



Monday, May 6

9:30-10:30	Opening and Welcome Addresses I. Steinbach ICAMS E. Weiler Ruhr-University Bochum H. Fischer ThyssenKrupp Steel Europe AG	Opening
10:30-11:00	Break	Break
11:00-11:40	H.D.K.H. Bhadeshia <i>Non-cubic ferrite</i>	M1 Chair I. Steinbach
11:40-12:20	V. Vitek <i>Bond-order potentials for bcc transition metals with attraction determined by bond integrals deduced from DFT and repulsion from the overlap of p electrons of closed-shell atoms of argon</i>	
12:20-12:50	J. Neugebauer <i>Materials design based on predictive ab initio thermodynamics</i>	
12:50-2:00	Lunch break	Break
2:00-2:40	D.G. Pettifor <i>Development of a magnetic bond-order potential for Mn phases</i>	M2 Chair M. Finnis
2:40-3:00	G.K.H. Madsen <i>Simplified models of electronic structure</i>	
3:00-3:20	T. Hammerschmidt <i>Bond-order potentials for large-scale atomistic simulations</i>	
3:20-3:40	J. Rogal <i>Atomistic modelling of phase transformation kinetics</i>	
3:40-4:10	Break	Break
4:10-4:50	G. Henkelman <i>t.b.a.</i>	M3 Chair J. Neugebauer
4:50-5:10	R. Janisch <i>Modelling and understanding the strength of grain boundaries based on ab-initio results</i>	
5:10-5:50	B.-J. Lee <i>Computational process design of high value-added {100} textured steel sheet</i>	
5:50-6:10	G. Sutmann <i>t.b.a.</i>	
6:10-6:15	Concluding remarks	
6:15-9:00	Poster session	Poster

Tuesday, May 7



9:00-9:40	M.W. Finnis <i>Progress in the theory of oxide scale growth</i>	T1 Chair H. Bhadeshia
9:40-10:10	G. Eggeler <i>Using advanced ingot metallurgy to contribute to a better understanding of NiTi shape-memory alloys</i>	
10:10-10:30	U. Preiss <i>A DFT informed phase field model for electrochemical systems</i>	
10:30-11:00	Break	Break
11:00-11:20	S.G. Fries <i>The Sapiens project: A four years trajectory inside thermodynamics</i>	T2 Chair R. Drautz
11:20-12:00	H.J. Seifert <i>Thermodynamic assessment and modeling of ternary Ti-Al systems</i>	
12:00-12:40	Y. Wang <i>Unique properties of ferroelastic systems having nanodomain structures</i>	
12:40-2:00	Lunch break	Break
2:00-2:40	E. Busso <i>A coupled diffusion-phase-field crystal-plasticity framework to study grain boundary cavitation in irradiated materials</i>	T3 Chair V. Vitek
2:40-3:00	A. Hartmaier <i>Scalebridging descriptions of mechanical properties of multiphase materials</i>	
3:00-3:20	A. Ma <i>Micromechanical modelling of plasticity and phase transformation in multi-phase polycrystalline metals</i>	
3:20-3:50	Break	Break
3:50-4:30	D. Raabe <i>Nanoscale phase transformations at martensite interfaces</i>	T4 Chair A. Hartmaier
4:30-5:00	W. Bleck <i>Understanding complex microstructure for various applications</i>	
5:00-5:20	F. Varnik <i>Multiscale modeling of solidification phenomena</i>	
5:20-5:30	Concluding remarks	