Findings
Joint between Caltech, ISU, and TTU

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1. SHEAR INDUCED STRUCTURE COMPLEXITY – MULTIPLE PHASES OF CARBON

Summary:

Previous reports from the literature indicate that under hydrostatic conditions amorphous diamond is obtained at pressures above 33 and 40 GPa from a glassy precursor, but was not quenchable. The reversible graphite to hexagonal diamond (lonsdaleite) transition has been reported at 16-30 GPa pressure; while an irreversible graphite to lonsdaleite transition has been reported at 17 and 19 GPa under shear (Blank & Estrin, 2014); at 19 GPa the sample also contained cubic diamond. An almost complete transformation from graphite to cubic diamond was reported under shear of 0.25 radians at 21-25 GPa (Blank & Estrin, 2014).

Our Quantum Mechanics (PBE DFT) simulations (Caltech) predict that shear strain can reduce uniaxial transformation stress by a factor of 1.62. In addition, we find that the existence of a grain boundary decreases the transformation stress by a factor of 1.58, i.e., total by a factor 2.55.

In our pressure-shear experiments (TTU), lead to several very exciting results for very low-pressure synthesis of hexagonal and amorphous diamonds.

Our continuum simulations (ISU) provide a model strain-induced kinetics of the phase transformations between graphite, cubic and hexagonal diamond, fullerene and amorphous diamond that is qualitatively consistent with the experiments.

1.1 Quantum Mechanics Atomistic simulations (Caltech)

To examine the atomistic mechanism of transformation of graphite into lonsdaleite (hexagonal diamond) under high pressures, we performed quantum mechanics simulations for perfect graphite and graphite with grain boundaries (GBs) under compressive and shear deformations. We observed the phase transformation from graphite to lonsdaleite structure at a high normal stress of 159.3 GPa for a perfect crystal. The shear deformation decreases the transformation normal stress from 159.3 GPa to 98.5 GPa. In addition, the existence of GBs decreases the transformation stress to 62.5 GPa.

Fig. 1 shows the stress-strain relationship for perfect graphite and graphite with GBs under uniaxial compression. The perfect graphite transforms to the lonsdaleite structure as the
normal stress increases to 159.3 GPa, i.e., at the total pressure of $159.3/3=53.1$ GPa. The structural changes are displayed in the subfigures in Fig. 1, where the sp2 carbon in graphite transforms to sp3 carbon in the lonsdaleite structure.

To examine how the existence of GB affects the phase transition, we constructed the GB models in the graphite structure. To be consistent with experimental observation, we construct the GB with the 5-member and 7 member rings. Two GBs are interested in each layer of graphite. The existence of GB decreases the critical normal stress from 159.3 GPa to 62.5 GPa, indicating that the GBs facilitate the phase transformation from graphite to lonsdaleite structure. The transition pressure with GBs is $62.5/3 = 20.8$ GPa, which is within range 16-30 GPa of experimentally observed transition pressure. The transformed lonsdaleite structure from GB model is displayed in the subfigure of Fig. 1.

Figure 1. Stress-strain relationship for perfect graphite and graphite with GBs under uniaxial compression. The insert subfigures are the snapshot at the critical strains that graphite transforms to lonsdaleite phase. The existence of GB decreases the critical normal stress from 159.3 GPa to 62.5 GPa.
To examine how the shear affects the phase transition, we first compressed the perfect crystal perpendicular to the layer direction by 30%, leading to the normal stress of 98.5 GPa. Then we sheared the system leading to the stress-strain relationship displayed in Fig. 2. As the shear strain increases from 0.04 to 0.06, the graphite structure transforms to the lonsdaleite structure, which leads to the stress discontinuity in the stress-strain curve as shown in Fig. 2. The structural changes are displayed in the subfigures of Fig. 2, which indicates the phase transition. Thus, the shear deformation will also facilitate the phase transformation from graphite to lonsdaleite structure.

1.2 Experimental work (TTU)

Continue working with shear on graphite as reported last year, the TTU group has found multiple phases from sheared graphite. The phases include cubic diamond, fullerene, amorphous diamond, and hexagonal diamond.

1. **Hexagonal diamond**— Formation of hexagonal diamond starting at 0.2 GPa has been reported last year. Figure 3. Shows the in situ synchrotron X-ray diffraction measurements, which clearly indicated the formation of hexagonal diamond.
Fig. 3. The X-Ray diffraction image of graphite in situ at 0.2 GPa after 45° of anvil rotation. Right two images are respectively enlarged from the diffraction image area 1 and 2 as marked. The pressure is calculated from the gold (111) diffraction line.

