Supplemental Proceedings

Volume 2: Materials Properties, Characterization, and Modeling
Supplemental Proceedings

Volume 2:
Materials Properties, Characterization, and Modeling
Check out these new proceedings volumes from the TMS2012 Annual Meeting, available from publisher John Wiley & Sons:

3rd International Symposium on High Temperature Metallurgical Processing
CFD Modeling and Simulation in Materials Processing
Characterization of Minerals, Metals, and Materials
Electrometallurgy 2012
Energy Technology 2012: CO2 Management and Other Technologies
EPD Congress 2012
International Smelting Technology Symposium (Incorporating the 6th Advances in Sulfide Smelting Symposium)
Light Metals 2012
Magnesium Technology 2012
Supplemental Proceedings: Volume 1: Materials Processing and Interfaces
T.T. Chen Honorary Symposium on Hydrometallurgy, Electrometallurgy and Materials Characterization

To purchase any of these books, please visit www.wiley.com.
TMS members should visit www.tms.org to learn how to get discounts on these or other books through Wiley.
About this volume

The TMS 2012 Annual Meeting Supplemental Proceedings, Volume 2: Materials Properties, Characterization, and Modeling is a collection of papers from the 2012 TMS Annual Meeting and Exhibition, held March 11–March 15, in Orlando, California, U.S.A.

The papers in this volume were selected based on technical topic compatibility and represent fourteen symposia from the meeting. This volume, along with the other proceedings volumes published for the meeting, and archival journals, such as Metallurgical and Materials Transactions and the Journal of Electronic Materials, represents the available written record of the 65 symposia held at the 2012 TMS Annual Meeting.

The individual papers presented within this proceedings volume have not necessarily been edited or reviewed by the conference program organizers and are presented "as is." The opinions and statements expressed within the papers are those of the individual authors only and are not necessarily those of anyone else associated with the proceedings volume, the source conference, or TMS. No confirmations or endorsements are intended or implied.
# TABLE OF CONTENTS


## 2012 Functional and Structural Nanomaterials: Fabrication, Properties, Applications and Implications

### Carbon Nanomaterials

- Photo-Ignition of Liquid Fuel Spray and Solid Fuel through Carbon Nanotubes
  
  A. Badakhshan, and S. Danczyk

### 0-Dimensional Nanomaterials

- Citrate Mediated Wet Chemical Synthesis of Fe Doped Nanoapatites: A Model for Singly Doped Multifunctional Nanostructures
  
  R. Kasinath, M. Klem, and R. Usselman

### 1-Dimensional Nanomaterials and ZnO

- P-Type Conductive Behaviors of AlN Co-Doped ZnO Films Deposited by the Atomic Layer Deposition
  
  Y. Kim, K. Jeong, H. Yun, S. Yang, S. Lee, H. Lee, and G. Lee

- Zinc Oxide Nanorods by the Pulsed Plasma in Liquid and their Photocatalytic Property
  
  E. Omurzak, K. Taniguchi, and T. Mashimo

### Nanomaterials for Energy Technology

- 3D Multiwall Carbon Nanotubes (MWCNTs) for Li-Ion Battery Anode
  
  C. Kang, I. Lahiri, R. Baskaran, M. Choi, W. Kim, Y. Sun, and W. Choi
Structural Nanomaterials

Obtaining and Characterization of Nanostructured Al-Sr Master Alloys ..........................43
P. Gabriela, S. Vasile, D. Mitrica, and I. Gheorghe

Refinement of Ligaments of Nanoporous Ag Ribbons by Controlling the Surface Diffusion of Ag..................................................................................................................51
T. Song, Y. Gao, Z. Zhang, and Q. Zhai

Joint Session with "2012 Surface and Heterostructures"

Synthesis and Characterization of Core-Shell TaNx Nanocomposites ..........................59
L. Liu, K. Huang, Z. Wang, J. Hou, and H. Zhu

Poster Session

Effects of Calcination Conditions on Particle Size and Morphology of NiFe₂O₄ Nanoparticles Synthesized by Solid-State Reaction .................................................................67
Z. Zhang, Y. Liu, G. Yao, D. Wu, and J. Ma

Raman Spectroscopy of Graphene and Plasma Treated Graphene under High Pressure.................................................................................................................................75
A. Hadjikhani, J. Chen, S. Das, and W. Choi

