

Table of Contents

Participants

Committees

Preface

Bridging Different Length and Time Scales in Diffusion Problems Using a Lattice Monte Carlo Method

I.V. Belova and G.E. Murch 1

Electro-Mechano-Chemistry; Transport Problem in Four Time Scales

M. Danielewski, M. Pietrzyk and B. Wierzba 11

Concurrent Multiscale Kinetic Monte Carlo-Continuum Models for the Evolution of Solids via Diffusion

S.P.A. Gill and P.E. Spencer 19

Comparison of the Strain Distribution Obtained from Multi Scale and Conventional Approaches to Modelling Extrusion

Ł. Madej, P. Hodgson and M. Pietrzyk 25

Energetic Landscapes and Diffusion Properties in FeCu Alloys

F. Soisson and C.C. Fu 31

Multi-Lattice Kinetic Monte Carlo Simulation of Interface Controlled Solid-State Transformations

C. Bos, F. Sommer and E.J. Mittemeijer 41

Cluster Dynamics Modeling of Materials: Advantages and Limitations

A. Barbu and E. Clouet 51

Interdiffusion of Two L1₀ Phases without Long-Range Order Decrease: Experiments and Molecular Dynamics Simulations

C. Goyhenex, R.V.P. Montsouka, M. Kozłowski and V. Pierron-Bohnes 59

Orientation of Interstitials in Clusters in α -Fe: A Comparison between Empirical Potentials

M.C. Marinica and F. Willaime 67

Anisotropy of the Vacancy Migration in Ti, Zr and Hf Hexagonal Close-Packed Metals from First Principles

G. V $\acute{e}$ rit $\acute{e}$, F. Willaime and C.C. Fu 75

Monte Carlo Simulation of Texture and Microstructure Transformation during Annealing of Steel

H.L. Li, J.T. Park and J.A. Szpunar 83

A Phase Field Model for grain Growth and Thermal Grooving in Thin Films with Orientation Dependent Surface Energy

N. Moelans, B. Blanpain and P. Wollants 89

An Extensive Study of Charge Effects in Silicon Doped Heterofullerenes

M. Matsubara and C. Massobrio 95

Interface Shape Change and Shift Kinetics on the Nanoscale

Z. Erd $\acute{e}$ lyi, D.L. Beke, G.A. Langer and A. Csik 105

Analysis of Oxygen Segregation at Metal-Oxide Interfaces Using a New Lattice Monte Carlo Method

I.V. Belova, G.E. Murch, N. Muthubandara and A. Öchsner 111

Materials Hardness Estimation by Simulation of the Indentation Process

M. Sychalski, T. Wejrzanowski and K.J. Kurzydłowski 119

Stability of Hollow Nanospheres: A Molecular Dynamics Study

A.V. Evteev, E.V. Levchenko, I.V. Belova and G.E. Murch 125

First Principles Study of Al(100) Twisted Interfaces

R. Sot and J. Piechota 131

Interface Dynamics of Melt Instabilities on Semiconductor Surface

B. Datsko, V. Meleshko, Z. Świątek, I. Mohylyak, L. Lityńska-Dobrzyńska and P. Zięba 137

Grain Boundary Migration in Nanocrystalline Iron

T. Wejrzanowski, M. Sychalski, R. Pielaszek and K.J. Kurzydłowski 145

Mutiscale Plastic Deformation near a Fatigue Crack from Diffraction

Y. Sun, R. Barabash, H. Choo, P.K. Liaw, Y. Lu, D.W. Brown and G.E. Ice 151