2. **Cubic diamond**-- From the synchrotron X-ray diffraction of the quenched sample, Figure 4, we clearly see the typical diffraction peak at 2.06 Å, which indicates the existence of cubic diamond. X-ray Phonon Spectrum measurements over the large area of the sheared graphite sample, Fig 5, indicate that large amount of SP³ bonding has been formed while small amount of SP² phase remains. We searched in the sheared graphite sample and identified a piece of crystal in the shape close to rectangular of edge lengths ~50 nm from low resolution TEM image (Figure 6). High resolution TEM measurements (also in Figure 7) indicates the d-spacing of the displayed crystal planes are ~2.06 Å within error range of the system, which is typical distance of the (111) plane of a cubic diamond. The angles between these planes from 68° to 70°, which is identical to the calculated angles between [111] planes of a cubic diamond.

We further performed the EELS measurements of this crystal. Compared to the spectra measured on pure nanocrystalline diamond and graphite (Figure 8), we found that it contains mainly the spectrum of the σ* bond corresponding to diamond, with minimal π* bonding, which may from the graphite residual on the diamond crystal.

The existence of the minimal graphite also causes the left peak drift of the σ* bond (addition of background). Based on these experimental evidences, we firmly believe that the compression and shear operation has resulted in the formation of cubic diamond phase.

Fig. 4. The XRD pattern from a sheet of quenched sample recovered from the cell (without materials from the anvil). The weak diffraction is believed to come from the residual high pressure phase. The ring marked with the red arrow is 2.062 Å (a line of diamond). A broad ring ranging from ~5.9 Å to 3.9 Å is also observed in this pattern, which reflects the complexity of the retained materials.
Fig. 5. The XPS of graphite before and after shear at pressures.

Fig. 6. Low resolution TEM image with SAED pattern find in the sheared graphite sample.

Fig. 7. High resolution TEM of sheared sample. Inset: the FFT in the area showing crystal planes.
Fig. 8. The EELS of the quenched sample from sheared graphite (top) compared to that of nanocrystalline diamond (middle) and pure graphite (bottom).

3. **Fullerenes, Amorphous diamond, carbon fiber/graphene** – High resolution TEM measurements also revealed the formation of fullerenes, amorphous diamond, carbon fiber/graphene (Figure 9).
Figure 9.
1.3 Continuum modeling of phase transformations in carbon (ISU)

Fig. 10. Scheme of phase transformations in the five-phase model. G(1) or (1) represents graphite, hD(3) or (3) means hexagonal diamond, F(2) or (2) is fullerene, aD(4) or (4) stands for amorphous diamond, and cD(5) or (5) is cubic diamond.

Based on iterative interaction with TTU and Caltech group, the following model for strain-induced phase transformations (PTs) in carbon is developed. Fig. 10 shows the scheme of PTs from low pressure phases to high pressure phases among five phases. Since each high pressure phase is observed in the normal conditions, we consider reverse PTs only occurs at negative pressures under the nonhydrostatic condition. Since we do not consider the negative pressures in this paper, we ignore the reverse PTs in Fig. 1 and in the governing equations. For example, the graphite (using symbols G(1) or (1)) can transform into fullerene (2) and hexagonal diamond (3), and we do not discuss the reverse PTs from (2) or (3) to (1). Other PTs include those from hexagonal diamond (3) to amorphous diamond (4), from fullerene (2) to amorphous diamond (4), and from amorphous diamond (4) to cubic diamond (5).

The governing equations for strain-induced PTs among the above phases have been derived based on our developed microscale theory for strain-induced PTs. All material parameters have been determined in an iterative loop with TTU and Caltech.
Fig. 11. The variation of concentrations $c_i$ of different phases versus an accumulated plastic strain $q$ at a fixed pressure $p$ starting from the initial graphite phase. The fixed pressure $p$ is 3 GPa (a), 4 GPa (b), 5 GPa (c), 6 GPa (d).

Fig. 11 shows the variation of concentration $c_i$ of different phases with an increasing accumulated plastic strain under several fixed pressure for the initial phase as graphite. At a low pressure in the Fig. 11a, the strain-induced PT occurs only from graphite to hexagonal diamond. At $q=2.5$, the whole sample transforms to hexagonal diamond. When we fix $p$ at pressure of 4 GPa in Fig. 11b, the fullerene can appear along with hexagonal diamond and the rate of reduction in graphite increases. At $q=1$, there is only a very small amount of graphite in Fig. 11b and hexagonal diamond and fullerene reached stationary concentrations. At $p=5$ GPa in Fig. 11c, coexistence of four phases takes place at $q=0.5$ but cubic diamond still did not appear. With increasing $q$, concentration of amorphous diamond increases and all other phases decreases. Graphite disappears first, then fullerene, and hexagonal diamond tends to disappearance at very
large $q$. At a fixed pressure of 6 GPa, after disappearance of graphite, cubic diamond nucleates at $q=1$, along with initially formed fullerene and hexagonal and amorphous diamond. Fullerene disappears at $q=1.5$. Cubic diamond grows from amorphous diamond, but concentration of amorphous diamond continues to grow in expense of hexagonal diamond.