RTS Noise Analysis in Fin-type Silicon-Oxide-High-k-Oxide-Silicon Flash Memory .................................................................81

Atmospheric-Pressure Plasma Sintering of Silver Nanopaste Screen-Printed on PI .................................................................................................87
K. Kim, W. Myung, and S. Jung

Electrical Characterization in Pillar Type Silicon-Oxide-Nitride-Oxide-Silicon Flash Memory using Bandgap Engineering Method ..................................................95
S. Lee, S. Yang, J. Oh, H. Yun, K. Jeong, Y. Kim, H. Lee, and G. Lee
The Post-Annealing Effects of N-Doped ZnO Films Deposited by the Atomic Layer Deposition

K. Jeong, Y. Kim, H. Yun, S. Yang, S. Lee, Y. Kim, H. Lee, and G. Lee

Computational Thermodynamics and Kinetics

Thermodynamics

Determinants of Thermal Stability in Nano-sized Binary Alloys

C. Yang, and Y. Mai

Thermodynamic Modeling of Peirce-Smith Converter Slag at the Chagres Smelter, Chile

N. Cardona, P. Mackey, P. Coursol, R. Parada, and R. Parra

Phase-Field Simulations in Alloys I

Phase Field Modeling of Coherent Zirconium Hydrides Reorientation under Applied Load

L. Zhang, L. Thuinet, A. Legris, A. Debacker, and A. Ambard

Phase-Field Simulations in Alloys II

Numerical Modeling of Dendritic Growth During Solidification of Alloys Using Lattice Boltzmann and Cellular Automaton Methods

M. Eshraghi, and S. Felicelli

Poster Session

A Kinetic Study of the Leaching of Germanium Dust and Fume by Sulfuric Acid

W. Wang, J. Peng, Z. Zhang, L. Chu, and G. Lai

Establishment and Analysis of the Composite Key Stratum Model Layer on the Winkler Foundation

H. Pan, S. Li, P. Zhao, and T. Zhang
Convex Projection to Estimate Heat Content of Cold Charges in Peirce-Smith Converting .................................................................................................151
A. Navarra, A. Pubill Melsió, and J. Kapusta

Defects and Properties of Cast Metals

Metal Cleanliness

Films and Bifilms – An Update ........................................................................161
J. Campbell

Fluid Flow and Inclusion Entrapment in the Runner Steel During Ingot Casting ..............................................................................................169
L. Zhang, Y. Chen, and S. Yang

Modeling of Die Filling of Low-Pressure Die-Cast Aluminum Alloy Wheels .................................................................................................177
J. Duan, D. Maijer, S. Cockcroft, C. Reilly, K. Nguyen, and D. Au

Quench Sensitivity of 2024, 6063 and 7075 .......................................................185
E. Tan, A. Tarakci, and D. Dispinar

Effect of Different Casting Parameters on the Cleanliness of High Manganese Steel Ingots Compared to High Carbon Steel ........................................193
P. von Schweinichen, Z. Chen, D. Senk, and A. Lob

Tensile Properties, Porosity and Melt Quality Relation of A356 ..................201
D. Dispinar, S. Akhtar, A. Nordmark, F. Syvertsen, M. Di Sabatino, and L. Arnberg

Investigation on Non-metallic Inclusions of Q420 Ingots Cast by Bottom Teeming ............................................................................................209
Y. Luo, J. Zhang, C. Xiao, and J. Yang

Porosity

Effect of Porosity on Deformation, Damage, and Fracture of Cast Steel ..........217
C. Beckermann, and R. Hardin

Detection and Influence of Shrinkage Pores and Non-Metallic Inclusions on Fatigue Life of Cast Aluminum Alloys ...............................................225
Y. Tijani, A. Heinriet, W. Stets, and P. Voigt
Relationship between Pores Volume (by Density Measurements) and Pores Area (on Fracture Surfaces) of A356 Fatigue Specimens..............................233
   A. Morri, L. Ceschini, I. Svensson, and S. Seifeddine

Non Homogenous Microstructure of Cast Iron Components – Challenge For Fatigue Evaluation of Non-Destructively Tested "Defect Free" Components ..................................................241
   A. Heinriet, J. Eufinger, W. Stets, A. Sobota, and H. Loeblich

Hot Tearing

The Importance of Solidification Structure with Respect to Hot Tearing during Continuous Casting of Steels.........................................................251
   R. Pierer, W. Rauter, and C. Bernhard

