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as of 31-Jan-2022

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Title: Experimental and Computational Investigations of Deformation Behavior of Icosahedral Boron-Rich Ceramics
Begin Performance Period: 07-Dec-2017
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Report Term: 0-Other
Submitted By: Ghatu Subhash
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STEM Degrees: 5 **STEM Participants:** 2

Major Goals: Research efforts under the current project broadly focused on investigating the mechanics of deformation in ceramics, with special emphasis on icosahedral ceramics (B4C and B6O), using analytical, computational and experimental techniques. The five major objectives pursued were:
(a) development of new analytical models to investigate penetration behavior of rods into ceramic targets that overcomes limitations of the existing models,
(b) investigating the origins of amorphization in boron carbide through computational and experimental means,
(c) understanding the mechanical response of boron suboxide and other p-block hexaborides through experimental and computational methods,
(d) an in-depth computational investigation of shock response of boron carbide in various crystal orientations, and
(e) utilizing semi-empirical hardness models to analyze boron carbide polymorphs across the homogeneity range (~8.8 to 20 atomic percent carbon) and develop an improved model for hardness prediction.

Accomplishments: • A comparative study of four pressure-sensitive phenomenological constitutive models (Mohr–Coulomb (MC), Drucker-Prager (DP), extended-MC, and Johnson–Holmquist (JH-2)) found that only the extended-MC model (developed by the PI ‘s group from previous funding) captures the entire spectrum of material response well beyond HEL with a single equation: i.e., linear response at low pressures, experimentally observed nonlinear response at higher pressures up to HEL, and the pressure-independent response beyond HEL. This study was published in the International Journal of Impact Engineering [1].

• The newly developed analytical model for long rod impact on ceramic targets agrees well with experimental data and includes a formulation for dwell/interface defeat, a feature that is absent in most penetration models. The model can also be used to quantify the effects of amorphization in boron carbide and predict the ballistic performance of an amorphization-resistant boron carbide. Finally, the model is universally applicable to a wide range of structural ceramics and can be used in the absence of experimental data to characterize comminuted ceramics. Results from this study were published in the International Journal of Impact Engineering [2].

• A 3-dimensional Raman mapping of indentations in boron carbide revealed a positive correlation between high levels of residual stress and the number of detected amorphized regions. Finite element simulations conducted to estimate the indentation-induced residual stress fields in the absence of amorphization and cracking underpredicted the average residual pressure observed through Raman spectroscopy. Thus, amorphization was inferred to increase pressure in the material. This pressure was interpreted as evidence for volumetric expansion of the amorphized material which is less ordered and hence exerts compressive forces on the surrounding crystalline matrix. This study was published in Journal of the American Ceramic Society [3].

• Quantum mechanical (QM) and molecular dynamics (MD) simulations were pursued to understand the amorphization phenomenon in boron carbide. These investigations revealed a new rationale for explaining the origin of new features in the Raman spectrum of boron carbide under high-pressure conditions. Centered on a thermodynamic approach, the proposed theory argues that amorphization occurs under conditions of high pressure near zones of high stress concentration due to temperatures exceeding the melting point. The MD simulations, which confirm melting of boron carbide at compressive pressures of ~70 GPa, also show that recrystallization back to the original structure does not occur when the applied pressure is released. Results from this study were published in Journal of Applied Physics [4].

• Realizing the vast volume of knowledge base developed over more than two decades by the PI's team, The PI has summarized the vast literature available on icosahedral ceramics and has critiqued various theories on amorphization. This summary was published in 68-page review article in Progress in Materials Science [5] .

• The analysis of boron suboxide (B6O), another icosahedral ceramic, produced through hot pressing (HP) and spark plasma sintering (SPS) techniques revealed the following: First, a quasistatic compressive strength of 5 GPa was obtained for HP B6O sample, which is the highest ever reported for this material. Second, simulated XRD results for twinned B6O showed the occurrence of a strong peak at $2\theta=37^{\circ}$, which can be utilized to track the volume fraction of nanotwinning in fabricated B6O samples. Finally, based on the analysis of critical shear stress for nanotwinned B6O under biaxial shear simulations, an optimum twin spacing of 0.89 nm was determined. These results, published in Acta Materialia [6], suggest high potential for B6O as a structural ceramic.

• To further probe into the origins of high strength in icosahedral ceramics, an analysis into the ground state bonding in p-block hexaborides was investigated. The analysis revealed icosahedral separation and localization of equatorial bonding as the main predictors of elastic moduli. This work demonstrated that susceptibility to nanotwinning relies on key bonding traits. These findings may aid in the development of new models for nanotwinning in structural ceramics. The results from this study have been published in Physical Review Materials [7].

• In the MD-based investigation of shock response of boron carbide, the P-V shock Hugoniot of the ceramic was derived from Rayleigh lines constructed at various impact velocities. Further, it was revealed that boron carbide undergoes local heating beyond the melting point at high shock intensities. Therefore, temperature, in addition to high pressure, was inferred to be a significant driver of amorphization in boron carbide. This study was published in Physical Review B [8].

• A detailed analysis of shock wave profiles which spanned across the elastic and shock deformation regimes in boron carbide was conducted. The Hugoniot elastic limit along [111] was determined to be 60 GPa, which reduced to 24 GPa at 47° to [111]. The equation of state of boron carbide (i.e., shock-velocity versus particle-velocity relationship) thus determined from the atomistic scale cohered well with experimental data. The axial stress-volumetric strain hysteresis curves along the two orientations through the loading stage, Hugoniot state, and release were also determined. Finally, the MD-derived shock Hugoniot and hydrostat curves aligned well with experimental data up to 140 GPa. Thus, the hydrostat of boron carbide derived in this work provides an accurate basis for assessing residual strength of boron carbide under shock conditions. The manuscript documenting this study is currently under review in Physical Review B [9].

• Boron carbide exhibits numerous polymorphs and variability in stoichiometry. The contributions of these compositions towards the hardness of boron carbide is unknown. The analysis of boron carbide polymorphs using semi-empirical models found intrinsic hardness to be primarily a function of stoichiometry, with polymorphism having a lower influence. Hardness estimates also exhibited substantial sensitivity to the model used (differing by as much as 9 GPa) indicating that the search for new super-hard materials should be guided by more than just one model. Further, bond resistance model was observed to offer the best conformance to experimental data. This study was published in Journal of the American Ceramic Society [10].

• The second phase of the above study resulted in a new intrinsic hardness model that provided better predictability than previous bond-strength (BS) and electronegativity (EN) models. In addition, the exponents quantifying the dependence of intrinsic hardness on bond length, bond density, electronegativity, and coordination numbers were found to be quite flexible in fitting to a given experimental dataset in multiple ways at a constant quality of fit. This characteristic of the exponents explains from a numerical perspective, the diversity of parameter–

exponent combinations observed in the existing hardness models. The results from this study were published in Journal of Material Science [11].

• After several years of effort, a monograph was finally published in April 2021, titled, “Dynamic Response of Advanced Ceramics”, Wiley Publishers; 358 pages [12].

• A book chapter was also published summarizing failure mechanisms in brittle materials under quasi-static and dynamic loads, Springer publishers [13]

The above references are listed under PRODUCTS.

Training Opportunities: Many graduate and undergraduate students were trained during this period. Their training and professional development included:
1. Relevant course work to conduct rigorous scientific research which also counted towards completion of their degree requirements,
2. Use of relevant experimental, characterization and analytical tools and computational methods on supercomputers.
3. Report writing and manuscript preparation summarizing their research results
4. Technical presentations of their research to the sponsors and at major conferences.
5. Mentoring new students and training them on equipment
6. Developing safety protocols and safe operation of equipment

Results Dissemination: The results were disseminated through 11 journal publications, 1 book, 1 book chapter and 33 conference/non-conference proceedings, and 3 PhD theses. The details are given under “Products”.

Honors and Awards: Students:
• Cody Kunka [13], Matthew W DeVries [14], and Salil Bavdekar [15] successfully defended their PhD thesis.
• Amith Adoor Cheenady successfully defended PhD research proposal.
• Matthew W DeVries received “MAE Graduate Student Research Award”.
• Matthew W DeVries began career at Corvid Technologies in September 2019.

Dr. Ghatu Subhash received the following recognitions:
-University of Florida Doctoral Dissertation Advisor/Mentoring Award-2020-2021 (Feb 2021)
-Herbert Wertheim College of Engineering Doctoral Dissertation Advisor/Mentoring Award, University of Florida (Nov 2020).
-B.J. Lazan Award, Society for Experimental Mechanics (SEM) “for innovative contributions to experimental mechanics and development of in-depth understanding of multiaxial dynamic response of ceramics and soft materials” (2021)
-Fellow of ACerS - The American Ceramic Society (2020)
-University of Florida Research Foundation Professor, University of Florida (2020-2023)
-Frocht Award, Society for Experimental Mechanics (SEM) - in recognition of outstanding achievements as an educator. The award recognizes the Experimental Mechanics Educator of the Year and is in recognition of the technical stature and the high personal regard in which the awardee is held by the experimental mechanics community (2018)
-National Academies of Engineering, Science and Medicine Panel member for ‘Ballistic Science and Engineering’ at the Army Research Laboratories, National Research Council - 2015-2019; served on three panels in 2015, 2017 and 2018.
-Appeared in a PBS documentary “Secrets of Spanish Florida” - aired nationwide on Dec 26, 2017 (9-11pm) while discussing the impact response of Coquina, the material with which the oldest fort in USA, Castillo de San Marcos, in St. Augustine was built.

Protocol Activity Status:

Technology Transfer: During this period, the PI collaborated with three ARL researchers on three publications. These interactions elevated our understanding and also exposed ARL researchers our approaches and experiences:
• Drs. Dr. Sikhanda Satapathy [2], Dr. Philip Jannotti [3] and Dr. Christopher Haines [9]. Two Journal publications involved collaboration with Assistant Professor Qi An from University of Nevada, Reno.
• The PI and his students have presented the research results at the Armor Ceramics Symposia, organized by Drs Jerry LaSalvia and Jeff Swab of ARL, International Conference and Exposition on Advanced Ceramics and Composites conference (ICACC 2018, 2019 and 2020), Daytona Beach, FL. Several ARL researchers attend this conference.
• A free copy of the published book by the PI "Dynamic Response of Advanced Ceramics" was shipped to Drs. Christopher Haines, Jerry LaSalvia and Phillip Jannotti of ARL.

