel Mason (O1.2) UK Atomic Energy Authority	Andrew Warwick (O2.1) UK Atomic Energy Authority
Mark Gilbert (O5.2) UK Atomic Energy Authority	Sam Murphy (O3.3) Lancaster University	Brian Wirth (O1.7) University of Tennessee, Knoxville
Akira Hasegawa (O1.4) IMR, Tohoku University	Duc Nguyen-Manh (O1.6) UK Atomic Energy Authority	Jan Wróbel (O4.6) Warsaw University of Technology
Xunxiang Hu (O3.4) Sichuan University	Takuji Oda (O4.3) Seoul National University	Sojeong Yang (O4.1) Seoul National University
Atsushi M. Ito (O2.7) National Institute for Fusion Science, Japan	Pär Olsson (O2.8) KTH Royal Institute of Technology	Hong-Bo Zhou (O1.5) Beihang University
Shin Kajita (O2.4) The University of Tokyo	Sehyeok Park Seoul National University	Steve Zinkle (O1.1) University of Tennessee
Keonwook Kang (O2.5) Yonsei University		

Final agenda

Monday 29th January	Tuesday 30th January	Wednesday 31st January
Session 1.1 **Topic: Optimised modelling and experimental validation** **(9:00-10:30)** Session Chairs: Jaime Marian, David Cereceda	**Session 2.2** **Topic: Material Response theory** **(9:00-10:30)** Session Chairs: Philip Edmondson, Luca Reali	**Session 2.3/4.3** **Topic: Material Response Theory/Machine Learning** **(9:00-10:30)** Session Chairs: Sam Murphy, Akira Hasegawa
O1.1: **Steve Zinkle (Uni. Tennessee, ORNL),** Fundamental Experimental Studies for Benchmarking Models and Improved Understanding of Radiation Effects in Materials O1.2: **Daniel Mason (UKAEA)**, Simulated Transmission Electron Microscopy of highly irradiated metals O1.3: **Michael Short (MIT)**, Quantifying Radiation Damage with Stored Energy for Faster Testing of Hypotheses of Primary Radiation Damage Resistance	O2.4: **Shin Kajita (Uni. Tokyo),** Helium irradiation and co-deposition effects on tungsten O2.5: **Keonwook Kang (Yonsei University)**, Hydrogen Effect On The Behavior of a Single Dislocation in BCC Tungsten: Atomistic Study O2.6: **Jaime Marian (UCLA)**, Modeling irradiation creep under fusion reactor operation	O2.7: **Atsushi Ito (NIFS)**, Regenerated ZBL Potential and Its Effect on Sputtering Yield (pre-recorded video presentation) O2.8: **Pär Olsson (KTH, Sweden)** Microstructure and magnetization evolution in bcc iron via direct first-principles predictions of radiation effects O4.6: **Jan Wróbel (WUT, Poland)**, The development of ML potentials for Ta-Ti-V-W high-entropy alloys for fusion applications

Coffee & Tea break 10:30-11:00	Coffee & Tea break 10:30-11:00	Coffee & Tea break 10:30-11:00
Session 1.2 **Topic Optimised modelling and experimental validation** **(11:00-13:00)** Session Chairs: Brian Wirth, Sophia von Tiedemann	**Session 3.1** **Topic: Transmutation impacts** **(11:00-13:00)** Session Chairs: Mark Gilbert, Hong-Bo Zhou	**Session 5** **Topic: General topics in fusion materials modelling** **(11:00-13:00)** Session Chairs: Daniel Mason, Atsushi Ito
O1.4: **Akira Hasegawa (Tohoku University)**, Current Status of Neutron Irradiation Data and Future Prospects for Modeling Studies of Tungsten and Tungsten Alloys	O3.1: **Sophia von Tiedemann (Uni. Birmingham)**, Prediction of transmutants in relevant fusion materials and modelling their impact on material properties	O5.1: **Jaime Marian (UCLA)**, Simulations of structural material evolution under pulsed irradiation conditions typical of IFE reactors
O1.5: **Hong-Bo Zhou (Beihang University)**, Multiscale modeling of evolution of defect structure and corresponding mechanical properties of tungsten induced by neutron irradiation	O3.2: **David Cereceda (Villanova Uni.),** Effects of the chemical environment and energetics of point defects on transmuting tungsten-based alloys	O5.2: **Mark Gilbert (UKAEA),** Nuclear data applications for fusion materials modelling and ongoing needs
O1.6: **Duc Nguyen-Manh (UKAEA)**, Predictive composition stability of advanced structural materials for nuclear applications	O3.3: **Sam Murphy (Uni. Lancaster)**, Atomistic Simulation of Solid Tritium Breeder Materials	O5.3: **Jae-Min Kwon (KFE)**, Digital Twin Technologies to Accelerate Fusion R&D
30-minute discussion	30-minute discussion	30-minute discussion

