Available online at www.sciencedirect.com

ScienceDirect

Procedia Engineering 204 (2017) 360–366

Procedia Engineering

www.elsevier.com/locate/procedia

14th Hypervelocity Impact Symposium 2017, HVIS2017, 24-28 April 2017, Canterbury, Kent, UK

Correlation between hot spots and 3-D defect structure in single and polycrystalline high-explosive materials

Cameron Hawkins[a]*, Oliver Tschauner[b,c], Zachary Fussell[a,b,c], Jesse Smith[d]

[a]*National Security Technologies, P.O. Box 98521, Las Vegas, NV 89193, USA, *email: HAWKINMC@nv.doe.gov*
[b]*High Pressure Science and Engineering Center UNLV, 4505 Maryland Pkwy, Las Vegas, NV 89154, USA*
[c]*University of Nevada, Las Vegas (UNLV), 4505 Maryland Pkwy, Las Vegas, NV 89154, USA*
[d]*Advanced Photon Source, 9700 S. Cass Ave, Argonne, IL 60439, USA*

Abstract

A novel approach that spatially identifies inhomogeneities from microscale (defects, con-formational disorder) to mesoscale (voids, inclusions) is developed using synchrotron x-ray methods: tomography, Lang topography, and micro-diffraction mapping. These techniques provide a non-destructive method for characterization of mm-sized samples prior to shock experiments. These characterization maps can be used to correlate continuum level measurements in shock compression experiments to the mesoscale and microscale structure. Specifically examined is a sample of C4. We show extensive conformational disorder in gamma-RDX, which is the main component. Further, we observe that the minor HMX-component in C4 contains at least two different phases: alpha- and beta-HMX in spatially variable amounts. PETN sprayed film was found to be very homogeneously fine grained with modest preferred orientation of crystallites and modest rotational disorder of nitro-groups.

Peer-review under responsibility of the scientific committee of the 14th Hypervelocity Impact Symposium 2017.

Keywords: high-explosive materials; shock physics; x-ray diffraction; tomography; lang-topography

1. Introduction

The formation of hot spots in highly energetic (HE) materials during the initial stages of detonation is one of the key components in understanding the detonation process. HE materials are usually not refined single crystals, but compounds of crystallites of one to a few HE-compounds and binders. Impedance mismatch between binder and

*Corresponding author email address:hawkinmc@nv.doe.gov

1877-7058
Peer-review under responsibility of the scientific committee of the 14th Hypervelocity Impact Symposium 2017.
10.1016/j.proeng.2017.09.778

crystallites can be influential on the response of material to shock. In addition, accidental but unavoidable inhomogeneities such as cracks, voids, grain boundaries, inclusions of fluid or solid phases in the crystallites, and crystal lattice defects, can affect the initial response of the material to shock and can operate as locations for hot spot formation. Thus, correlating the given, initial inhomogeneities to hotspot formations is key to understanding the initial stages of detonation [1,2]. Such correlation, quantitatively established, helps to provide an understanding of the performance of HEs; therefore allowing them to become more reproducible, more reliable, and safer.

2. Introduction

During dynamic compression, localized stress and temperature in aggregate samples are affected by defects, voids, impurities and other heterogeneities that exist prior to shock. These crystal lattice defects produce weak points by inducing lattice strain. In a solid without internal structural degrees of freedom, such as an FCC metal, such local strain would induce small scale reverberations. In molecular solids, such as most HE materials, the local strain around the defects can be relaxed by changes in the conformational state of the molecules. In other words, the excess free energy from induced strain will be converted in part into an increase in inner energy. In HE materials, different conformational states of molecules have different sensitivities to shock [3]. Thus, defects induce local strain, which then induce changes in sensitivities. We examine the extent of such changes of conformation around defects in HE materials, as well as the nature of these conformational changes in terms of sensitivity.

Local changes in the molecule structure that have higher sensitivity to shock can therefore lend themselves to detonation. Chen and You et al. examine the surface of beta-HMX crystallites and show that the presence of a layer of delta-HMX, which is highly sensitive, as well as the thickness of this layer, controls the bulk sensitivity of HMX [4,5,6]. Current techniques of spatially resolved defect characterization (TEM darkfield, LEEDS) are destructive and cannot be applied to samples prior to shock experiments. Furthermore, these methods are restricted to very small length scale (nm) whereas characterization of samples prior to shock needs to extend to mm-scale or beyond. Characterization of voids and impurities in HE samples is presently restricted to sub-mm length scale and lacks correlation of impurity location with impurity phase identification. There is a need for nondestructive characterization techniques that cover the mesoscale (mm to μm) and microscale (μm to nm) to provide a way to understand the stress and temperate evolution upon shock loading.

3. Tomography and Topography

A combination of x-ray tomographic and topographic techniques along with a highly-spatially resolved structure analysis were utilized to map mesoscale and microscale structure and defects, such as voids and inclusions. These techniques use the high-energy micro-focused synchrotron beamline 16-IDB at HPCAT within the Advanced Photon Source (APS) at Argonne National Lab (ANL). Available energies beyond 30 keV provide full transmission of the x-rays through samples of cm-scale thickness and radial extension.

Synchrotron X-ray tomography, provides a 2D electron density distribution with μm-resolution, which can be applied to single crystal, polycrystalline and/or powdered samples. This method detects voids and cracks on the mesoscale, as well as density differences in polycrystalline aggregates of single or multiple phases. The 2D tomography map can be used to identify regions that could generate local temperature or stress excursion during shock. Compressed sensing, which provides sub-micrometer spatial resolution of density contrasts (voids, cracks, inclusions), was applied to the tomogram technique and improved the efficiency of collection by a factor of 10 to 50 without compromising the spatial resolution. This provided a more time-efficient method for tomographic imaging which allows much larger sized samples to be characterized.

The topography technique builds on recent Lang-topography innovations to provide a fully 3D quantitative assessment of defect structure, orientation, and induced strain in polycrystalline aggregates. Lang topography is a single crystal diffraction-based technique of mapping defect location and density in solids, which probes variation in Bragg-intensity as a function of local strain [7,8]. The Lang method shows the spatial distribution of crystal defects (point defects, dislocations, domain-walls) through the strain that these defects induce in a particular crystal lattice plane.