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Participant Type: PD/PI
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Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
National Academy Member: N

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Person Months Worked: 2.00 **Funding Support:**
Project Contribution:
National Academy Member: N

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Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
National Academy Member: N

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Person Months Worked: 2.00 **Funding Support:**
Project Contribution:
National Academy Member: N

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Project Contribution:
National Academy Member: N

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Project Contribution:

National Academy Member: N

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Person Months Worked: 6.00 **Funding Support:**
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Participant Type: Other Professional
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Person Months Worked: 1.00 **Funding Support:**
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Publication Location:
Article Title: Nanotwinning and Amorphization of Boron Suboxide
Authors: Cody Kunka, Qi An, Nicholas Rudawski, Ghatu Subhash, James Zheng, Virginia Halls, Jogender Singh
Keywords: Nanotwinning Boron suboxide Boron carbide Amorphization Density functional theory
Abstract: Recently, researchers discovered that in contrast to isolated twins, periodic twins with nanoscale spacing can dramatically improve mechanical properties. Incorporation of “nanotwinning” into icosahedral solids improves their strength and stability. In this manuscript, we assert that boron suboxide, while far less studied than boron carbide (i.e., the most popular icosahedral solid), possesses higher propensity for nanotwinning and higher theoretical promise. For boron suboxide, the influence of processing on twin spacing is explored through mechanical testing and transmission electron microscopy. Quantum-mechanical simulations are then performed to suggest a critical twin spacing that would maximize performance and to show how to track experimental nanotwinning with x-ray diffraction. Finally, transmission electron microscopy and Raman spectroscopy show that amorphization, the localized loss of crystallinity, drives mechanical failure in ways unique to boron suboxide.
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Date Submitted: 8/6/19 12:00AM Date Published: 6/1/18 4:00AM
Publication Location:
Article Title: Icosahedral superstrength at the nanoscale
Authors: Cody Kunka, Xiaokun Yang, Qi An, Ghatu Subhash
Keywords: boron suboxide, icosahedral solids, p-block hexaborides, nanotwinning, bonding strength
Abstract: Materials that exhibit extreme hardness, low mass density, and high thermal/chemical stability can often be modeled as simple modifications to the ?-rhombohedral phase of boron. To facilitate the development and discovery of these multipurpose, structural ceramics, the current work reveals fundamental physics on the bonding and deformation of p-block hexaborides, an important and representative subclass of icosahedral solids. Icosahedral separation and localization of equatorial bonding are identified as predictors of both elastic moduli and strength. This work explores the role of nanotwinning in mechanical performance of ceramics. This work demonstrates (1) that susceptibility to nanotwinning relies on key bonding traits and (2) that nanotwinning minimally affects elasticity and high-periodicity inelasticity. Overall, this work rationalizes both the mechanical performance of a of these materials and the cutting-edge mechanism of nanotwinning through fundamental, physics-based a
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Publication Location: United States
Article Title: Deformation behavior and amorphization in icosahedral boron-rich ceramics
Authors: Amnaya Awasthi, Ghatu Subhash
Keywords: icosahedral ceramics, Boron carbide, boron suboxide, boron, amorphization, raman spectra, DFT
Abstract: The article reviews contemporary knowledge of atomic structures, mechanical properties and deformation mechanisms of a range of boron-rich ceramics, including different allotropes of boron, polymorphs of boron carbide, and futuristic materials such as boron suboxide, “BAM” materials and their derivatives. Many icosahedral boron-rich ceramics are prone to “amorphization”, which causes loss of strength and catastrophic failure. This article presents a critique of established approaches that explain the amorphization phenomena. Main highlights include the demystification of Raman spectrum of amorphized boron carbide using a multi-scale atomistic computational approach and investigation into connection between shock conditions and rise in temperature. We probe avenues for enhancing performance of these ceramics well beyond contemporary thresholds, by proposing research pathways using rigorous computational material informatics.
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Publication Location:
Article Title: High-pressure deformation and amorphization in boron carbide
Authors: Amnaya P. Awasthi, Ghatu Subhash
Keywords: boron carbide, amorphization, Raman spectra, Molecular dynamics, DFT
Abstract: Icosahedral boron-rich solids fall second in hardness to diamondlike structures and possess low density, high thermal, and mechanical stability at high temperatures, and superior industrial manufacturability. A common deleterious feature called “presssure-induced amorphization,” limits their performance in high-velocity projectile applications. This article discusses spectral characteristics of amorphized states of boron carbide, with the goal of understanding the mechanistic layout of pressure-induced amorphization. Shock studies of boron carbide have proposed phase transformation at high pressures, but no conclusive evidence has been corroborative to prove the existence of new high-pressure phases. We propose a new rationale toward deciphering the amorphization phenomenon in boron carbide centered on a thermodynamic approach to explain atomic interactions in amorphous islands. Quantum mechanical simulations are utilized to understand the impact of stresses on Raman spectrum.
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Article Title: A unified model for dwell and penetration during long rod impact on thick ceramic targets
Authors: Salil Bavdekar, Ghatu Subhash, Sikhanda Satapathy
Keywords: Dwell, Penetration Model, ceramic targets, Dynamic expanding cavity model
Abstract: An improved model for long rod penetration into thick ceramic targets is presented by combining modi? ed version of the Walker–Anderson model with dynamic expanding cavity model. This model is captures the dwell-penetration transition phenomena in ceramics effectively. The target response is assumed to occur in a hemispherical region containing nested comminuted, cracked and elastic regions of deformation. A dynamic expanding cavity model, recently developed by the authors, along with an exponential pressure-shear response of brittle materials in the form of the extended Mohr-Coulomb model, is used to capture the stress ?elds in these regions. Incorporating this constitutive model reduces the requirement on experimental data as it uses a single set of parameters to predict the response of many brittle ceramics. The predictions of the model are in good agreement with experimental result and is also used to quantify the e?ect of amorphization on boron carbide.
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Publication Location: United States
Article Title: Shocked ceramics melt: An atomistic analysis of thermodynamic behavior of boron carbide
Authors: Matthew DeVries, Ghatu Subhash, Amnaya Awasthi,
Keywords: Boron Carbide, Amorphization, MD simulations, Melting
Abstract: Macroscale experiments for structural response of materials often do not capture deformation features at the atomistic scale. This limitation is more pronounced in materials subjected to shock loading, especially in covalently bonded ceramics such as boron carbide, which exhibit pressure-induced amorphization. Perhaps because ceramics have high thermal resistance, temperature was never considered a prime factor influencing deformation mechanisms, leaving such phenomena unexplained. In this article, we probe fundamental material behavior using molecular dynamics (MD) to link nanoscale thermodynamics to amorphization during shock loading. For the first time, we have generated Rayleigh lines via MD shock simulations, subsequently constructing the shock-Hugoniot, which aligns well with experimental data. We estimate shock-induced temperature in ceramics to be well above their melting point, resolving a plethora of interconnected scientific issues pertaining to amorphization.
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Article Title: Intrinsic hardness of covalent crystals: a unified multiparametric framework
Authors: Amith Adoor Cheenady, Amnaya Awasthi, Ghatu Subhash
Keywords: Intrincsic Hardness, electronegativity, bond strength,
Abstract: Bond resistance, bond strength and electronegativity models have been widely utilized for predicting intrinsic hardness of novel covalent materials. Although these models are generally perceived to be distinct, this manuscript recognizes them to be drawing input parameters from the same basis set comprising of bond density, bond length, electronegativity, and coordination number, while primarily differing in the exponents assigned to them. A numerical bound on the feasible space of these exponents is derived, followed by a search operation of this space to determine optimal values. The resulting model yields hardness estimates in good conformance with experimental data for numerous binary and ternary ceramic compounds. The study also provides a plausible explanation for the diversity of parameter–exponent combinations in the existing intrinsic hardness models, that is derived from the variability exhibited by these exponents in capturing a given experimental dataset at a constant fitti
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Publication Location: United States
Article Title: Comparison of pressure-sensitive strength models for ceramics under ultrahigh confinement
Authors: Salil Bavdekar, Ghatu Subhash
Keywords: Confinement, Failure, HEL, Modelling/model Strength
Abstract: Four pressure-sensitive phenomenological constitutive models for brittle ceramics are compared to available experimental data over a wide range confinement pressures. The linear Mohr–Coulomb and Drucker Prager models are only applicable at low pressures. While the nonlinear strain-rate dependent Johnson–Holmquist (JH-2) model provides a reasonable fit to experimental data up to HEL for mostmaterials, it completely fails to capture the experimentally observed pressure and strain-rate independent strength saturation of ceramics at pressures beyond HEL. It is demonstrated that the extended Mohr–Coulomb model is the only model that can not only capture the linear response at low pressures, but also the experimentally observed nonlinear response at higher pressures up to HEL and the pressure-independent response beyond HEL with a single curve. Further, the constants used in this model are shown to be universal and applicable to most brittle materials.
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Article Title: Amorphization-induced volume change and residual stresses in boron carbide
Authors: Gregory Parsard, Ghatu Subhash, Phillip Jannotti
Keywords: 3D amorphization volume, indentation, residual stress, Raman spectroscpy
Abstract: The residual pressure surrounding quasistatic and dynamic Vickers indentations in boron carbide was quantitatively mapped using Raman spectroscopy. These maps were compared against similar maps of amorphization intensity and optical micrographs of deformed regions to determine the roles of amorphization and damage upon indentation-induced residual stress. A positive correlation was found between high levels of residual stress and the number of amorphized sites detected. Finite element simulations were conducted to model the indentation-induced residual stress fields in the absence of amorphization and cracking. The simulations underpredicted the average residual pressure observed through Raman spectroscopy, implying that amorphization contributes to increased pressure in the material. This pressure is interpreted as potential evidence of volumetric expansion of the amorphized material which is less ordered and hence exerts compressive forces on the surrounding crystalline matrix.
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Authors: Amith Adoor Cheenady, Amnaya Awasthi, Matthew DeVries, Christopher Haines, Ghatu Subhash
Keywords: Shock response, single crystal, elastic modulus
Abstract: The response of monocrystalline boron carbide to planar shock loading has been investigated using molecular dynamics simulations, along crystal orientations with the highest and lowest elastic moduli. While shocks of intensity lower than the HEL generate quasilongitudinal and quasitransverse waves, an elastic precursor trailed by inelastic waves is observed when HEL is exceeded. Bond breakage, accompanied by temperature rise, is observed to be the primary mode of deformation under the inelastic waves. Higher shock intensities generate a deformation shock front with considerable loss of crystalline order. At higher shock velocities, boron carbide is characterized by a convergence in the shock Hugoniot curves obtained along the two loading directions. Finally, it is shown that the simulation derived hydrostat curve presented in this work is coherent with experimental data up to 140 GPa and provides an accurate basis for assessing residual strength of boron carbide under shock conditions.
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Publication Location: United Stets
Article Title: Characterization of BAM-B4C composites prepared by spark plasma sintering
Authors: Rafael A. Riera, Salil Bavdekar, Matthew DeVries, Jogendar Singh, Ghatu Subhash
Keywords: BAM, boron carbide, SPS, hardness
Abstract: Aluminum magnesium boride (BAM) and boron carbide (B4C) have high strength, high hardness, and good impact resistance along with low mass density. Four BAM-B4C composite specimens (100% BAM, BAM + 10 wt% B4C, BAM + 20 wt% B4C, and BAM + 50 wt% B4C) were characterized using microscopy and spectroscopy. It was found that addition of B4C increased the mechanical properties of the composite. The BAM + 10 wt% B4C composite possessed the highest compressive strength while the BAM + 20 wt% B4C composite possessed the highest fracture toughness. Further addition of B4C lead to extensive phase segregation and cracking and degradation of its mechanical properties. The BAM + 10 wt% B4C composite possessed the highest compressive strength while the BAM + 20 wt% B4C composite possessed the highest fracture toughness. Any further addition of B4C lead to phase segregation and cracking within the composite microstructure, highly degrading its mechanical properties.
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Date Received: Conference Date: 08-Jun-2020 Date Published: 01-Feb-2021
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Paper Title: and Dynamic Mechanical Characterization of a Spark Plasma Sintered B6O-B4C Composite.
Authors: Kimia Ghaffari, Salil Bavdekar, Ghatu Subhash
Acknowledged Federal Support: **Y**