Fig. 12. The variation of concentrations $c_i$ versus accumulated plastic strain $q$ at stepwise increase in pressure. Initially the sample is in graphitic form. At the fixed pressure $p=4$ GPa, $q$ is increased from 0 to 3; then $p$ is increased to 5 GPa and $q$ varies from 3 to 6; and then at $p=6$ GPa $q$ changes from 6 to 9.

In contrast to Fig. 11, in Fig. 12 the pressure is also stepwise increased at some values of the accumulated plastic strain $q$. At pressure $p=4$ GPa and $q$ not greater than 3, the curves in Fig. 12 are consistent with Fig. 11b. However, once $q$ is greater than 3 at $p=5$ GPa, it is different from the Fig. 11c, because the initial phases at $p=5$ GPa are fullerene and hexagonal diamond rather than graphite. The amorphous diamond grows with a reduction of other two phases. In Fig. 12, there is no coexistence of four phases (in contrast to Fig. 11c), and at $q=9$, the sample mostly transforms amorphous diamond, and the small amount of hexagonal and cubic diamonds. With increasing strain and after disappearance of the hexagonal diamond, amorphous diamond will slowly transform to the cubic diamond.

2. COMPRESSION AND SHEAR OF LEAD (EXPERIMENTS FROM TTU AND CONTINUUM THEORY FROM ISU)

For better understanding the stress and stain field in the sample chamber of a rotational diamond anvil cell, we first explored the shear effect on one of the softest solid material, lead. By application of large plastic shear on a lead sample in a rotational diamond anvil cell, we studied the pressure self-multiplication and the stress deviation phenomena, along with the consequential effects on a phase transformation. It is indicated that pressure can be promoted by the gradual addition of shear [1]. The stress deviation in the sample along different Chi angles is minimal and within the systematic error range. It is thus specified that a quasi-hydrostatic condition is generated in the sample chamber. Moreover, surprisingly, under such shear-controlled pressure elevation, the lead fcc-to-hcp phase transformation pressure is found to
initiate and complete respectively at 12.8 and 18.5 GPa, which is identical to those observed in hydrostatic compressions. The phenomena of the so-launched quasi-hydrostatic pressure, the self-multiplication, along with the consequential effects on the phase transformation properties by shear at pressures is expected to lead to further understanding of materials as well as to potential new technologies at extremes.

Fig. 13. Pressure in lead during anvil rotation at constant applied force. \( P_{\text{Pb}} \) and \( P_{\text{Pt}} \) are pressures calculated from EOS of Pb and Pt. Error of \( P_{\text{Pt}} \) is determined by the error of Pt’s unit cell volume.

The ISU group attempted to theoretically interpret the obtained at Texas Tech results, *in an iterative loop with experiment*. Our theory predicts that at deformation above recrystallization temperature, the effect of plastic shear should be absent because any accumulation of defects will be eliminated by recrystallization. For lead, recrystallization temperature is below room temperature. Thus, effect of shear should be negligible, which is consistent with experiments. This is conceptual confirmation of our theory. Pressure-self multiplication effect during shear without PT and at constant applied force should be caused by redistribution of stresses between sample and gasket: pressure reduces in gasket and, to keep the same force, should be increased in a sample. Large pressure gradient is expected in a Zr gasket because of relatively high yield strength. Thus, this is a system behavior rather than material behavior. The low yield strength in shear of lead (~0.01 GPa), negligible with the operating pressure of ~10 GPa, explains negligible non-hydrostaticity of stresses in experiment.
3. SHEAR AND COMPRESSION OF BORON CARBIDES ALLOYED WITH OTHER ELEMENTS (THEORY CALTECH, EXPERIMENT TTU)

Caltech has been using QM theory to predict the stability and ductility of Boron Carbides alloyed with other elements, such as Si, N, P, As, O, and S. This is discussed in detail in the Caltech separate report.