Hot Tearing Susceptibility in DC-Cast Aluminum Alloys ..................259
   N. Jamaly, A. Phillion, S. Cockcroft, and J. Drezet

Solidification Phenomena during Casting of Stainless Steel/Cast Iron Composites .................................................................267
   T. Lucey, R. Wuhrer, P. Huggett, K. Moran, W. Yeung, and M. Cortie

Hot Tear Susceptibility of Al-Mg-Si Alloys with Varying Iron Contents ......275
   L. Sweet, M. Easton, J. Taylor, C. Davidson, L. Lu, M. Couper, and D. StJohn

The Analytical Model of Microsegregation for Solute Elements in Solidifying Mushy Zone of Steel........................................................283
   C. Xiao, J. Zhang, and Y. Luo

Solidification Structure and Segregation

A Multi-Scale 3D Model of the Vacuum Arc Remelting Process ..............291
   K. Pericleous, G. Djambazov, M. Ward, L. Yuan, and P. Lee

Identification of Defect Prone Peritectic Steel Grades by Analyzing the High Temperature Phase Transformations .................................299
   P. Presoly, R. Pierer, and C. Bernhard

Effect of Deformation on Microsegregation in Cast Structure of Bearing Steel ...........................................................309
   M. Basirat, and H. Fredriksson
Effects of Section Size And Cooling Rate on Microstructure and As-Cast Properties of Investment Cast CO-CR Biomedical Alloy


Molecular-Dynamics Simulations of NI-Based Superalloys

C. Woodward, J. Lill, D. Trinkle, and M. Asta

Numerical Simulation on Solidification Microstructure of Cast Steel using Cellular Automaton Method

B. Su, Z. Han, B. Liu, Y. Zhao, B. Shen, and L. Zhang

Microstructure Simulation in Pressurized Solidification during Squeeze Casting of Aluminum Alloy A356

Y. Li, Z. Han, A. Luo, A. Sachdev, and B. Liu

Modeling of Melt Mixing Phenomena in Cast Iron with Dual Graphite Structure

S. Lekakh, J. Qing, and V. Richards

Ductility, Creep, Stress and Cracks

Thermal-Mechanical Model Calibration with Breakout Shell Measurements in Continuous Steel Slab Casting

J. Iwasaki, and B. Thomas

Effect of Cooling Structure on Stress Distribution of Copper Plates of Slab Continuous Casting Mold

X. Meng, W. Wang, and M. Zhu

Reasonable Temperature Schedules for Cold or Hot Charging of Continuously Cast Slabs

Y. Li, P. Lan, K. Liu, H. Sun, H. Chen, and J. Zhang

Deformation Prediction of a Heavy Hydro Turbine Blade During Casting Process with Consideration of Martensitic Transformation

J. Kang, T. Wang, T. Huang, and B. Liu

Novel Processes and Applications

Automated Vision System for Inspection of Surface Casting Defects Based on Advanced Computer Techniques

S. Swillo, and M. Perzyk
Deformation, Damage, and Fracture of Light Metals and Alloys

Session I

A Macroscopic Yield Function Coupled with Crystal Plasticity Theory for Modeling Forming of AZ31 Magnesium Alloy Sheets

Session II

Effect of Corrosion on the Strength of Fillet Arc Welded Cu-Lean AA7xxx Joints

Micro-Shear Stress and Damage Predictions from Hydrostatic Stress Loading of Aluminum Alloys 7075, 7039, and 7020

Session III

Deformation Twinning Activation of Ti-6Al-4V under Different Loading Conditions
Impact Response and Dislocation Substructure of Ti-6Al-4V Alloy at Cryogenic Temperatures.................457
   W. Lee, T. Chen, and S. Huang

Session IV

Low Temperature Superplastic Deformation of Mg-Bi-Si Alloys...............465
   S. Remennik, A. Katsman, and D. Shechtman

Session V

Microstructure, Texture and Mechanical Properties of Mg-Gd-Nd-Y-Zn Alloy Manufactured under Various Thermomechanical Treatments.....................471
   X. Hou, Z. Cao, and L. Wang

Poster Session

Correlation between Melt Quality and Fatigue Properties of 2024, 6063 and 7075 .................................................................479
   E. Tan, A. Tarakcilar, and D. Dispinar