DISSERTATIONS:

Publication Type: Thesis or Dissertation
Institution: University of Florida
Date Received: Completion Date: 8/20/18 9:09PM
Title: Quantum and Experimental Mechanics of Icosahedral Ceramics
Authors: Cody Kunca
Acknowledged Federal Support: **Y**

Publication Type: Thesis or Dissertation
Institution: University of Florida
Date Received: Completion Date: 2/21/19 10:10PM
Title: A unified analytical model for the dynamic response of structural ceramics to impact and penetration
Authors: Salil Bavdekar
Acknowledged Federal Support: **N**

Publication Type: Thesis or Dissertation
Institution: University of Florida
Date Received: Completion Date: 5/14/19 9:11PM
Title: Amorphization of Boron Carbide: Influence of Gran Size, Secndary Phases and High Pressure
Authors: Mathew DeVries
Acknowledged Federal Support: **Y**

Partners

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I certify that the information in the report is complete and accurate:
Signature: Ghatu Subhash
Signature Date: 9/7/21 4:36AM

Project Summary - Grant # ARO-W911NF-18-1-0040.
(Reporting Period: September 2017 – August 2021)

Experimental and Computational Investigations of Deformation Behavior of Icosahedral Boron-Rich Ceramics

Ghatu Subhash
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Objective

Research efforts under the current project broadly focused on investigating the mechanics of deformation in ceramics using analytical, computational and experimental techniques. The five major objectives pursued were (a) development of a new analytical model to study penetration of rods into ceramic targets that overcomes limitations of existing models, (b) investigating the origins of amorphization in boron carbide through computational and experimental means, (c) understanding the mechanical response of boron suboxide and other p-block hexaborides through experimental and computational methods, (d) an in-depth computational investigation of shock response of boron carbide, and (e) utilizing semi-empirical hardness models to analyze boron carbide polymorphs across the homogeneity range (~8.8 to 20 atomic percent carbon) and develop an improved model for hardness prediction.

Approach

- The performance of four pressure-sensitive phenomenological constitutive models (Mohr–Coulomb (MC), Drucker-Prager (DP), extended-MC, and Johnson–Holmquist (JH-2)) were compared to available experimental data for various ceramic materials at a wide range of confinement pressures. In the subsequent study, an analytical model was developed to investigate the penetration of long rods into semi-infinite ceramic targets. The model is based on the principle of momentum balance along the centerline of penetration. An improved dynamic expanding cavity model (d-ECM) and the extended-MC model were utilized to capture the shear stress behavior in the comminuted ceramic targets.

- The influence of amorphization on indentation-induced residual stress in boron carbide was studied by 3-dimensional mapping of residual pressure around quasistatic and dynamic Vickers indentations using Raman spectroscopy. The maps thus generated were compared against those of amorphization intensity and optical micrographs of deformed regions.

- Quantum mechanical (QM) simulations were utilized to understand the impact of applied stresses on Raman spectra of boron carbide, while molecular dynamics (MD) simulations of volumetric compression were used to understand thermodynamic aspects of amorphization. Through this approach, a new theory of amorphization in boron carbide was proposed which overcame the significant gaps present in the existing theories.

- The mechanical response of Hot Pressed (HP) and Spark Plasma Sintered (SPS) boron suboxide (B_6O) was characterized through quasistatic/dynamic indentation and quasistatic compression. The trends in properties were explained through Scanning Electron Microscopy (SEM), High Resolution Transmission Electron Microscopy (HR-TEM), X-Ray Diffraction (XRD), Raman spectroscopy and measurements of porosity, grain size, nanotwinning and amorphization. Biaxial shear deformation of nanotwinned B_6O crystals were analyzed through QM simulations to determine an optimum twin spacing that would sustain the highest shear stress.

Next, non-twinned and nanotwinned p-block hexaborides ($(B_{12})ii$, i=O, S, P, As) were studied through QM simulations and theoretical estimates of their lattice parameters, covalent radii, bulk and shear moduli, microhardness, shear strengths and toughness were obtained. The correlations of these physical quantities with each other and with the lengths of the various bonds present in these crystals were investigated. Shear deformation of non-twinned and nanotwinned varieties of these crystals were also studied.

- The shock response of boron carbide was comprehensively studied using MD in two phases. In the first phase, planar, normal impact experiments were simulated in LAMMPS to understand the phenomenon of shock induced amorphization. The simulation setup involved a cuboidal super-cell of single-crystal boron carbide ($B_{11}C_pCBC$) with dimensions 50x56x269 Å impacting a rigid wall at velocities ranging from 0.5 to 4.5 km/s. The temporal and spatial variation of temperature, density, pressure, and particle velocity in the domain was determined.

  The second phase of the study involved understanding the nature of the various waves generated in boron carbide under shock conditions, the influence of crystal orientation on shock response, and investigating the complete shock load-unload hysteresis cycle. To meet these objectives, the prior study was extended to larger domains and longer time scales, and a finite-length shock pulse was generated and propagated in the domain, which loaded the pristine material to the Hugoniot state and unloaded it, thus simulating the complete hysteresis cycle. Two crystal orientations — corresponding to the highest ([111], along the three-atom chain in boron carbide) and lowest (47° to [111]) elastic moduli — were investigated to understand the anisotropic response of the ceramic under shock conditions.

- QM simulations and estimates from three semi-empirical hardness models (bond resistance model (BR), bond strength model (BS), and electronegativity (EN) model) were utilized to investigate the influence of polymorphism and stoichiometry on the intrinsic hardness of boron carbide, reveal the sensitivity of the estimates to the model used, and test their conformance to experimental data. A neighborhood search subroutine was developed in MATLAB to identify the bonds that exist between the atoms in a unit cell of the crystal and calculate intrinsic hardness as per these models. These hardness estimates were then compared to experimental data.

  The BR, BS and EN models comprise of exponents that quantify the dependency of intrinsic hardness of a covalent crystal on four quantities at the scale of the unit cell — electronegativities and coordination numbers of atoms comprising the crystal, bond lengths, and bond density in the unit cell. A new intrinsic hardness model was proposed based on a numerical analysis of these exponents that constitute the models.

Relevance to Army

Accomplishments for Reporting Period

- The comparative study of the four pressure-sensitive phenomenological constitutive models found that only the extended-MC model captures the linear response at low pressures, experimentally observed nonlinear response at higher pressures up to HEL, and the pressure-independent response beyond HEL with a single curve (see Fig. 1). This study was published in the *International Journal of Impact Engineering* [1].

- The newly developed analytical model for rod-ceramic target impact agrees well with experimental data (see Fig. 2) and includes a formulation for dwell/interface defeat, a feature that is absent in most penetration models. The model can also be used to quantify the effects of amorphization in boron carbide and predict the ballistic performance of an amorphization-resistant boron carbide (see Fig. 2). Finally, the model is universally applicable to a wide range of structural ceramics and can be used in the absence of experimental data to characterize comminuted ceramics. Results from this study were published in the *International Journal of Impact Engineering* [2].

- The 3-dimensional Raman mapping of indentations in boron carbide revealed a positive correlation between high levels of residual stress and the number of detected amorphized sites (see Fig. 3). Finite element simulations conducted to estimate the indentation-induced residual stress fields in the absence of amorphization and cracking underpredicted the average residual pressure observed through Raman spectroscopy. Thus, amorphization was inferred to increase pressure in the material. This pressure was interpreted as evidence for volumetric expansion of the amorphized material which is less ordered and hence exerts compressive forces on the surrounding crystalline matrix. This study was published in *Journal of the American Ceramic Society* [3].

- The QM and MD based analysis of the amorphization phenomenon in boron carbide revealed a new rationale for explaining the origin of new spectral features in the Raman spectrum of the ceramic under high-pressure conditions. Centered on a thermodynamic approach, the proposed theory argues that amorphization occurs under conditions of high pressure near zones of high stress concentration due to temperatures exceeding the melting point. The MD simulations, which confirm melting of boron carbide at compressive pressures of ~70 GPa, also show that recrystallization back to the original structure does not occur when the applied pressure is released (see Fig. 4). Results from this study were published in *Journal of Applied Physics* [4] and *Progress in Materials Science* [5].

- The analysis of B_6O produced through HP and SPS techniques revealed the following. Firstly, a quasistatic compressive strength of 5 GPa was obtained for HP B_6O sample, which is the highest ever reported for this material. Secondly, simulated XRD results for twinned B_6O showed the occurrence of a strong peak at $2\theta=37^{\circ}$, which can be utilized to track the volume fraction of nanotwinning in fabricated B_6O samples (see Fig. 5(a)). Finally, based on the analysis of critical shear stress for nanotwinned B_6O under biaxial shear simulations, an optimum twin spacing of 0.89 nm was determined (see Fig. 5(b)). These results, published in *Acta Materialia* [6], suggest high potential for B_6O as a structural ceramic.

- The analysis of the ground state bonding in p-block hexaborides revealed icosahedral separation and localization of equatorial bonding as the main predictors of elastic moduli. This work demonstrated that susceptibility to nanotwinning relies on key bonding traits and that nanotwinning minimally affects high periodicity inelasticity. These findings aid in the development of the first model for nanotwinning in structural ceramics. The results from this study have been published in *Physical Review Materials* [7].

- In the MD-based investigation of shock response of boron carbide, the P-V shock Hugoniot of the ceramic was derived from Rayleigh lines constructed at various impact velocities (see Fig. 6(a)). Further, it was revealed that boron carbide undergoes local heating beyond the melting point at high shock intensities (see Fig. 6(b), which plots the peak temperature attained under shock loading against the shock stress). Therefore, temperature, in addition to high pressure, was inferred to be a significant driver of amorphization in boron carbide. This study was published in *Physical Review B* [8].

- Next, a detailed analysis of shock wave profiles which spanned across the elastic and shock deformation regimes in boron carbide was conducted. The Hugoniot elastic limit along [111] was determined to be 60 GPa, which reduced to 24 GPa at 47° to [111]. The equation of state of boron carbide (i.e., shock-velocity versus particle-velocity relationship) thus determined from the atomistic scale is presented in Fig. 7 along with experimental data. Note that in Fig. 7, results along [111] are denoted 'Prl' (for parallel orientation) while those at 47° to [111] are denoted 'Obl' (for oblique orientation). The axial stress-volumetric strain hysteresis curves along the two orientations through the loading stage, Hugoniot state and release were also determined (see Fig. 8). Finally, the MD-derived shock Hugoniot and hydrostat curves (see Fig. 9) aligned well with experimental data up to 140 GPa. Thus, the hydrostat of boron carbide derived in this work (see Fig. 9) provides an accurate basis for assessing residual strength of boron carbide under shock conditions. The manuscript documenting this study is currently under review in *Physical Review B* [9].