Using the ReaxFF derived from QM, Caltech was able to carry out shear transformations with systems having scales of 25 nm (200,000 atoms) where they observed transformations from a single crystal to twins to amorphous bands 2 to 3nm thick that then cavitate to form microscopic cracks. They find that the origin of this brittle failure is reaction of the inter-icosahedral CBC chains with a broken C-B between two icosahedra that fractures the icosahedra. They find that the fractured icosahedra have 5 to 10% higher density than the crystal, which leads to tension and cavitation, explaining the observed amorphous band failure.

Caltech has shown with QM studies that replacing the CBC chains with Si2 chains makes BCSi system much more ductile. In addition, changing the B11C1 icosahedra to B10Si2 to obtain the (B10Si2)(Si2) structure analogous to Boron Carbide also seems to be more ductile. Caltech is working with collaborators at UC Riverside and Rutgers to synthesize these alloys which will then be provided to TTU for experimental tests. TTU has already done experiments with the P doped Boron Carbide.

We anticipate experimental tests of the Caltech predictions over the next year, and perhaps some continuum modeling to complement the ongoing atomistic modeling.

Other Collaborative Efforts of ISU

1. Collaborative efforts between ISU and V. Blank group from the Technological Institute for Superhard and Novel Carbon Materials (Moscow, Russia)

Shear and transformation bands in the fullerene [2]

Shear transformation-deformation bands have been revealed (Fig. 14) consisting of shear-strain-induced nanocrystals of linearly-polymerized fullerene and polytypes, the triclinic, monoclinic, and hcp C$_{60}$, and amorphous structures. Thus, plastic straining arrests five high pressure phases under normal pressure, which may be important for their engineering applications. Localized shear deformation looks contradictory because high pressure phases of C$_{60}$ are stronger than the initial low pressure phase. However, this was explained by transformation-induced plasticity during localized PTs which occurs because of a combination of applied stresses and internal stresses due to a volume reduction during PTs. Localized PTs and plastic shear deformation promote each other producing positive mechanochemical feedback and cascading structural changes. Obtained results demonstrate that transformation kinetics cannot be analyzed in terms of prescribed shear and methods to measure local shear should be developed.
2. Collaborative Efforts between ISU and NIST (Dr. James Warren)

Thermodynamically consistent phase field theory of phase transformations with anisotropic interface energies and stresses [4,5]

The main focus here is to introduce, in a thermodynamically consistent manner, an anisotropic interface energy into a phase field theory for PTs. Previous theories have assumed the free energy density (i.e., gradient energy) is an anisotropic function of the gradient of the order parameters in the current (deformed) state, which yields a nonsymmetric Cauchy stress tensor. This violates two fundamental principles: the angular momentum equation and the principle of material objectivity. Here, it is justified that for a noncontradictory theory the gradient energy must be an isotropic function of the gradient of the order parameters in the current state, which also depends anisotropically on the direction of the gradient of the order parameters in the reference state. A complete system of thermodynamically consistent equations is presented. We find that the main contribution to the Ginzburg-Landau equation resulting from small strains arises from the anisotropy of the interface energy, which was neglected before. The explicit expression for the free energy is justified. An analytical solution for the nonequilibrium interface and critical nucleus has been found and a parametric study is performed for orientation dependence of the interface energy and width as well as the distribution of interface stresses.

Fig. 15: (a) Distribution of the dimensionless biaxial interface stress $\sigma_{st}(y)$ for and several crystallographic directions for bcc Li and Fe.
3. Collaborative Efforts between ISU and Geophysical Laboratory of Carnegie Institution of Washington (Dr. Russel Hemley)

Large elastoplasticity under megabar pressure: formulation and application to compression of a sample in a diamond anvil cell

Our joint comprehensive paper [10] based on the results reported in the first year have been submitted and published in International Journal of Plasticity.

Individual ISU work on development of the new methods and approaches

One of the main goals of the project is to develop and verify nanoscale phase field approach (PFA) to phase transformations (PTs) between multiple phases, dislocation nucleation and motions, and interaction between PT and dislocational plasticity and twinning. The following breakthrough results are obtained in these directions.