Emeritus Professor George D.W. Smith Honorary Symposium

Steels I

Microstructural Characterisation of Nanometre Scale Irradiation Damage in High-Ni Welds.................................................................489
   J. Hyde, P. Styman, C. English, G. Smith, K. Wilford, T. Williams,
   R. Boothby, and H. Thompson

Ulthahigh Strength Pearlritic Microstructures: Contributions by George D. W. Smith.........................................................................503
   G. Krauss, S. Miller, E. De Moor, and D. Matlock

Atom Probe Analyses of Advanced Sheet Steels..................................513
   K. Seto, D. Saxey, and G. Smith
Steels II and Superalloys

High Strength Conductors for High Field Magnets ........................................... 521
  K. Han, R. Walsh, V. Toplosky, and J. Lu

Initial Age Hardening and Nanostructural Evolution in a Cu-Ni-P Alloy .......... 529
  Y. Aruga

From Macro to Nano, Understanding Mechanical Behavior across Length Scales: A Structural Materials Division Symposium in Honor of Robert Ritchie

Fatigue

A Comparison of Cast Aluminum Bulkhead Fatigue Resistance: The Effect of Specimen Geometry ................................................................. 539
  A. Campbell, and J. Allison

Small Scale Mechanical Behavior and Theory

Mechanical Behavior at the Limit of Strength ..................................................... 547
  J. Morris

Deformation and Fracture

Tensile Deformation of Quenched and Partitioned Steel - A Third Generation High Strength Steel ................................................................. 555
  J. Coryell, J. Campbell, V. Savic, J. Bradley, S. Mishra, S. Tiwari, and L. Hector

Mechanical Behavior of Novel Materials

Adhesion of Nickel-Titanium Shape Memory Alloy Wires to Polymeric Materials: Theory and Experiment ......................................................... 563
  L. Hector, F. Antico, and P. Zavattieri

xiii
General Poster Session

Session I

Mechanical Behavior of Porous NiAl Fabricated by Unidirectional Solidification ..............................................................579
J. Lee, S. Hyun, M. Kim, T. Ide, and H. Nakajima

Phase Decomposition in Isothermally-Aged Fe-Cr Alloys....................581
V. Lopez-Hirata, E. Avila-Davila, H. Dorantes-Rosales,
and M. Saucedo-Muñoz

Investigation of the Polymer Composite Materials Reinforced by Hybrid Carbon and Basalt Fibers........................................589
N. Chikhradze, G. Abashidze, and L. Japaridze

Wettability and Interfacial Microstructure of Pb-Free Sn3.5Ag Alloy Powders on Cu Substrate..................................................595
J. Zhao, W. Zhang, T. Song, Y. Gao, and Q. Zhai

Existence of Niobium in Ductile Iron and Its Effect on the Morphology of Graphite Ball.........................................................603
X. Sun, Z. Yin, L. Chang, Q. Hua, and Q. Zhai

Mechanical Properties of Nanocomposites Based on PA6 Blends .............613
P. Agrawal, G. Brito, B. Cunha, S. Cavalcanti, E. Araújo,
and T. Mélo

Effect of Carbon on Structural Changes in Ni$_3$Al Phase.......................621
A. Janas, E. Olejnik, B. Grabowska, and J. Nawrocki

Integrative Materials Design: Performance and Sustainability

Processing and Properties of Advanced Steels & Sustainable Design, Life-Cycle Analyses, and Recycling

The Contribution of Niobium Bearing Steels and Enhanced Sustainability ....631
S. Jansto
Materials Design Approaches and Experiences III

Non-ferrous Alloys and Processes

C. Hutchinson

High Strength Steels

Alloy Design of 9% Cr Steel for High Efficiency Ultra-Supercritical Power Plants .................................................................649
F. Abe

Microstructural Studies on Thermomechanically Processed Plain Carbon Dual Phase Steel .................................................................659
A. Singh, S. Nath, M. Bhardwaj, V. Pancholi, and G. Chaudhari

Joining and Microstructure-Property Relationships

Heat Treatment Effects on Creep Behavior of Directionally Solidified CM247LC Superalloy .................................................................667
K. Hsu, H. Wang, W. He, C. Kuo, H. Bor, and C. Wei

Mechanical Behavior at Nanoscale I

In-situ Technique on Deformation Process

Localized Crystal Rotation in Gum Metal at Ideal Strength ....................675
S. Kuramoto, T. Furuta, D. Satoyama, E. Withey, and J. Morris