- The analysis of boron carbide polymorphs using semi-empirical models found intrinsic hardness to be primarily a function of stoichiometry, with polymorphism having a lower influence. Hardness estimates also exhibited substantial sensitivity to the model used (differing by as much as 9 GPa) indicating that the search for new super-hard materials should be guided by more than just one model. Further, bond resistance model was observed to offer the best conformance to experimental data (see Fig. 10). This study was published in *Journal of the American Ceramic Society* [10].

- The second phase of this study resulted in a new intrinsic hardness model that provided better predictability than BS and EN models (see Fig. 11). In addition, the exponents quantifying the dependence of intrinsic hardness on bond length, bond density, electronegativities and coordination numbers were found to be quite flexible in fitting to a given experimental dataset in multiple ways at a constant quality of fit. This characteristic of the exponents explain from a numerical perspective, the diversity of parameter–exponent combinations observed in the existing hardness models. The results from this study were published in *Journal of Material Science* [11].

Collaborations and Technology Transfer

- Journal publications [6] and [7] involved collaboration with Assistant Professor Qi An from University of Nevada, Reno.
- Journal publication [2] involves collaboration with Dr. Sikhanda Satapathy from Army Research Laboratory.
- The book *Dynamic Response of Advanced Ceramics* [12] was co-authored with Prof. Dipankar Ghosh, Old Dominion University (ODU), Norfolk, VA.

Research plans for next reporting period

Graduate Students Involved During Reporting Period

- Cody Kunka (Ph.D, graduated)
- Matthew W DeVries (Ph.D, graduated)
- Salil Bavdekar (Ph.D, graduated)
- Amith Adoor Cheenady (Ph.D, current)

Awards, Honors and Appointments

- Cody Kunka [13], Matthew W DeVries [14], and Salil Bavdekar [15] successfully defended their PhD thesis.
- Amith Adoor Cheenady successfully defended PhD research proposal.
- Matthew W DeVries received “MAE Graduate Student Research Award”.
- Matthew W DeVries began career at Corvid Technologies in September 2019.
- Professor Subhash received the following awards and recognitions during this reporting period:
    a. *University of Florida Doctoral Dissertation Advisor/Mentoring Award*-2020-2021 *(Feb 2021)*
    b. *Herbert Wertheim College of Engineering Doctoral Dissertation Advisor/Mentoring Award, University of Florida (Nov 2020).*
    c. *B.J. Lazan Award, Society for Experimental Mechanics (SEM) “*for innovative contributions to experimental mechanics and development of in-depth understanding of multiaxial dynamic response of ceramics and soft materials” (2021)
    d. *Fellow of ACerS - The American Ceramic Society* (2020)
    e. *University of Florida Research Foundation Professor*, University of Florida *(2020-2023)*
    f. *Frocht Award, Society for Experimental Mechanics (SEM)* - in recognition of outstanding achievements as an educator. The award recognizes the ***Experimental Mechanics Educator of the Year*** and is in recognition of the technical stature and the high personal regard in which the awardee is held by the experimental mechanics community (2018)
    g. *National Academies of Engineering, Science and Medicine Panel member for ‘Ballistic Science and Engineering’ at the Army Research Laboratories, National Research Council* - 2015-2019; served on three panels in 2015, 2017 and 2018.
    h. *Appeared in a PBS documentary “Secrets of Spanish Florida”* - aired nationwide on Dec 26, 2017 (9-11pm) while discussing the impact response of Coquina, the material with which the oldest fort in USA, Castillo de San Marcos, in St. Augustine was built.

Technology Transfer

During this period, the PI collaborated with three ARL researchers on three publications. These interactions elevated our understanding and also exposed ARL researchers our approaches and experiences:

- Drs. Dr. Sikhanda Satapathy [2], Dr. Philip Jannotti [3] and Dr. Christopher Haines [9]. Two Journal publications involved collaboration with Assistant Professor Qi An from University of Nevada, Reno.
- The PI and his students have presented the research results at the Armor Ceramics Symposia, organized by Drs Jerry LaSalvia and Jeff Swab of ARL, International Conference and Exposition on Advanced Ceramics and Composites conference (ICACC 2018, 2019 and 2020), Daytona Beach, FL. Several ARL researchers attend this conference.
- A free copy of the published book by the PI “*Dynamic Response of Advanced Ceramics”* was shipped to Drs. Christopher Haines, Jerry LaSalvia and Phillip Jannotti of ARL.

Resulting Journal Publications, Books and Thesis Dissertations During Reporting Period

Journal Publications

[1] S. Bavdekar and G. Subhash, “Comparison of pressure-sensitive strength models for ceramics under ultrahigh confinement,” *International Journal of Impact Engineering*, vol. 118, 2018, doi: 10.1016/j.ijimpeng.2018.04.007.

[2] S. Bavdekar, G. Subhash, and S. Satapathy, “A unified model for dwell and penetration during long rod impact on thick ceramic targets,” *International Journal of Impact Engineering*, vol. 131, 2019, doi: 10.1016/j.ijimpeng.2019.05.014.

[3] G. Parsard, G. Subhash, and P. Jannotti, “Amorphization-induced volume change and residual stresses in boron carbide,” *Journal of the American Ceramic Society*, vol. 101, no. 6, pp. 2606–2615, 2018, doi: 10.1111/jace.15417.

[4] A. P. Awasthi and G. Subhash, “High-pressure deformation and amorphization in boron carbide,” *Journal of Applied Physics*, vol. 125, no. 21, 2019, doi: 10.1063/1.5091795.

[5] A. Awasthi and G. Subhash, “Deformation behavior and amorphization in icosahedral boron-rich ceramics,” *Progress in Materials Science*, vol. 112, 2020, doi: 10.1016/j.pmatsci.2020.100664.

[6] C. Kunka *et al.*, “Nanotwinning and amorphization of boron suboxide,” *Acta Materialia*, vol. 147, pp. 195–202, 2018, doi: 10.1016/j.actamat.2018.01.048.

[7] C. Kunka, X. Yang, Q. An, and G. Subhash, “Icosahedral superstrength at the nanoscale,” *Physical Review Materials*, vol. 2, no. 6, 2018, doi: 10.1103/PhysRevMaterials.2.063606.

[8] M. DeVries, G. Subhash, and A. Awasthi, “Shocked ceramics melt: An atomistic analysis of thermodynamic behavior of boron carbide,” *Physical Review B*, vol. 101, no. 14, 2020, doi: 10.1103/PhysRevB.101.144107.

[9] A. A. Cheenady, A. Awasthi, M. DeVries, C. Haines, and G. Subhash, “Shock Response of Single-crystal Boron Carbide Along Orientations with the Highest and Lowest Elastic Moduli,” *Physical Review B (under review)*.

[10] A. A. Cheenady, A. Awasthi, and G. Subhash, “Intrinsic hardness of boron carbide: Influence of polymorphism and stoichiometry,” *Journal of the American Ceramic Society*, doi: 10.1111/jace.17420.

[11] A. A. Cheenady, A. Awasthi, and G. Subhash, “Intrinsic hardness of covalent crystals: a unified multiparametric framework,” *Journal of Materials Science*, vol. 56, no. 20, 2021, doi: 10.1007/s10853-021-06084-w.

Books and Thesis Dissertations

[12] G. Subhash, D. Ghosh, and A. Prakash, *Dynamic Response of Advanced Ceramics*. 2021. doi: 10.1002/9781119599807.

[13] C. Kunka, “Quantum and Experimental Mechanics of Icosahedral Ceramics,” PhD thesis defense, Mechanical and Aerospace Engineering, University of Florida, Gainesville, 2018.

[14] M. Devries, “Amorphization of Boron Carbide: Influence of Grain Size, Secondary Phases, and High Pressure,” PhD thesis defense, Mechanical and Aerospace Engineering, University of Florida, Gainesville, 2019.

[15] S. Bavdekar, “A Unified Analytical Model for the Dynamic Response of Structural Ceramics to Impact and Penetration,” PhD thesis defense, Mechanical and Aerospace Engineering, University of Florida, Gainesville, 2019.

Book Chapters

[13] S. Bavdekar and G. Subhash, "Failure mechanisms of brittle materials under quasi-static and dynamic loads: Overview" In: Voyiadjis G.Z. (eds) Handbook of Damage Mechanics. Springer, New York, NY. https://doi.org/10.1007/978-1-4614-8968-9_80-1; 1-29 (2021)

Conference Proceedings

[16] Ghaffari, K., Bavdekar, S., Subhash, G. Static and Dynamic Mechanical Characterization of a Spark Plasma Sintered B6O-B4C Composite. *Dynamic Behavior of Materials, Volume 1: Proceedings of the 2020 Annual Conference on Experimental and Applied Mechanics 1, 79, 2021*

Conference Presentations

[1] G. Subhash, A.P. Awasthi, C. Kunka, "Comparison of structure and deformation mechanisms in boron carbide and boron suboxide", *2018 SEM Annual Conference and Exposition on Experimental and Applied Mechanics*, June 4–7 2018, Greenville, SC. (Presented by G. Subhash)
[2] S. Bavdekar, G. Subhash. "Comparison of Pressure-Sensitive Strength Models for Ceramics under Ultrahigh Confinement", *2018 SEM Annual Conference and Exposition on Experimental and Applied Mechanics*, June 4–7, 2018, Greenville, SC. (Presented by S. Bavdekar)
[3] C. Kunka, "Comparison of Structure and Deformation Mechanisms in Boron Carbide and Boron Suboxide", *2018 SEM Annual Conference and Exposition on Experimental and Applied Mechanics*, June 4–7 2018, Greenville, SC. (Given as substitute for G. Subhash)
[4] C. Kunka, "Superstrength through Icosahedral Bonding", *2018 SEM Annual Conference and Exposition on Experimental and Applied Mechanics*, June 4–7 2018, Greenville, SC.
[5] C. Kunka , "Superstrength through Icosahedral Bonding", *Mach Conference*, April 4, 2018, Annapolis MD.
[6] A.P. Awasthi, G. Subhash, "Deciphering constitutive states of amorphized boron carbide", *Mach Conference*, April 4, 2018, Annapolis MD.
[7] G. Subhash, A.P. Awasthi, C. Kunka, "Ultra-hard ceramics: Can we make them any harder?" Indian Institute of Science, Bangalore, February 2018. (Presented by Ghatu Subhash)
[8] C. Kunka, "Nanotwinning in Boron Suboxide", *42nd International Conference and Expo on Advanced Ceramics and Composite*, Daytona Beach, FL, USA. January 21–26, 2018
[9] M. Coovert, G. Parsard, G. Subhash. Influence of Amorphization on Residual Stress Development in Boron Carbide via Quasi-static and Dynamic Vickers Indentation. *42nd International Conference and Expo on Advanced Ceramics and Composite*, Daytona Beach, FL, USA. January 21–26, 2018. (Presented by S. Bavdekar)
[10] S. Bavdekar, G. Subhash. An Extended Mohr-Coulomb Model for Ultrahigh Pressure Response of Structural Ceramics. *42nd International Conference and Expo on Advanced Ceramics and Composite*, Daytona Beach, FL, USA. January 21–26, 2018. (Presented by Ghatu Subhash)
[11] C. Kunka, A.P. Awasthi, G. Subhash, "Dynamic Response of Boron Suboxide", *International Mechanical Engineering Congress and Exposition, ASME* November 2017, Tampa, FL (Presented by C. Kunka).
[12] G. Subhash, A.P. Awasthi, G. Parsard, C. Kunka, "Deciphering the Link between Deformation Behavior and Raman Spectra for Polymorph-Level Tailoring of Boron Carbide", *International Mechanical Engineering Congress and Exposition, ASME* November 2017, Tampa, FL (Presented by G. Subhash).
[13] M. DeVries, "Using molecular dynamics to investigate the atomistic response of boron carbide under shock", *2019 SEM Annual Conference and Exposition on Experimental and Applied Mechanics*, June 3-6 2019, Reno, NV.

