ACEX2011
ABSTRACT BOOK

IRONIX
GLOBAL EVENTS CONSULTING

5TH INTERNATIONAL CONFERENCE
ON ADVANCED COMPUTATIONAL ENGINEERING AND EXPERIMENTING
ACE-X 2011
4, 5 & 6 JULY, 2011 ALGARVE - PORTUGAL

IRONIX CONFERENCES MANAGEMENT
we organise conferences!

Edited by:
IRONIX CONFERENCES
www.ironix-conferences.com

nanomaterials.

[1] R.D. Groot and P.B. Warren. J. Chem. Phys., 107, 4423-4435, (1997).
[2] M. Meunier. J. Chem Phys. 123, (2005).
[3] A. Maiti. J. Wescott, P. Kung. Molecular Simulation, 31, 2-3 (2005).
[4] Wescott, P. Kung, A. Maiti Applied Physics Letters 90, 033116 (2007)

SS9

ACEX360

Mr. Seyed Vahid Hosseini
K. N. Toosi University of Technology
IRAN

Molecular Dynamics Simulation of Dislocation Behavior during Nano-Machining Process on a Bicrystal with a Grain Boundary

Seyed Vahid Hosseini1, a, Mehrdad Vahdati2, b, Ali Shokuhfar2, c
1Ph.D Student of Mechanical Engineering, K. N. Toosi University of Technology, Tehran, Iran.
2Professor of Mechanical Engineering, K. N. Toosi University of Technology, Tehran, Iran.
aMscmechanic@hotmail.com , bVahdati@kntu.ac.ir , cShokuhfar@kntu.ac.ir

Abstract
Atomistic details about dislocation interaction with grain boundary have attracted much attention during the last several decades. This is because the mechanical properties of the polycrystalline materials are greatly affected by the interaction of lattice dislocations with grain boundaries and the results from the grain boundary studies have greatly contributed to the design of structural materials. Recently, atomistic simulation techniques have successfully progressed to achieve atomic scale understanding of micro mechanism. In particular, the simulation techniques have enabled detailed analyses of dislocation nucleation and defect interactions during nanoscratching process, including the interaction mechanism of dislocations with twin boundaries and a mechanism for misfit dislocation creation, and the role of grain boundaries in the nano-polycrystals during deformation. In this paper, the nano-machining of copper with and without a grain boundary is compared to study the effect of the grain boundary on machining characteristics using molecular dynamics simulation with EAM potentials. Also, interaction of dislocations with a Σ=5 (210) [001] grain boundary that is parallel to the scratching direction was investigated. Furthermore, the transmission of the dislocations across the grain boundary was analyzed during the ploughing process of rigid tool on the specimen. The results showed that the dislocation transmitted across the grain boundary during nanomachining process and left a step in the boundary plane. Also, results suggested that a partial dislocation in the first grain merged into the grain boundary and it was dissociated into another partial dislocation in second grain and a grain boundary dislocation, introducing a step in the grain boundary. Finally, the behavior of tool forces are affected when the generated dislocation are reach to the grain boundary.

SS9

ACEX097

Prof. Luisa Maria Rocha Durães
University of Coimbra,
PORTUGAL

Modeling and simulation of radial combustion propagation of Fe2O3/Al thermite systems

P. Brito1,2, L. Durães1, A. Portugal1
1 CIEPQPF, Dept. of Chem. Engineering., Faculty of Sciences & Technol., University of Coimbra, Pólo II, Rua Sílvio Lima, 3030-790 Coimbra - Portugal
2 Dept. of Chem. & Biolog. Technol., School of Technol. & Management, Polytech. Inst. of Bragança, Campus de Santa Apolónia, PO Box 1134, 5301-857 Bragança - Portugal

Abstract
In previous works [1-2], a one-dimensional model was built to simulate the non-steady radial combustion propagation on thin disk shaped samples of Fe2O3/Aluminum thermite mixtures and was successfully tested. Now, the purpose is to extend the referred model to the more sensible two-dimensional features of the samples, maintaining the main characteristics of the previous model: zero order kinetics, conductive/radiative heat transfer, assumption of phase transitions, temperature and composition variation of all system properties during propagation. Therefore, an adaptive numerical algorithm that conjugates a Method of Lines (MOL) strategy based on finite differences space discretizations, with a collocation scheme based on increasing level dyadic grids is applied for the solution of the problem. The model validation implies the comparison of numerical results with available experimental data obtained in similar conditions. Thus, the particular integration method proves to cope satisfactorily with the steep travelling thermal wave in 1D and 2D spatial domain supports, either for trivial uniform mixing conditions, as in complex examples developed to feature more sophisticated circumstances, such as non-homogeneous reactant mixing [1], and selective pseudo-random directional flame extinction, which realistically replicate the observed experimental phenomena.

[1] P. Brito, L. Durães, J. Campos, A. Portugal, Chem. Eng. Sci., 62, 5078 (2007).
[2] L. Durães, P. Brito, J. Campos, A. Portugal, in Computer Aided Chemical Engineering, Vol. 21A, p. 365, Marquardt, W., Pantelides, C., Eds. (Elsevier, 2006).

SS9

VIP-ACEX031

Prof. Noorhana Yahya
Universiti Teknologi PETRONAS,
MALAYSIA

Forward Modeling of Seabed Logging by Finite Integration (FI) and Finite Element (FE) Methods

N. Yahya1, M.N.Akhtar2, and N.Nasir2
1Department of Fundamental and Applied Science,
2Department of Electrical and Electronic Engineering, Universiti Teknologi PETRONAS
31750, Bandar Seri Iskandar, Malaysia

Abstract
Seabed electromagnetic (EM) modelling for the detection of deep target hydrocarbon reservoir is still remains a challenge for oil and gas industry. More precise and accurate electromagnetic (EM) methods are required for the better detection of hydrocarbon reservoir. Finite integration method (FIM) and Finite element method (FEM) were chosen for 3D modelling of seabed logging to get more precise EM response from hydrocarbon reservoir. The purpose of EM modelling was to investigate the total electric and magnetic fields instead of scattered electric and magnetic fields, which shows accurate and precise resistivity contrast at target depth of 3000m below seafloor. Finite integration method and finite element method was applied on our proposed seabed model having square area (20´20km). It was observed that finite integration method shows 6.52% resistivity contrast at target depth of 1000m where as finite