Deformation/strength at Nanoscale and Li-induced Deformation

Study of Dislocation Climb at Nanovoids in BCC Metal .......................683
M. Bhattacharya, A. Dutta, A. Giri, N. Gayathri, and P. Barat
Poster Session

Processing of ta-C Protective Films on a Mold for Glass Lenses

S. Oh, and Y. Kim

Effects of Ti on Electronic Structure and Mechanical Property of Uranium: a First-Principles Study

J. Qi, Y. Ren, G. Wu, J. Zhang, and K. Chou

Mechanical Behavior for Different Cutting Directions on Copper and Rhodium Single Crystals

S. Kano, and A. Korenaga

Investigation of the Crystal Structure on the Nanomechanical Properties of Pulsed Laser Deposited NbN Thin Films

M. Mamun, A. Farha, Y. Ufuktepe, H. Elsayed-Ali, and A. Elmustafa

Nanomechanical Properties of Hydrogen Implanted AlN for Layer Transfer by Ion-Induced Splitting

M. Mamun, K. Tapily, O. Moutanabbir, D. Gu, H. Baumgart, and A. Elmustafa

Nanomechanical Properties of Atomic Layer Deposition Sb₂Te₃ Thin Films

M. Mamun, D. Gu, D. Nminibapiel, H. Baumgart, H. Robinson, V. Kochergin, and A. Elmustafa

The Role of Stacking Fault Energy and Deformation Twinning on the Indentation Size Effect of FCC Pure Metals and Alloys

D. Stegall, and A. Elmustafa

Investigation of the Indentation Size Effect in FCC Metals Using Activation Volume Analysis

D. Stegall, and A. Elmustafa

Nanoindentation Investigation of VO₂ Films Synthesized by Reactive Bias Target Ion Beam Deposition (RBTIBD)

M. Mamun, S. Kittiwatanakul, K. Zhang, H. Baumgart, J. Lu, S. Wolf, and A. Elmustafa
Minerals, Metals and Materials under Pressure

**Damage and Microstructure**
Continuum Scale Material Modeling under Large Strain, Strain Rates and Pressure Incorporating Microstructure Effect

N. Bonora, A. Ruggiero, G. Iannitti, and S. Dichiaro

N. Bonora, A. Ruggiero, G. Iannitti, and S. Dichiaro

Stochastic Methods in Materials Research

**Session I**
Research on Prediction of the Stability of Partially Stabilized Zirconia Prepared by Microwave Heating Using Levenberg Marquardt-Back Propagation Neural Network

L. Liu, S. Guo, D. Li, J. Peng, G. Chen, and L. Xu

Stochastic Geometry and Transformation Kinetics Theories: Basics and Results

P. Rios, and E. Villa

**Symposium in Memory of Patrick Veyssière:**
Understanding the Mechanisms Controlling Plastic Flow

**Plastic Flow**
Finite Element Implementation of a Self-Consistent Polycrystal Plasticity Model: Application to α-Uranium

M. Knezevic, R. McCabe, R. Lebensohn, C. Tomé, and B. Mihaila

**Intermetallic Alloys**
Some Long-Period Superstructures and the Related Motion of Dislocations in Al-Rich TiAl Single Crystals

T. Nakano, S. Hata, K. Hayashi, and Y. Umakoshi

xvii
Deformation Mechanisms

A Comparison of Dislocation Microstructures Formed during Severe Plastic Deformation of an Al-2.5 Mg Alloy at Room and Cryogenic Temperatures and Their Effect on Alloy’s Room-Temperature Strength .................................................805
  J. Singh, A. Sarkar, G. Sharma, and J. Chakravartty

Ultrasonic Fatigue of Advanced Materials and Systems

Ultrasonic Fatigue of Metals and Alloys I

Damage Mechanisms in the VHCF Regime in Quasi Defect-Free Metals Regarding Different Levels of Microstructural Inhomogeneity .......................815
  M. Zimmermann, and H. Christ

Comparison of Fatigue Property of Metallic Materials under Conventional and Ultrasonic Testing Methods ........................................................................823

Ultrasonic Fatigue of Metals and Alloys II; Very High Cycle Fatigue of Composites and MEMS

Ultrasonic Fatigue of Ti6Al4V in the Very High Cycle Fatigue Regime ..........831
  S. Heinz, G. Wagner, F. Balle, and D. Eifler