[14] M. DeVries, “Reactive molecular dynamics simulations of shock of boron carbide”, *Mach Conference 2019*, April 3-5 2019, Hopkins Extreme Materials Institute, Annapolis, MD.
[15] M. DeVries, “Atomistic response of boron carbide under shock impact conditions using molecular dynamics”, *43rd International Conference and Expo on Advanced Ceramics and Composites (ICACC)*, Jan 27- Feb 1 2019, Daytona Beach, FL.
[16] A.P. Awasthi, M. DeVries, G. Subhash, “Ceramics under high pressures: Compression characteristics of B_4C using molecular dynamics”, *43rd International Conference and Expo on Advanced Ceramics and Composites (ICACC)*, Jan 27- Feb 1 2019, Daytona Beach, FL.
[17] A. Cheenady, A. Awasthi, G. Subhash, “Hardness Prediction in Icosahedral Boron Rich Ceramics”, *43rd International Conference & Exposition on Advanced Ceramics and Composites (ICACC)*, Jan 27–Feb 1 2019, Daytona Beach, FL.
[18] G. Subhash, “Molecular Dynamics Simulation of Shock Induced Temperature Rise and Loss of Shear Strength in Boron Carbide” *29th International Workshop on Computational Mechanics of Materials* (IWCMM29) Centre for Advanced Academic Studies Dubrovnik, Croatia, September 15-18, 2019.
[19] G. Subhash, “Shock and High-Pressure Response of Boron Carbide: Experiments and Constitutive Modeling” *American Society of Mechanical Engineers - International Mechanical Engineering Congress and Exposition (ASME-IMECE 2019)*, Nov 11-14, 2019, Salt Lake City, Utah, USA.
[20] G. Subhash, A. Awasthi, M. Devries, “Thermodynamics of Pressure-Induced and Shock-Induced Amorphization in Boron Carbide-Unraveling the Mystery Through MD Simulations and Experimental Data” (Invited), *44th International Conference & Exposition on Advanced Ceramics and Composites (ICACC)*, Jan 27-30, 2020, Daytona Beach, FL.
[21] S. Bavdekar, S. Satapathy, G. Subhash, “A Unified Analytical Model for the Dynamic Response of Armor Ceramics to Impact and Penetration”, *44th International Conference & Exposition on Advanced Ceramics and Composites (ICACC)*, Jan 27-30, 2020, Daytona Beach, FL.
[22] A. Cheenady, M. DeVries, A. Awasthi, G. Subhash, “Influence of Crystal Orientation on Shock Response of Boron Carbide”, *44th International Conference & Exposition on Advanced Ceramics and Composites (ICACC)*, Jan 27-30, 2020, Daytona Beach, FL.
[23] A. Cheenady, M. DeVries, A. Awasthi, G. Subhash, “Influence of Crystal Orientation on Shock Response of Boron Carbide”, *2020 Southeast Graduate Student Symposium of the Society for Experimental Mechanics*, June 15-16 2020, Virtual Symposium.
[24] A. Cheenady, M. DeVries, A. Awasthi, G. Subhash, " Influence of Crystal Orientation on Shock Response of Boron Carbide ", *Mach Conference*, April 7, 2021, Annapolis MD.

Non-Conference Presentations

[1] A.P. Awasthi, G. Subhash, “New directions for deciphering pressure-induced amorphization in boron-rich ceramics”, Hopkins Extreme Materials Institute (HEMI), Johns Hopkins University, MD.
[2] C. Kunka, "Quantum and Experimental Mechanics of Boron-Rich, Icosahedral Ceramics.", Group 01851 (Materials Mechanics & Tribology), April 18 2018, Sandia National Laboratories.
[3] C. Kunka, "Quantum and Experimental Mechanics of Boron-Rich, Icosahedral Ceramics.", Group 05219 (MEMs Technologies), April 19 2018, Sandia National Laboratories
[4] C. Kunka, "Quantum and Experimental Mechanics of Boron-Rich, Icosahedral Ceramics.", Center for Integrated Nanotechnology (CINT), July 2 2018, Sandia National Laboratories
[5] C. Kunka, "Quantum and Experimental Mechanics of Boron-Rich, Icosahedral Ceramics.", Group on Experimental Testing in Materials Science, June 29 2018, Los Alamos National Laboratories.
[6] M. DeVries, “Amorphization of boron carbide: Influence of grain size, secondary phases, and high pressure”, PhD dissertation defense, May 14 2019, University of Florida, Gainesville, FL.
[7] S. Bavdekar “A unified analytical model for the dynamic response of structural ceramics to impact and penetration”, PhD dissertation defense, February 21 2019, University of Florida, Gainesville, FL.

[8] G. Subhash. "Pressure-induced amorphization in ultrahard ceramics: A thermodynamics-based theory for boron-rich icosahedral ceramics", Invited seminar at Naval Research Laboratories, Washington, DC, Sept 5, 2019.
[9] A. Cheenady, "Intrinsic Hardness and Shock Response of Boron Carbide", PhD proposal defense, April 21, 2020, University of Florida, Gainesville, FL.

Seminars at Universities and Laboratories

1. Naval Research Laboratories, Washington, DC, "Pressure-induced amorphization in ultrahard ceramics: A thermodynamics-based theory for boron-rich icosahedral ceramics" (Sept 5, 2019)
2. University of Texas, Austin, Department of Aerospace Engineering and Engineering Mechanics, "Pressure-induced amorphization in ultrahard ceramics: A thermodynamics-based theory for boron-rich icosahedral ceramics" (Feb 14, 2019)
3. Texas A&M University, Materials Science and Engineering Department, "Deformation Mechanisms in Ultrahard Ceramics: A Comprehensive Experimental, DFT and MD Investigation," (Oct 8, 2018)
4. University of Houston, Texas, Mechanical Engineering Department, "Deformation Mechanisms in Ultrahard Ceramics: A Comprehensive Experimental, DFT and MD Investigation," Houston, TX (Sept 27, 2018)
5. Johns Hopkins University/MEDE/, Baltimore, MD "New insights into Amorphization in Boron Carbide" (Apr 9, 2018)

Keynote or Invited Presentations at Conferences

1. Invited (by Invitation Only) presentation on "Thermodynamics of Pressure-Induced and Shock-Induced Amorphization in Boron Carbide-Unraveling the Mystery Through MD Simulations and Experimental Data", S4: Armor Ceramics - Challenges and New Developments; Session title: Quasi-Static and Dynamic Behavior IV, January 28, 2020; 44th International Conference and Exposition on Advanced Ceramics and Composites conference (ICACC 2020), Daytona Beach, FL,January 26-31, 2020,
2. Invited (by Invitation Only) presentation on "Bonding Structure and Deformation Mechanism in Ultrahard Icosahedral Ceramics", at the 43rd International Conference and Exposition on Advanced Ceramics and Composites (ICACC 2019) 'SYMPOSIUM 10: Ceramics Modeling, Genome and Informatics, Feb 28-31, 2019, Daytona Beach, FL.
3. Invited Presentation (40 min) at the ASME-IMECE 2018 conference "Amorphization in Boron Carbide: Experimental and Computational Study" Session 12-3-1 (Mechanical Characterization in Extreme Environments-1), Sept 15, 2018, Pittsburg, PA.
4. Invited Presentation (40 min) "Experimental and Computational Spectroscopy for Deciphering Amorphization in Boron Carbide due to Dynamic Loading", in Dynamic Behavior of Materials VIII – Effect of Microstructure on Dynamic Response II, at TMS 2018, Phoenix, AZ, 13 March 2018.
5. Conference Keynote Lecture (invited) "Bonding, Structure and Deformation Mechanisms in Ultra-Hard Ceramics", at Ceramics 2018, Rome, 14-15 May, 2018.
6. Invited Speaker "Ultrahard Ceramics: Can we make them any harder?" at the Discussion Meeting on "Mechanics/Materials Interface" Evolve Back Resorts, Coorg, Karnataka, India, Feb.18-22, 2018, Organized by the Indian Institute of Science, Bangalore, India.
7. Conference Plenary Presentation "Experimental and Computational Spectroscopy for Characterizing Deformation Modes in Icosahedral Boron-rich Ceramics", at the International Conference on Molecular Spectroscopy (ICMS 2017), 8-10 December 2017, Kottayam, Kerala, India.
8. Session Keynote Speaker "Deciphering Amorphization in Boron Carbide using Experimental and Computational Spectroscopy" of the Session on 'Dynamic response and failure of advanced materials -5', (topic 12-16), Organized by Prof. Luoyu Roy Xu of University of New Mexico, at the ASME-IMECE, Tampa, FL, November 5-9, 2017

Figures

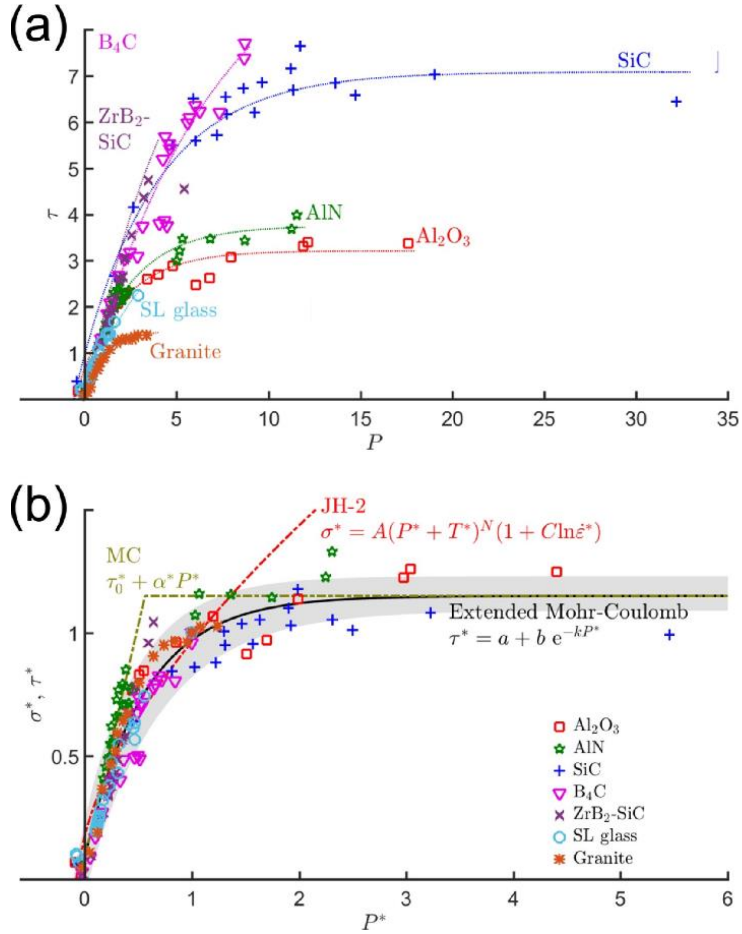

Figure 1. (a) Experimental data for intact ceramics. (b) Experimental data normalized by the corresponding P_{HEL} and τ_{HEL} values along with the MC, JH-2 and extended-MC models [1]. The bilinear MC model is unable to capture the inelastic response at higher pressures while the JH-2 model fails to capture the pressure independent strength saturation beyond HEL. The extended-MC model captures the material response over the entire range in a single curve. The 99% confidence interval for this model is represented by the grey band.

