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14. ABSTRACT

New three-dimensional dislocation-density based crystalline plasticity formulations was used with grain-boundary (GB) kinematic interfacial schemes, void nucleation and growth formulations, specialized three-dimensional computational models, nonlinear fracture methodologies, and in-situ experiments to predict how combinations of ductile failure modes initiate and evolve, at different physical scales, to complete rupture in f.c.c. and b.c.c. systems with a focus on aluminum alloys. The proposed methodology provides an integrated framework to simultaneously

15. SUBJECT TERMS

High strain-rate; failure, crsytalline plasticity, dislocation-density

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a. REPORT	b. ABSTRACT	c. THIS PAGE			Mohammed Zikry
UU	UU	UU	UU		19b. TELEPHONE NUMBER 919-515-5237

Report Title

Final Report: Microstructurally Based Prediction of High Strain Failure Modes in Crystalline Solids

ABSTRACT

New three-dimensional dislocation-density based crystalline plasticity formulations was used with grain-boundary (GB) kinematic interfacial schemes, void nucleation and growth formulations, specialized three-dimensional computational models, nonlinear fracture methodologies, and in-situ experiments to predict how combinations of ductile failure modes initiate and evolve, at different physical scales, to complete rupture in f.c.c. and b.c.c. systems with a focus on aluminum alloys. The proposed methodology provides an integrated framework to simultaneously handle different interrelated physical mechanisms, such as a myriad of representative dislocation-density interactions with high and low angle GB interfaces, the growth and coalescence of a population of voids, and how these interactions can lead to either intergranular or transgranular failure.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
08/31/2014	3.00	Prasenjit Khanikar, Yi Liu, M.A. Zikry. Experimental and computational investigation of the dynamic behavior of Al–Cu–Li alloys, Materials Science and Engineering: A, (05 2014): 0. doi: 10.1016/j.msea.2014.02.089
08/31/2014	4.00	M. A. Zikry, Prasenjit Khanikar. Predictions of High Strain Rate Failure Modes in Layered Aluminum Composites, METALLURGICAL AND MATERIALS TRANSACTIONS A, (10 2013): 0. doi: 10.1007/s11661-013-2016-0
09/30/2014	5.00	W.M. Lee, M.A. Zikry. Microstructurally induced computational and material instabilities, International Journal of Plasticity, (01 2014): 0. doi: 10.1016/j.ijplas.2013.06.011
11/06/2015	8.00	Shoayb Ziaei, Qifeng Wu, Mohammed A. Zikry. Orientation relationships between coherent interfaces in hcp–fcc systems subjected to high strain-rate deformation and fracture modes, Journal of Materials Research, (8 2015): 0. doi: 10.1557/jmr.2015.207
11/06/2015	7.00	S. Ziaei, M. A. Zikry. Modeling the Effects of Dislocation–Density Interaction, Generation, and Recovery on the Behavior of H.C.P. Materials, METALLURGICAL AND MATERIALS TRANSACTIONS A, (11 2014): 0. doi: 10.1007/s11661-014-2635-0

TOTAL: **5**

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

1. Failure Modes in Crystalline Systems, TMS Annual Meeting, Nashville, TN, March, 2016
2. Dynamic Fracture of Crystalline Material Systems, TMS Annual Meeting, Orlando, FL, March, 2015
3. Dynamic Fracture Modes in Crystalline Materials, World Computational Mechanics Congress, Barcelona, Spain July, 2014
4. Behavior of High Temperature H.C.P. Materials, TMS Annual Meeting, San Diego, CA, February, 2014
5. High Strain-Rate Failure Modes in Crystalline Alloys, Army Research Office Workshop, Baltimore, MD, September, 2013
6. Intergranular and Transgranular Failure Modes in Crystalline Materials, Society of Engineering Science, Brown University, Providence, RI, July, 2013
7. Failure Modes in Layered Crystalline Materials, TMS 2013, San Antonio, 2013
8. Failure Modes in Layered Crystalline Materials, ASME IMECE 2012, Houston, 2012
9. Experimental and Microstructurally-Based Computational Investigation of the High Strain-Rate Behavior of High Strength Aluminum Alloys, The Metals Society, Orlando, FL, March, 2012

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received	Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received		Paper
06/25/2016	1.00	W.M. Lee, M.A. Zikry. Microstructurally Induced Computational and Material Instabilities, INTERNATION Journal of Plasticity (12 2013)
06/25/2016	2.00	M.A Zikry, P. Khanikar. PREDICTIONS OF HIGH STRAIN-RATE FAILURE MODES IN LAYERED ALUMINUM COMPOSITES, METALLURGICAL AND MATERIALS TRANSACTIONS A (08 2013)
06/25/2016	6.00	. HIGH STRAIN-RATE INTERFACIAL BEHAVIOR OF LAYERED METALLIC COMPOSITES, Mechanics of Materials ( )

TOTAL: **3**

Number of Manuscripts:

Books

Received	Book

TOTAL:

Received	Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

1. Fellow, American Association for the Advancement of Science (AAAS), one of only 14 engineers in 2015
2. RJ Reynolds Research Award (NCSU) for Distinguished Research and Education, 2015
3. UCSD Mechanical/Aerospace Engineering Alumni Impact, 2016