In-Situ Characterization of the Damage Evolution of Welded Aluminum Alloy Joints during Very High Cycle Fatigue (VHCF) with Nonlinear Ultrasonic Technique ..................................................................................839
  M. Cremer, M. Zimmermann, and H. Christ

Ultrasonic Fatigue of Aluminum Matrix Composites (AMC) in the VHCF-Regime ...............................................................................................................847
  G. Wagner, M. Wolf, and D. Eifler

Ultrasonic Fatigue Testing System Combined with Online Nondestructive Testing for Carbon Fiber Reinforced Composites ........................................855
  D. Backe, F. Balle, T. Helfen, U. Rabe, and S. Hirsekorn
TMS2011 General Poster Session

Magnetic Materials for Energy Applications

Phase Transformation and Magnetic Properties of Pr$_2$Co$_7$ Intermetallics........865
N. Mliki, R. Fersi, and L. Bessais

TMS2011 General Abstracts: Structural Materials Division

Applications

Hot Deformation Behavior of Ti-6Al-4V Alloy with $\alpha$-Martensite Starting Microstructure..................................................................................................................873
H. Matsumoto, B. Liu, S. Lee, Y. Li, K. Sato, Y. Ono, and A. Chiba

Author Index.................................................................................................................877

Subject Index..................................................................................................................883
The proceedings contained in this section have not been edited or reviewed by the conference program organizers. The opinions and statements expressed in the proceedings are those of the authors only and are not necessarily those of the editors or TMS staff. No confirmations or endorsements are intended or implied.
PHOTO-IGNITION OF LIQUID FUEL SPRAY AND SOLID FUEL THROUGH CARBON NANOTUBES

Badakhshan A¹, Danczyk S. A.²

¹ Jacobs Technology, ROSS Group, 8 Draco Dr., Edwards AFB, CA 93524
² Air Force Research Lab, RZSA, 10 Saturn Blvd, Edwards AFB, CA 93524
Approved for public release by Air Force Research Lab; distribution unlimited

Abstract

We have studied the ignition of liquid fuel and simulated solid rocket fuels (SRF) by the photo-ignition of single wall carbon nanotubes (SWCNTs). Our investigation includes the effect of solid additives such as aluminum nano-particles and solid oxidizers such as ammonium perchlorate (AP) on the photo-ignition characteristics. We found that by mixing CNT with other nanoparticles and powdered material, the ignition parameters such as; burn temperature and burn duration can be tailored to meet ignition requirements. We believe this approach in photo-ignition of a fuel spray and solid fuels provides a suitable method for ignition of liquid rocket engines and solid rocket motors. Among the advantages of this approach are a compact, light weight, and robust ignition method and it enables distributed ignition of fuel sprays.

Keyword: photo-ignition, fuel ignition, carbon nanotubes, liquid fuel spray, rocker fuel

Introduction

The first report on photo-ignition of single wall carbon nanotubes (SWCNTs) by a camera flash appeared in 2002 [1]. It was suggested that Fe nanoparticles within SWCNTs play an important role in the photo-ignition process [2]. Subsequently, others reproduced some of the aforementioned results and offered that SWCNTs could be used as ignition agents for a variety of liquid fuels, including those of interest in liquid rocket engines [3-5]. It was also proposed that SWCNTs could facilitate distributed ignition of liquid sprays [3]. In an earlier work, we showed that liquid fuel can be ignited through photo-ignition of SWCNTs [6]. Other applications of photo-ignition of SWCNT have also been reported [7-9]. More recently other reports on the photo-ignition of the gaseous fuel and air mixture showed distributed ignition [10,11]. There has been a recent report on the photo-ignition of graphene oxide for fuel ignition applications [12]. In this report, we will describe the experimental procedure as well as the results for achieving photo-ignition of a liquid fuel spray and a solid fuel by SWCNTs.

Experimental Setup and Instrumentation

Samples of the carbon nanotubes (CNTs) with different nanoparticle Fe content that was used in this study were from Unidym Inc., Houston, Texas. The samples were as grown ("raw") CNT and contained different impurities (mostly Fe and carbon...
particles) and the CNT content is expected to be predominantly SWCNT [13]. The term CNT is used in this report instead of SWCNT to indicate the raw SWCNT samples.