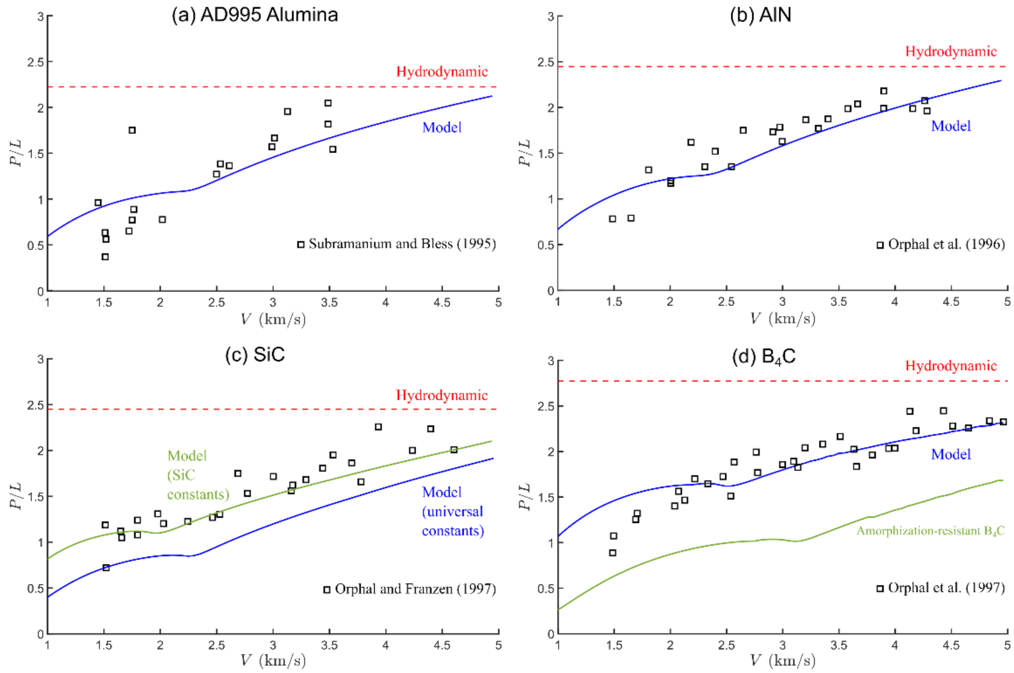

Figure 2. Comparison of experimental data and model results for normalized depth of penetration as a function of impact velocity for a long tungsten projectile (L/D = 20) impacting different structural ceramics [2].

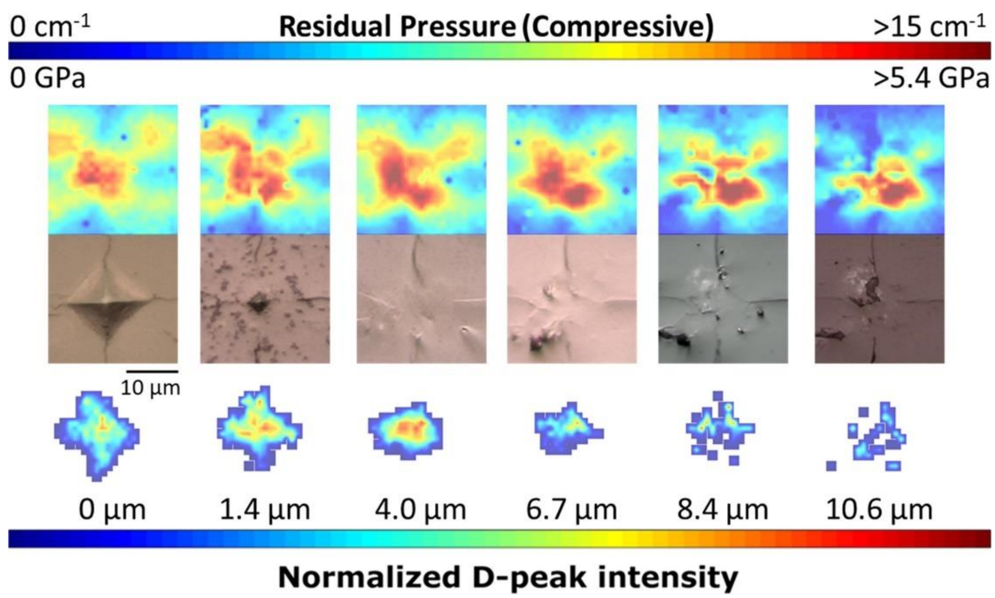

Figure 3. Maps of residual pressure (top) and amorphization (bottom) on surfaces at various depths below a 4.9 N Vickers indentation on boron carbide [3].

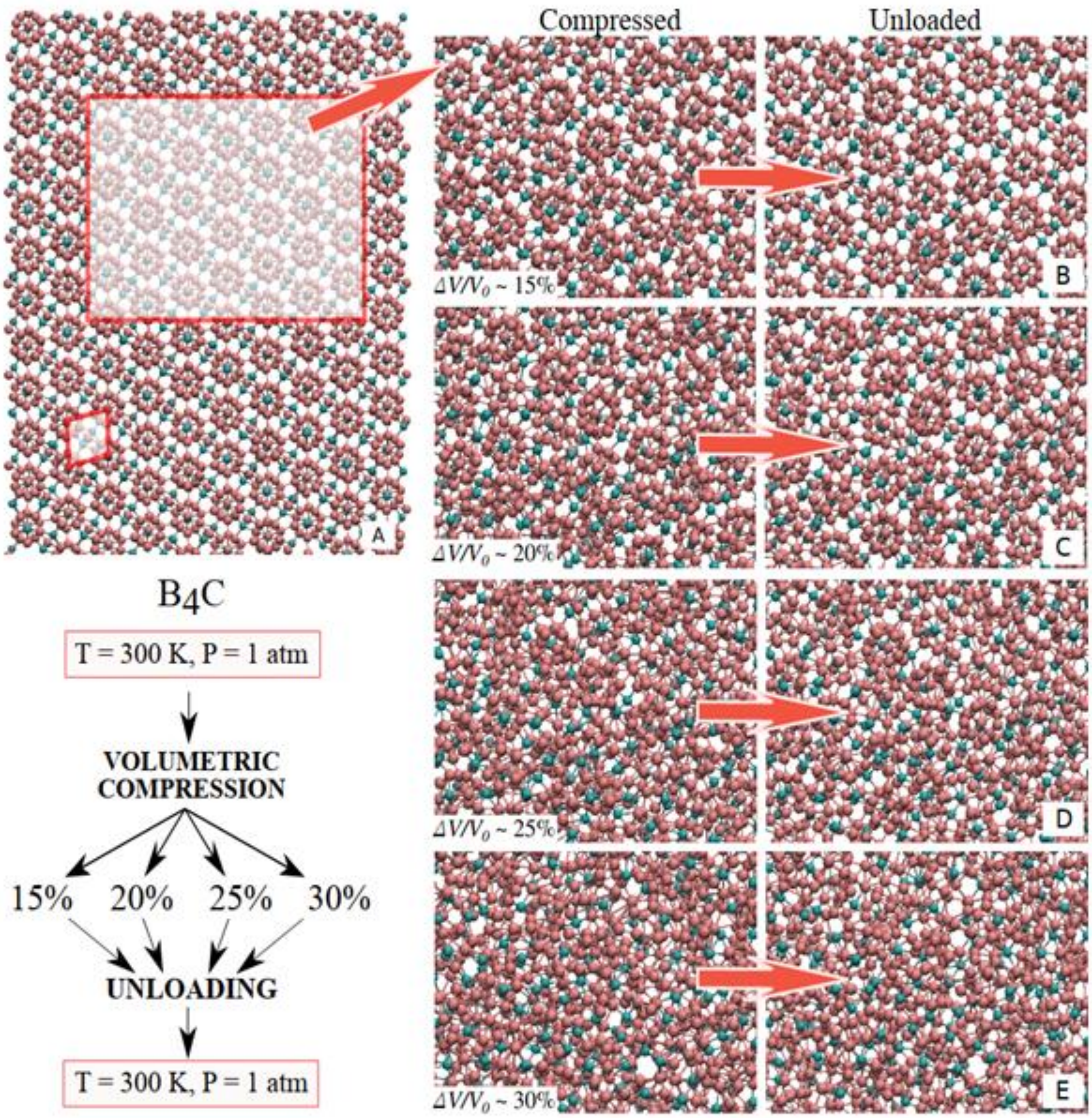

Figure 4. (A) Rectangular MD computational domain and underlying rhombohedral lattice of boron carbide. The rectangular inset is a window of observation for structural changes that occur when the overall structure is subjected to volumetric strains and unloaded. Four different cases shown for volumetric compressive strain ($\Delta V/V_0$) of about (B) 15%, (C) 20%, (D) 25% and (E) 30%. A very small residual structural change is seen when the system is unloaded from $\Delta V/V_0$ = 15%, temperature T~725 K, pressure P~30 GPa. There is perceptible residual structural disorder when unloaded from $\Delta V/V_0$ = 20%, T~1100 K, P~34 GPa which clearly becomes more pronounced for $\Delta V/V_0$ = 25%, T~1400 K, P~45 GPa, while at $\Delta V/V_0$ = 30%, T~2100 K, P~70 GPa, the resulting structure has almost no residual structural order after unloading. For more information, see references [4] and [5].

