



EUROPEAN COMMISSION
DIRECTORATE GENERAL JRC
JOINT RESEARCH CENTRE
Institute for Transuranium Elements (Karlsruhe)
Material Research Unit

Karlsruhe, 24 March 2011

WORKSHOP

MATERIALS MODELLING AND SIMULATIONS FOR NUCLEAR FUELS

MONDAY 29 SEPTEMBER 2008

08:00	TRANSPORTATION TO FZK-FTU	BUS SERVICE
08:45-09:00	WELCOME	T. FANGHÄNEL (ITU)
INTRODUCTION		
09:00-09:20	GNEP FUELS CAMPAIGN MODELING AND SIMULATION ROAD MAP	U. CETIN (LANL), K. PASAMEHMETOGLU (INL)
09:20-09:40	DISCOVERY AND DESIGN OF ADVANCED NUCLEAR FUELS	M. STAN (LANL)
09:40-10:00	COMPUTATIONAL MATERIALS SCIENCE NETWORK (CMSN) PROJECT ON "MULTISCALE SIMULATION OF THERMO-MECHANICAL PROCESSES IN IRRADIATED FISSION-REACTOR MATERIALS"	D. WOLF (INL)
10:00-10:20	THE F-BRIDGE PROJECT	C. VALOT (CEA)*
10:20-10:40	COFFEE / TEA BREAK	
SESSION I. FIRST PRINCIPLE CALCULATIONS		
10:40-11:00	XANES AND THE ELECTRONIC STRUCTURE OF ACTINIDE OXIDES	C. SUZUKI (JAEA)
11:00-11:20	FIRST-PRINCIPLES MODELLING OF HE BEHAVIOUR IN UO ₂	Y. YOUNSUK, O. ERIKSSON, P. OPPENEER (UU)
11:20-11:40	WIEN2K CALCULATIONS OF HE IN UO ₂ AND PUO ₂	D. SEDMIDUBSKY, O. GEDEON (ICT)

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11:40-12:00	CASTEP CALCULATIONS FOR HE IN NUCLEAR FUELS	D. PARFITT, R. GRIMES (IC)*
12:00-12:20	VASP CALCULATIONS FOR PERFECT AND DEFECTIVE ACTINIDE NITRIDES AND OXIDES	D. GRYAZNOV (ITU), E. HEIFETS, E. KOTOMIN, Y. MASTRIKOV, Y. ZHUKOVSKII (ISSP)
12:20-12:40	INVESTIGATION USING DENSITY FUNCTIONAL THEORY OF THE BEHAVIOR OF RARE GASES IN SILICON CARBIDE	M. BERTOLUS (CEA)
12:40-13:30	LUNCH	FZK CANTEEN
13:30-13:50	STABILITY AND MIGRATION MECHANISMS OF POINT DEFECTS AND VOLATILE ELEMENTS IN URANIUM CARBIDE (VASP CALCULATIONS)	M. FREYSS, B. DORADO (CEA)
13:50-14:10	EXAFS INVESTIGATIONS OF SOLID SOLUTIONS	M. WALTER (ITU)
14:10-14:30	INTERACTION OF THE OXYGEN MOLECULE WITH THE UN(001) SURFACE: AB INITIO MODELING	D. BOCHAROV (ISSP)
14:30-14:50	FIRST PRINCIPLES MODELLING OF DEFECT MIGRATION IN URANIUM NITRIDE AND TRANSURANUS PREDICTION OF FUEL PERFORMANCE	S.N.RASHKEEV (INL), E.A.KOTOMIN (ISSP), Y.MASTRIKOV (ISSP), P.VAN UFFELEN (ITU)
14:50-15:10	COFFEE / TEA BREAK	
SESSION II. CLASSICAL MOLECULAR DYNAMICS SIMULATIONS		
15:10-15:30	MICROSCOPIC PROCESSES IN OXIDE FUELS: INSIGHTS FROM SIMULATION	S. PHILLPOT (UF)
15:30-15:50	MOLECULAR DYNAMICS STUDY OF XENON BEHAVIOUR WITH COMPLEX POINT DEFECT CLUSTERS IN UO ₂	L. VAN BRUTZEL, A. CHARTIER (CEA)
15:50-16:10	HELIUM DIFFUSION IN UO ₂	K. GOVERS, S. LEMEHOV, M.VERWERFT (SCK)
16:10-16:30	QUANTITATIVE MEASUREMENT OF HELIUM IN NUCLEAR FUELS	E. MAUGERI, J.-Y. COLLE, J.-P. HIERNAUT, T. WISS (ITU)
16:30-18:00	POSTER SESSION	
19:00	WORKSHOP DINNER OFFERED BY ITU	HOTEL RESIDENZ