The experimental setup consists of a Canon camera flash, model Speedlight 580 EXII compact Xe-arc, as ignition light source, a pulse energy meter from GenTec, SUN series EM-1 with ED-500 detector head. The light source provided a 22-step intensity setting with 0.1 to 7-ms duration at the lowest to the highest light setting with a maximum of about 5 J/cm² per flash. The experimental setup is shown in Figure 1.

![Experimental Setup Diagram](image)

**Figure 1**—The experimental setup for the study of photo-ignition effect in SWCNT.

The data acquisition system Win600, a 16 channel digital scope/DAQ system from Hi-Techniques, was equipped with a photodiode detector as a trigger. The light from the camera flash provided a synchronization pulse through a digital delay/pulse generator. A high-speed pyrometer with a 6 μs response time, model KGA 740 HS, from Mikron Infrared Inc. of Oakland, NJ, covering 300-2300° C, was used to determine the temperature of a millimeter size spot of the sample.

Phantom V7.1, a high-speed camera from Vision System, which is capable of capturing up to 4800 picture/s at full-frame, was used to capture the images of the photo-ignition process for characterization purposes. The minimum ignition energy (MIE) was determined as the fluence was progressively increased until the onset of ignition.

**Sample Preparation**

Encapsulated CNT samples were prepared by placing the samples in a transparent container 0.75 cm³ in volume (D=7 mm L=20 mm). If there are enough CNTs in the container the gaseous byproducts of the photo-ignition of CNTs (mostly CO₂ or CO) would pressurize the capsule beyond 30 PSI and it would rupture and release its burning contents at the vicinity of the fuel spray and cause ignition of the spray.
Results and Discussion

Table I shows the MIE measurement by set up of figure 1 for samples grown under nearly identical conditions by the same vendor. Samples R0554 and R0215 were used in the experiments that are subsequently reported, unless stated otherwise.

Table I. Minimum Ignition energy for SWCNT samples with different Fe content in air

<table>
<thead>
<tr>
<th>Sample Code</th>
<th>Fe Content of Sample (Wt%)</th>
<th>Sample Appearance</th>
<th>Min Ignition Energy Fluence (mJ/cm²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R0554</td>
<td>50%</td>
<td>like soot, velvet black, fluffy</td>
<td>69±7</td>
</tr>
<tr>
<td>R0215</td>
<td>43</td>
<td>like soot, velvet black, fluffy</td>
<td>71±7</td>
</tr>
<tr>
<td>R0532</td>
<td>39</td>
<td>like soot, velvet black, fluffy</td>
<td>84 ±10</td>
</tr>
<tr>
<td>R0220</td>
<td>30</td>
<td>like soot, velvet black, fluffy</td>
<td>100 ±10</td>
</tr>
<tr>
<td>R0471</td>
<td>18</td>
<td>like soot, velvet black, fluffy</td>
<td>180±13</td>
</tr>
<tr>
<td>P0232</td>
<td>12</td>
<td>gray/black powder</td>
<td>&gt;750*</td>
</tr>
<tr>
<td>D0381</td>
<td>5</td>
<td>gray/black powder</td>
<td>&gt;750*</td>
</tr>
</tbody>
</table>

* no ignition was observed up to the maximum available fluence for the pulse duration setting.

Figure 2- Photo-ignition of Hexane+Acetone (50% each) in a sequence of images taken at 2000 frames per second (FPS), where t=0 indicates the peak of the flash.
Encapsulated CNT were used with the fuel ignition setup in testing the photo-ignition of the liquid fuel in order to keep the CNT samples dry. If there is enough CNT in the capsule (D=7 mm, L=20 mm), the ignition of CNTs would pressurize the capsule and it would burst and release its burning contents. Fig. 2 shows the liquid fuel ignition experiments, where the ignition capsule containing CNT was held close to the path of the fuel spray nozzle from an ultrasonic atomizer. Upon photo-ignition and rupture of the capsule the fuel and the burning particles impinge upon one another creating ignition of the fuel spray and oxygen mixture in multiple spots along the path of the spray.

![Figure 2- Ignition Capsule setup](image)

**Figure 2** - Schematic diagram showing the ignition capsule setup with the ultrasonic atomizer and the path of the fuel spray.