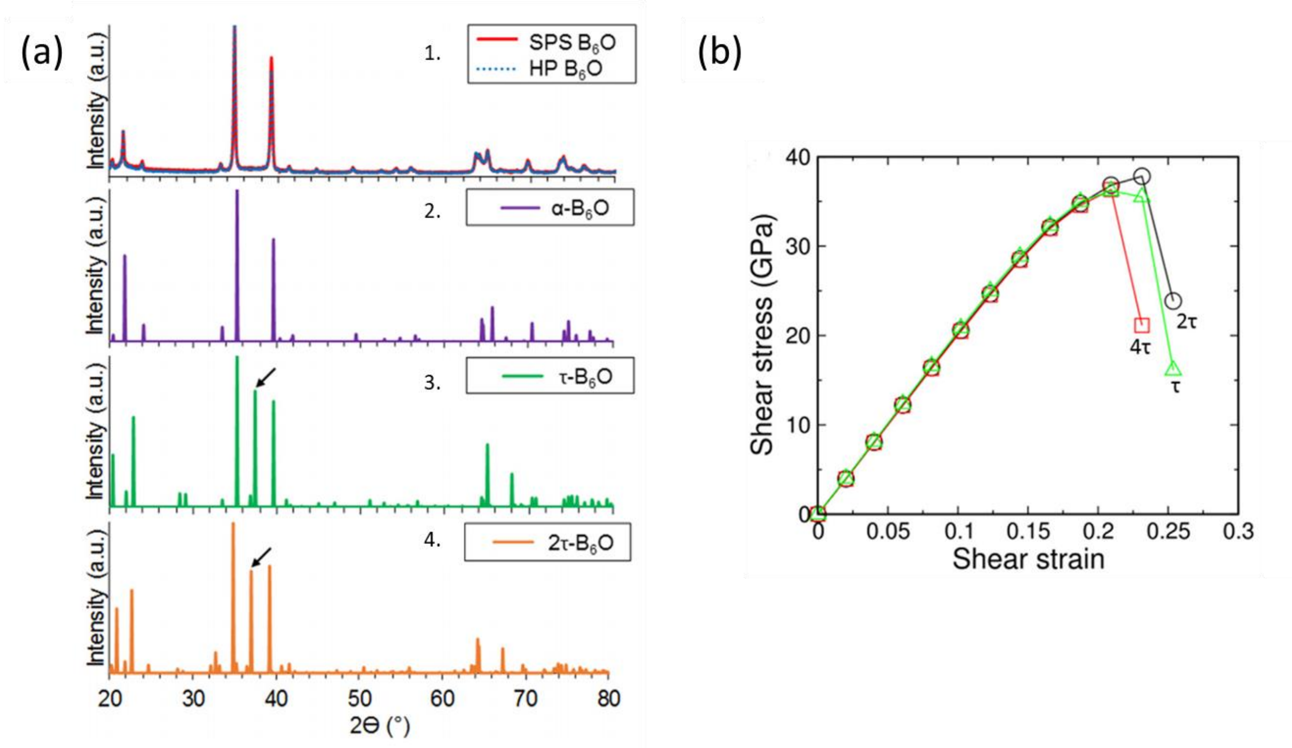

Figure 5. (a) X-ray diffraction (XRD) of (1) experimental B_6O, (2) simulated α- B_6O, (3) simulated τ- B_6O (i.e., β- B_6O), and (4) simulated 2τ- B_6O suggest limited nanotwinning in experimental samples. The unique peak at 2θ=37˚ in τ - B_6O and 2τ - B_6O correlates with nanotwinning regardless of twin spacing. (b) A twin spacing of 0.89nm is seen to sustain the highest shear stress under a biaxial shear loading. For more information, see reference [6].

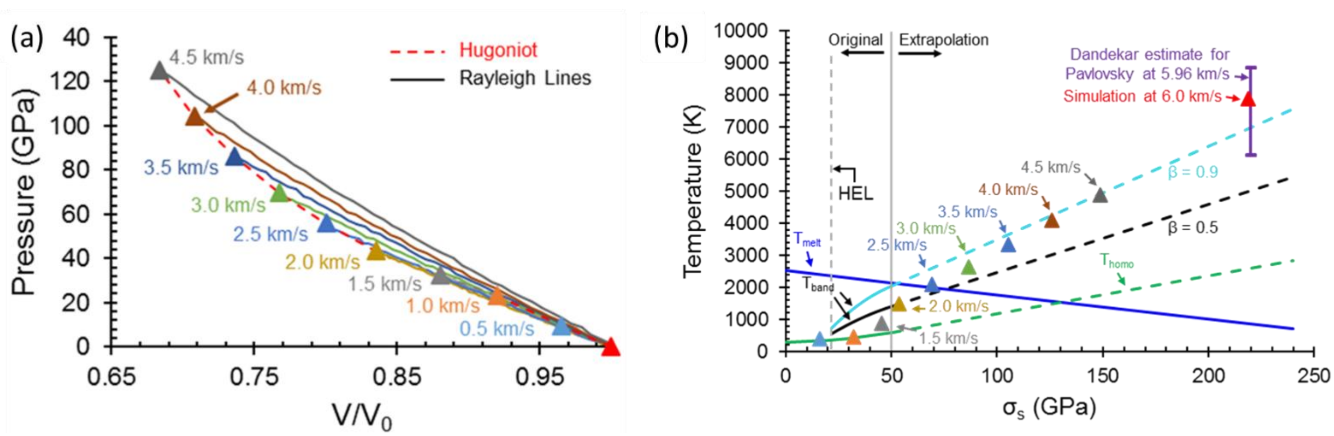

Figure 6. (a) The P-V shock Hugoniot of boron carbide is derived from Raleigh lines constructed at various impact velocities. (b) Temperature as a function of shock stress for simulated boron carbide systems (triangles); plotted alongside melting temperature of boron carbide (solid deep blue line), and homogeneous shock and shear localization temperature contributions estimated by Zhao et al. (2016) (solid lines). Dashed lines indicate linear extrapolations into the high stress regime. Also included at high stresses are the prediction of temperature rise made by Dandekar (2001) for Pavlovsky (1971) data at 5.96 km/s impact velocity, as well as the corresponding temperature rise for simulated 6.0 km/s shock. For more information, see reference [8].

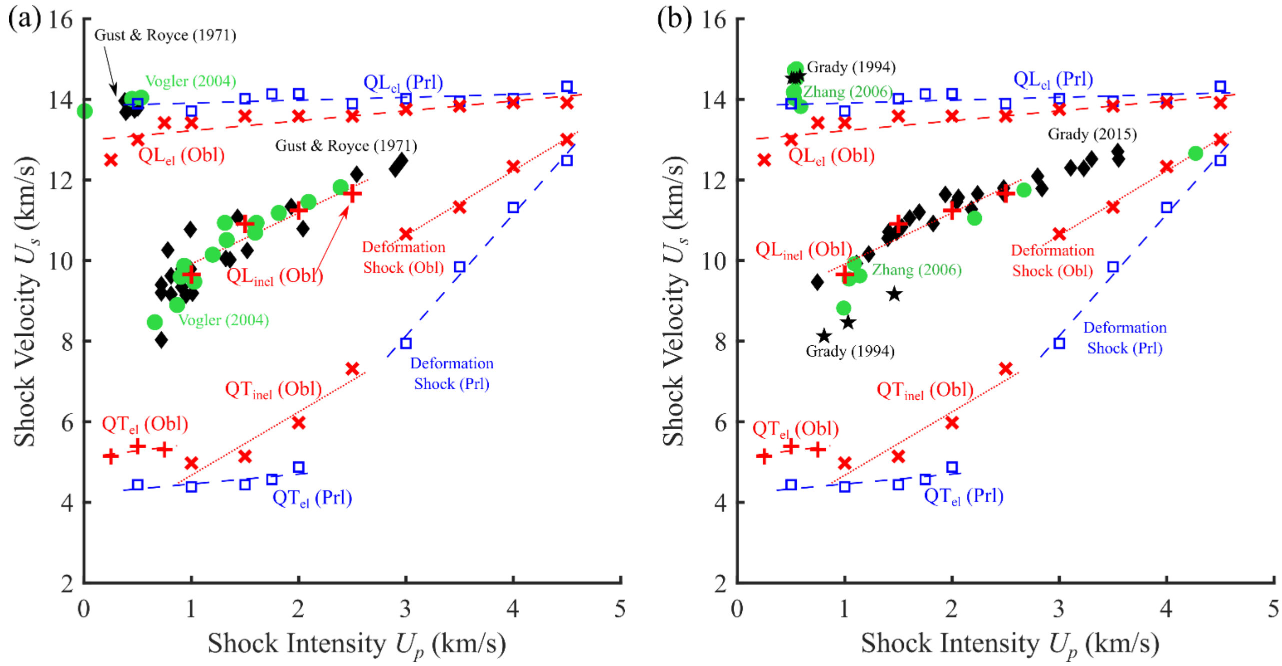

Figure 7. The simulation-derived U_s-U_p relationships [9] along the parallel ([111]) orientation ('Prl', hollow (□) symbols) and oblique (47° to [111]) orientation ('Obl', open (×,+) symbols) in boron carbide compared with experimental measurements (filled symbols) from (a) Gust and Royce (1971) and Vogler et al. (2004) and (b) Grady (1994, 2015) and Zhang et al. (2006). Subscripts 'el' and 'inel' identify the waves as elastic and inelastic, respectively. The MD-derived elastic precursor velocities along both crystal orientations ('QL$_{el}$') agree with experimental measurements (see top left corner in both panels). The inelastic wave velocity along the oblique orientation ('QL$_{inel}$') also coheres well with experimental data. For a detailed explanation of the wave profiles, see reference [9].

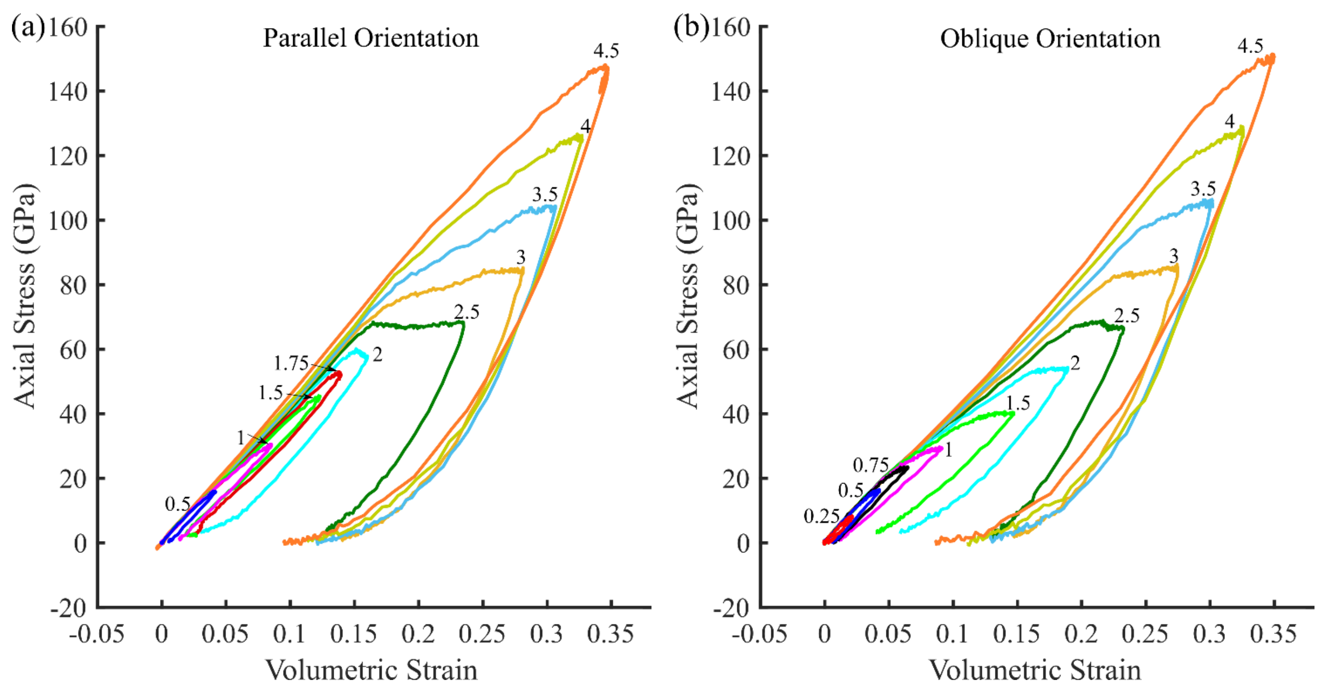

Figure 8. A compilation of axial stress versus volumetric strain response curves at all shock intensities (numbered beside the curves in km/s) investigated in reference [9] along (a) parallel ([111]) and (b) oblique (47° to [111]) orientations.