TUESDAY 30 SEPTEMBER 2008

08:00-08:30	TRANSPORTATION TO FZK-FTU	BUS SERVICE
SESSION II. CLASSICAL MOLECULAR DYNAMICS SIMULATIONS (CONT.)		
08:40-09:00	OXYGEN DIFFUSION MECHANISMS IN NON-STOICHIOMETRIC URANIUM DIOXIDE	E. YAKUB (OSEU), D. STAICU (ITU)
09:00-09:20	THERMAL CONDUCTIVITY OF (U,Pu)O ₂ WITH PU CONTENT FROM 0% TO 100%	C. COZZO, D. STAICU (ITU)
09:20-09:40	FISSION GAS BEHAVIOUR IN UO ₂	R. GRIMES, D. PARFITT (IC)
09:40-10:00	SIMULATION OF THERMAL SPIKES IN UO ₂	K. GOVERS, S. LEMEHOV, M. VERWERFT (SCK)
10:00-10:20	COFFEE / TEA BREAK	
SESSION III. THERMODYNAMICS		
10:20-10:40	NON-CONGRUENT EVAPORATION IN HIGH-TEMPERATURE URANIUM-BEARING FUELS	I. IOSILEVSKIY (MIPT)
10:40-11:00	THE UO ₂ -ZrO ₂ PHASE DIAGRAM	D. MANARA (ITU)
11:00-11:20	THE MEPHISTA THERMODYNAMIC DATABASE	M. BARRACHIN (IRSN)
11:20-11:40	ACTINIDE OXIDES VAPOUR PRESSURES ABOVE PURE AND MIXED OXIDES	P. GOTCU, J.-P. HIERNAUT, J.-Y. COLLE, R.J.M. KONINGS (ITU)
SESSION IV. MESOSCOPIC AND MACROSCOPIC MODELS		
11:40-12:00	INVESTIGATION OF MODEL FOR STRESS CORROSION CRACKING OF CLADDING MATERIALS	Y. KAJI (JAEA)
12:00-12:20	APPLICATION OF MATERIALS MODELS TO SIMULATE MICROSTRUCTURAL EVOLUTION IN FUELS	V. TIKARE (SNL)
12:20-12:40	AN ATTEMPT TO SIMULATE HIGH BURNUP STRUCTURE IN UO ₂ FUEL WITH MONTE CARLO METHOD	O. JAE-YONG, K. YANG-HYUN, L. BYUNG-HO (KAERI)
12:40-13:30	LUNCH	FZK CANTEEN
13:30-13:50	NUMERICAL MODELING OF GASEOUS FISSION PRODUCT TRANSPORT AT THE MICROSCALE	T. BARTEL, M. T. LUSK (SNL)
13:50-14:10	NEW ADVANCED ANALYSES OF FISSION PRODUCT BEHAVIOUR IN TRISO PARTICLES	R. DUBOURG (IRSN)

14:10-14:30	SIMULATION OF CENTRELINE MELTING IN OPERATIONAL, DEFECTIVE NUCLEAR FUEL	M. J. WELLAND, W.T. THOMPSON, B.J. LEWIS (RMC)
14:30-14:50	MODELS OF EVAPORATION CONDENSATION IN FAST REACTOR	A. COURCELLE, F. VANNI (CEA)

SESSION V. FUEL BEHAVIOUR AND SIMULATION CODES

14:50-15:10	ATOMISTIC MODELING IN FRAPCON – A COMPARISON WITH EMPIRICAL MODELING	J. TULENKO (UF)
15:10-15:30	COFFEE / TEA BREAK	
15:30-15:50	SIMULATING CREEP DEFORMATION OF ZIRCALOY CLADDING UNDER DRY STORAGE CONDITIONS WITH TRANSURANUS	O. MARTIN (IE)
15:50-16:10	PERFORMANCE MODELLING OF CANDU NUCLEAR FUEL	M.H.A. PIRO, D.R. MORGAN, B.J. LEWIS, W.T. THOMPSON (RMC)
16:10-16:30	MODELLING OXIDATION OF DEFECTIVE UO_{2+x} FUEL	K. SHANEEN (RMC)
16:30-17:30	GENERAL DISCUSSION	
17:30	CLOSING OF THE WORKSHOP	

POSTER SESSION

DEVELOPMENT OF A MANDREL TEST FOR ADVANCED CLADDING MATERIALS

O. MARTIN, K.-F. NILSSON (IE)

THE MODES WITH THE KURDYUMOV'S SHARPENING IN THE URANIUM-PLUTONIUM FISSION ENVIRONMENT

V.D. RUSOV, V.A. TARASOV, T.L. BORIKOV, S.A. CHERNEGENKO (NPU)

GEOANTINEUTRINO SPECTRUM AND SLOW NUCLEAR BURNING ON THE BOUNDARY OF THE LIQUID AND SOLID PHASES OF THE EARTH'S CORE

V. D. RUSOV^{1,2}, V. A. TARASOV¹, T. N. ZELENTOVA^{1,2}, V. N. BOLSHAKOV¹, D. A. LITVINOV,¹ S. I. KOSENKO¹, O. A. BYEGUNOVA² (¹ NPU, ² UB)

THE GENERALIZED FEOKTISTOV'S CRITERION FOR NEUTRON MULTIPLYING MEDIUMS

V.D. RUSOV, V.A. TARASOV, S.A. CHERNEGENKO (NPU, UKRAINE)

A SELF STANDING GIBBS ENERGY MINIMIZATION PROCEDURE TO SOLVE CHEMICAL EQUILIBRIUM IN MULTIELEMENT MULTIPHASE NUCLEAR MATERIALS

M.H.A. PIRO, W.T. THOMPSON, B.J. LEWIS (RMC)

VASP CALCULATIONS FOR (U,Zr)N SOLID SOLUTIONS

D. GRYAZNOV (ITU), D. FUCHS (ISRAEL)

USING FIRST PRINCIPLE CALCULATIONS FOR NITRIDE FUELS IN A FUEL PERFORMANCE CODE

P. VAN UFFELEN (ITU), E. KOTOMIN (ISSP)

* To be confirmed