Graduate Students

NAME	PERCENT_SUPPORTED	Discipline
P. Khanikar	0.30	
S. Ziaei	0.30	
FTE Equivalent:	**0.60**	
Total Number:	**2**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
M.A. Zikry	0.10	
FTE Equivalent:	**0.10**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:...... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:...... 0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME
S. Ziaei, 0.3
P. Khanikar, 0.3

Total Number: **2**

Names of other research staff

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

Objective
The proposed research has as its major aim the development of an integrated computational and experimental framework for the investigation and control of failure mechanisms in b.c.c., h.c.p., and f.c.c. polycrystalline aggregate materials subjected to extreme changes in temperature, pressure, and strain-rates. A special focus is on high strength aluminum and titanium alloys due to their complex microstructures and their use in DoD applications.
Approach
• Development of large-scale three-dimensional computational formulations and new fracture formulations that accounts for the nucleation and propagation of intergranular and transgranular fracture
• Controlled in-situ scanning electron microscopy (SEM) and transmission electron microscopy (TEM), have been used to understand the thermo-mechanical response of polycrystalline aggregates.
• The new fracture methodology includes the effects of microstructural effects, such as grain texture, GBs, precipitates, and dispersed particles.
• The new fracture method is developed for high strain-rate applications. It is based on overlap method that overcomes limitations of current methods, such as XFEM and cohesive fracture.

Relevance to Army
• Future combat systems have to be deployable, high mobile, survivable, and adaptable to different environments and missions. The design of these heterogeneous systems, which could be comprised of different material systems with different interfaces, such as GBs, interphases, and bonded and joined surfaces, will have to be predicated on optimizing different material combinations for failure resistance due to extreme changes in momentum, energy, pressure, and strain-rate. If GB interfaces can be designed to dissipate momentum and energy, then failure initiation and growth can be blunted and potentially mitigated at different physical scales. This interfacial control could then result in the development of new failure resistant materials and systems.

• Material and system performance and durability under extreme loading conditions are of paramount importance to the Army and the DoD. Furthermore, the myriad of failure modes that can arise under different loading conditions and environments need to be accurately identified and innovative damage mitigation strategies and new failure resistant materials have to be developed. I have established contacts and collaborations with Army researchers at ARL-WMRD, ARL-CISD, TACOM, and the ARDEC at Picatinny Arsenal. I plan to continue to foster these relations to ensure that the proposed research has relevance to the basic research mission of the Army and the DoD. I will work closely with Army engineers and scientists to ensure that results from this research can be transitioned to the Army laboratories. I will continue to work with Drs. Cheeseman, Clayton, and Gazonas of WMRD to ensure Army relevance. Furthermore, I will continue collaborations with ALCAN, BAE, and Touchstone to continue industrial relevance and transitions for Army applications and systems.

Accomplishments for Reporting Period
• Major developments include computational validation of the high strain-rate and high-pressure applications. Other major accomplishments include:
• Validating criteria for initiation of fracture on cleavage planes
• New algorithms for crack propagation, growth, and rupture
• Comparison and validation with experimental observations/measurements
• New dislocation-density crystalline plasticity that accounts for dislocation-density interactions tailored to f.c.c. and b.c.c. systems
• Extending formulations to h.c.p. alloys that can be applied to titanium alloys
• Developing methodologies for aluminum alloys that account for layer thicknesses and interfacial effects, such as roll-bonded interfaces

Collaborations and Technology Transfer
• Collaboration and transitions of guidelines for aluminum design with Dr. Bryan Cheeseman, WMRD
• Collaborations with ALCAN (now Constellium), Touchstone, BAE in the development of new generations of aluminum alloys

Resulting Journal Publications During Reporting Period
S. Ziaei And M.A. Zikry (2015), Modeling The Effects Of Dislocation-Density Interaction, Generation, and Recovery on The Behavior of H.C.P. Materials, Metallurgical and Materials Transactions A, in press.

S. Ziaei, Q. Wu, and M.A. Zikry (2015), Orientation relationships between coherent interfaces in hcp–fcc systems subjected to high strain-rate deformation and fracture modes, Journal of Materials Research, Vol. 30, No. 15, pp. 2348-2359.
P. Khanikar and M.A. Zikry (2014), High Strain-Rate Interfacial Behavior of Metallic Layered Composites, Mechanics of Materials, 77, Page 52-66
P. Khanikar and M.A. Zikry (2014), Predictions of High Strain-Rate Failure Modes in Layered Aluminum Composites, Metallurgical Transactions A, 45, Page 60-71
P. Khanikar, Y. Liu, and M.A. Zikry (2014), Experimental and computational investigation of the dynamic behavior of Al–Cu–Li alloys, Materials Science and Engineering A, 604, 67-77

W.M. Lee, M.A. Zikry (2014), Microstructurally induced computational and material instabilities, International Journal of Plasticity.

Graduate Students Involved During Reporting Period
• S. Ziaei, Ph.D. student, graduated 2016
• P. Khanikar, Ph.D. student, graduated 2014

Awards, Honors and Appointments
• American Association for Advancement of Science Fellow, 2015
• RJ Reynolds Award for Research Excellence, North Carolina State University, 2015

Technology Transfer

Collaboration and transitions of guidelines for aluminum design with Dr. Bryan Cheeseman, WMRD
• Collaborations with ALCAN (now Constellium), Touchstone, BAE in the development of new generations of aluminum alloys