Fig. 3 shows the result of fuel ignition with the improved fuel and oxidizer mixing approach. In this case gaseous O₂ was introduced in a coaxial flow at a rate of 7 Lit/min with a swirl motion in order to produce an effective fuel and oxidizer mixing. The liquid fuel was injected at a rate of 3 cm³/min through a programmable syringe pump. This figure shows the following sequence of events:

- An ignition capsule (D=7 mm and L=20 mm) containing CNT and aluminum nanoparticles was attached to the flash of an instant camera and held close to the exit of the ultrasonic atomizer. Then the camera flash was activated and it lasted for approximately 1 ms.
- 2 ms after the peak of the flash the capsule ruptured along the seam and the burning “particles” were injected in the path of the fuel spray and O₂ mixture.
- At t=3 ms after the flash, burning particles were intersecting the spray mixture.
- At t=10 ms there was a volume of ignited fuel mixture.
- At t=15 ms the entire spray was in flame. In this case, the top of the flame at the exit of the injector has a diameter of about 1 cm.

The approach in Fig. 3 greatly improved the chance of a successful fuel ignition by CNTs (better than 90%) due to improved mixing of the fuel and the oxidizer. The choice of liquid fuel mixture was to get a better combustible due to acetone and produce a highly visible flame for imaging from Hexane. In this case, the speed of photo-ignition has improved as well. We believe with a proper fuel and oxidizer mixing, the fuel
ignition can be further improved toward 100% and this approach can lead to a distributed ignition similar to that of Fig. 2.

**Fuel Ignition for Simulated Solid Rocket Fuel**

Electrical ignition is widely used in solid rocket motors, where the electrical hot wire ignites an explosive bag which rapidly produces hot gases to achieve the required pressure and temperature for the ignition of the solid rocket fuel. Typically the solid fuel is a special blend of the fuel and the oxidizer that is cast into a rubber like hollow cylinder and it is designed to burn from inside out under high pressures and temperatures.

![Figure 4- Photo-ignition of CNT/MRF/SRF with a specific concentration exhibits a relatively large ignition plum which fills the glass container that is similar to void space inside a 2"x4" test rocket motor in size. These images were captured at 1000 FPS.](image)

We have successfully tested photo-ignition of SRF through photo-ignition of CNT. SRF was specially formulated to produce a rapid combustion similar to a typical solid rocket fuel, while being non-explosive due to safety considerations. Commercially available model rocket fuel used for hobby rocketry was also used for photo-ignition with similar results with and without encapsulation.

Fig. 4 shows an example of the photo-ignition of the SRF, which was encapsulated along with CNTs. The ignition capsule was attached to the camera flash at the top of a glass container. In this cases addition of a fraction of a gram of millimeter size SRF grains to the encapsulated mix increased the size of the ignition plume, as well as its burn temperature and duration.
Tailoring Ignition Parameters for Rocket Ignition Applications

In certain cases, the addition of a few milligrams of aluminum nanoparticles (Al-NPs) to the encapsulated CNT improved the probability of a successful ignition of the SRF. The Al-NPs had a nominal size of 18 nm and were passivated in order to prevent it from oxidizing. During the process of testing a mix of CNT, Al-NPs and grains of SRF, it was noted that different proportion of the three ingredients produced an igniter with different ignition properties such as ignition temperature, duration, pressure ramp up and ignition delay.

A typical encapsulated mixture included a few milligram of CNT, a small fraction of a gram of Al-NPs and a fraction of a gram of SRF in a 0.75 cm³ transparent ignition capsule. The function of CNT was to provide photo-ignition at a low light level (less than 0.1 J/cm²), while it produced substantial amount of gas to pressurize the capsule. The two part capsule that was used in this study ruptured at about 30 psi, as estimated through static measurements.

Al-NPs was easily ignited by CNTs and pyrometer data indicated that it produced a high ignition temperature (exceeding 1200° C), which burned well beyond 200 ms. Although, Al-NPs showed photo-ignition at a high photon flux (> 0.6 J/cm²) without CNTs, often the pressure built up within the capsule was not enough to rapidly rupture the capsule, rather it burned a hole through the wall of the capsule at a random location.

Al-NPs burn much longer than CNTs and at high enough temperature to ensure that they ignite the SRF particles/grains. Pyrometer data indicates that SRF particles burn at a very high temperature (approaching 2000° C), and they burn for substantially long time, well beyond 500-ms, depending on their size and their surface to volume ratio.

Figure 5- shows photo-ignition of CNT/Al-NPs/SRF with a relative concentration so that it exhibits a substantially long delay in the rupture of the ignition capsule. These images were captured at 2000 FPS and at an exposure time of 490 µs.