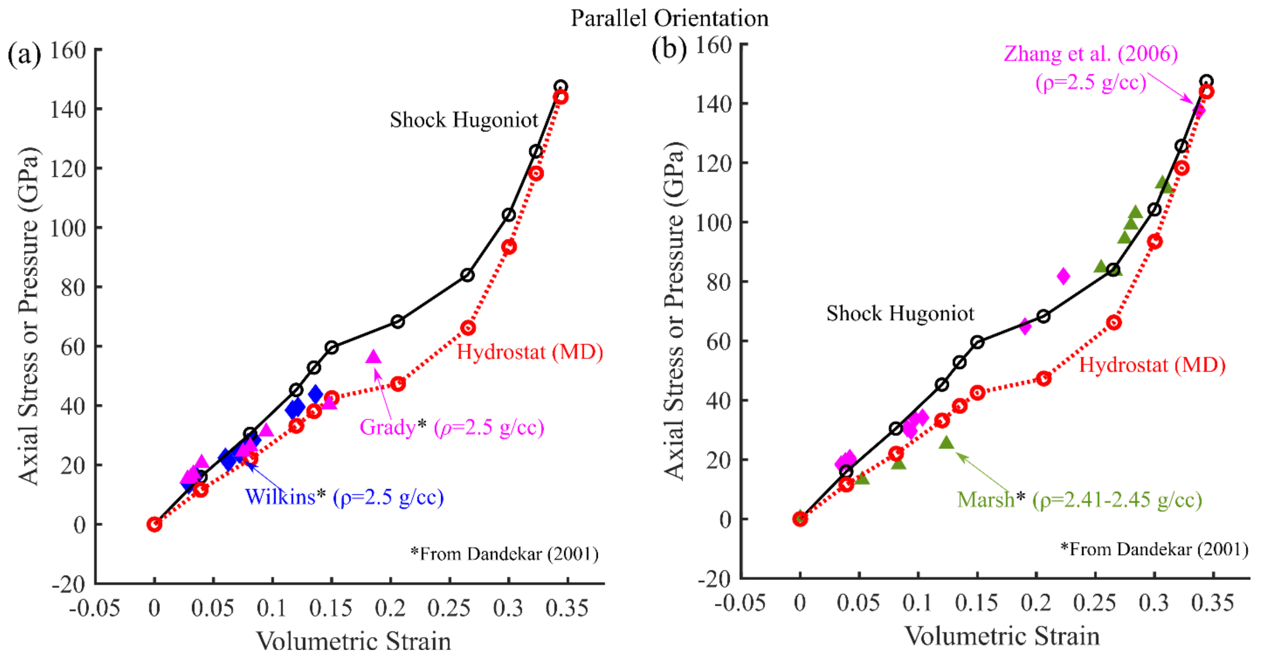

Figure 9. Comparison of the shock Hugoniot and hydrostat along the parallel orientation ([111] direction) [9] with experimental data from (a) Grady and Wilkins (Dandekar (2001)) and (b) Marsh (Dandekar (2001)) and Zhang et al. (2006). The MD-derived hydrostat coheres with experimental data for pressures as high as 140 GPa.

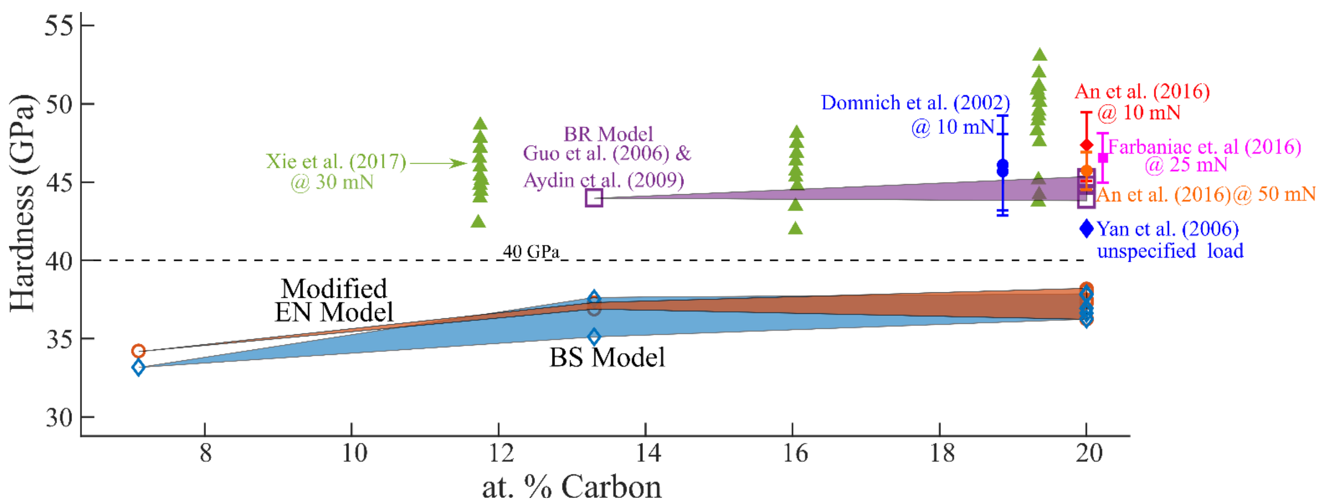

Figure 10. Comparison of hardness values for different stoichiometries of boron carbide predicted by BR (Aydin et al. (2009) and Guo et al. (2006)), BS and modified EN models (open symbols) with experimental data (filled symbols). Data colored blue were measured on single-crystal samples (Domnich et al. (2002) and Yan et al. (2006)) while the rest are nanoindentation studies (An et al. (2016), Farbaniac et al. (2016), and Xie et al. (2017)). The BR model is observed to best cohere with experimental data. For more information, see reference [10].

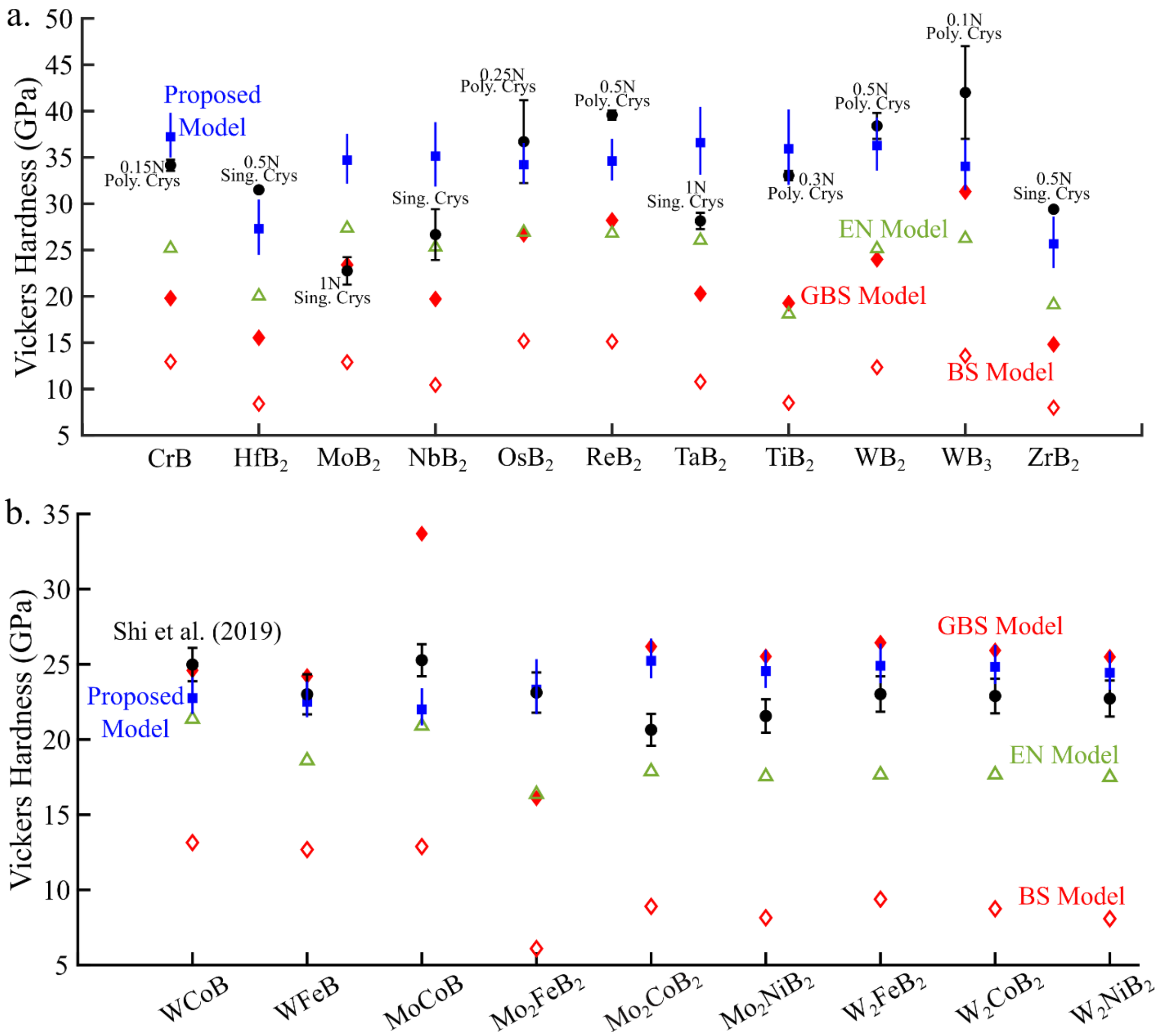

Figure 11. Hardness predictions from the new proposed model (squares), BS (open diamonds), generalized BS (closed diamonds) and EN (triangles) models along with experimental data (black circles) for (a) eleven transition metal borides, and (b) nine other borides from Shi et al. (2019). The blue bands quantify the sensitivity of the predictions to the parameters used in the proposed model. The proposed model is observed to provide better conformance with experimental data than BS, generalized BS and EN models. For more information, see reference [11].