Lunch 13:00-14:30 (1.5 hours for lunch) Coffee & Tea (14:00-14:30)	Lunch 13:00-14:30 (1.5 hours for lunch) Coffee & Tea (14:00-14:30)	Lunch 13:00-14:30 (1.5 hours for lunch) Coffee & Tea (14:00-14:30)
Session 1.3 **Topic Optimised modelling and experimental validation** **(14:30-16:00)** Session Chairs: Byeongchan Lee, Sojeong Yang	**Session 3.2/4.1** **Topic: Transmutation impacts/Materials response theory** **(14:30-16:00)** Session Chairs: Wahyu Setyawan, Keonwook Kang	**Session 6** **Topic** **(14:30-16:00)** Discussion lead: Mark Gilbert, Byeongchan Lee, Jaime Marian
O1.7: **Brian Wirth (Uni. Tennessee)**, Development of multi-scale computational frameworks to solve fusion materials science challenges	O3.4: **Xunxiang Hu (Sichuan Uni.)**, Nuclear Transmutation and its Impact on In-Service Performance of Tungsten	Closing and plans for review paper (section lead-authors, teams and timelines)
O1.8: **Phil Edmondson (Uni. Manchester)**, Optimising TBR for liquid breeder based fusion power plants	O4.1 **Sojeong Yang (Seoul Uni.),** Machine learning potential for studying sticking and reflection of low-energy hydrogen impingement on tungsten (110) surface	Hosting volunteers for next meeting
O1.9: **Chenxu Wang (Peking Uni.)**, Possibility and Challenge of Establishing Equivalent Methods to Predict Cavity Swelling in Alloys Induced by Neutron Irradiation	O4.2: **Huiqiu Deng (Hunan Uni.),** New machine learning Potentials for Fe-H-He and W-He Systems	

Short Break 16:00-16:15	Short Break 16:00-16:15	Meeting Close
Session 2.1 **Topic Material response theory (16:15-18:00)** Session Chairs: Steve Zinkle, Krishna Chaitanya Pitike O2.1: **Andrew Warwick (UKAEA),** Decoding the source of spatially fluctuating lattice strains O2.2: **Luca Reali (UKAEA)**, γ-photons and high-energy electrons: production by neutron irradiation and effects on nuclear materials O2.3: **Wahyu Setyawan (PNNL)**, Modeling of tritium permeation in Pd - coated V vacuum permeator 15-minute discussion	**Session 4.2** **Topic: Machine Learning (16:15-18:00)** Session Chairs: Duc Nguyen-Manh, Jan Wrobel O4.3: **Takuji Oda (Seoul National Uni.),** Isotope and nuclear quantum effects in hydrogen diffusion in bcc metals by machine learning potentials O4.4: **Krishna Chaitanya Pitike (PNNL),** Accurate Fe–He machine learning potential for studying He effects in bcc Fe O4.5: **Xiangyan Li (ISSP Hefei),** Interaction of vacancies, self-interstitial atoms, and helium/hydrogen with nanocavities in α-iron 15-minute discussion	
Social gathering (from 19:00)		
Sheraton Grand Incheon, Lotus 5 (3F) Beer and food		