1. Phase field approach to dislocation evolution at large strains: Computational aspects [3]

Computational aspects of the phase field simulations of dislocation nucleation and evolution are addressed. The complete system of equations for the coupled phase field approach to dislocation nucleation and evolution and nonlinear mechanics for large strains is formulated. Analytical solutions for a stationary and propagating single dislocation, dislocation velocity, core energy, and core width are found. Dislocation parameters for nickel are identified based on existing molecular dynamics simulations. In contrast to all previous efforts that are based on the spectral approach, finite element method (FEM) is utilized, which allowed us to treat large strain problems and non-periodic boundary conditions. The single dislocation order parameter profile and the stationary distance between two neighboring dislocations at a semicoherent sharp austenite–martensite interface are in perfect agreement with analytical expressions. The main focus is on proving that the new points of the developed theory can be confirmed in simulations, including possibility of obtaining the desired dislocation height for aligned and inclined dislocations, eliminating spurious stresses, resolving dislocation cores and interaction between cores of different dislocations. Mesh independence of the solutions is demonstrated and the effect of approximating finite element polynomials is analyzed, exhibiting possibility of significant numerical errors when special care is not taken of. Problems of nucleation and evolution of multiple dislocations along the single and multiple slip systems near martensitic lath (Fig. 16), and along the sharp austenite–martensite interface, the activity of dislocations with two different orientations in a nanograined material under shear and pressure, and the interaction between two intersecting dislocation systems are studied. Surface-modified partial dislocation was revealed. These problems represent the first step in the future study of interaction of phase transformation and dislocations.
2. Phase-field approach to nonequilibrium phase transformations in elastic solids via an intermediate phase (melt) allowing for interface stresses [6]

PFA for PTs between three different phases at nonequilibrium temperatures is developed. It includes advanced mechanics, thermodynamically consistent interfacial stresses, and interface interactions. A thermodynamic Landau–Ginzburg potential developed in terms of polar order parameters satisfies the desired instability and equilibrium conditions for homogeneous phases.
The interfacial stresses were introduced with some terms from large-strain formulation even though the small-strain assumption was utilized. The developed model is applied to study the PTs between two solid phases via a highly disordered intermediate phase (IP) or an intermediate melt (IM) hundreds of degrees below the melting temperature. In particular, the $\beta \leftrightarrow \delta$ PTs in HMX energetic crystals via IM are analyzed. The effects of various parameters (temperature, ratios of widths and energies of solid–solid (SS) to solid–melt (SM) interfaces, elastic energy, and interfacial stresses) on the formation, stability, and structure of the IM within a propagating SS interface are studied. Interfacial and elastic stresses within a SS interphase and their relaxation and redistribution with the appearance of a partial or complete IM are analyzed (Fig. 9). The energy and structure of the critical nucleus (CN) of the IM are studied as well. In particular, the interfacial stresses increase the aspect-ratio of the CN. Although including elastic energy can drastically reduce the energy of the CN of the IM, the activation energy of the CN of the IM within the SS interface increases when interfacial tension is taken into account. The developed thermodynamic potential is perfect for three phases but cannot be noncontradictory generalized for $n>3$ phases. This was done in the paper [7] described in the next item.

3. Multiple phase field theory for phase transformations [7]
Fig. 18. Minimum value of the sum of two order parameters, \((\eta_1 + \eta_2)_{\text{min}}\), versus \(k_E\) (ratio of the energy of solid-solid (SS) to solid-melt (SM) interfaces) for different \(k_\delta\) (ratio of the width of SS to SM interfaces) parameters and magnitude of the energy penalizing term \(K_{12}\) for two different initial conditions corresponding to SS interface and solid-melt-solid (SMS) interface. \((\eta_1 + \eta_2)_{\text{min}}=1\) for SS interface and \((\eta_1 + \eta_2)_{\text{min}}=0\) for SMS interface with complete melt between SS interface. Temperature is 100 K below the melting temperature. Strong scale effect (described by \(k_\delta\)) is observed, leading to different type of the transition between SS and SMS interface (continuous or discontinuous), degree of disordering within melt and different stability and metastability regions of the melt.

A critical outstanding problem on developing of phase field approach for temperature- and stress-induced phase transformations between arbitrary \(n\) phases is solved. PFA for multiphase materials, which with high and controllable accuracy satisfy all the desired conditions for arbitrary \(n\) phases, is developed. Instead of explicit constraints on the order parameters, we included in the simplest potential the terms that penalize the deviation of the trajectory in the order parameter space from the straight lines connecting each of the two phases. It describes each of the PTs with the single order parameter, which allows us to use an analytical solution for the propagating interface to calibrate each interface energy, width, and mobility. It reproduces the desired PT criteria via instability conditions; introduces interface stresses, and allows us to control the presence of the third phase at the interface between the two other phases. The developed approach unifies and integrates approaches developed in different communities (in particular, solidification and martensitic PTs) and is applicable to various PTs between multiple solid and liquid phases and grain evolution, and can be extended for diffusive, electric, and magnetic PTs.

FEM simulations have been performed for multiphase temperature-induced PTs with application to solid-solid PTs via nanometer size virtual or intermediate melt within the SS interface, hundreds of degrees below melting temperature. Simulations were performed for \(\beta\leftrightarrow\delta\) PTs via intermediate melt in HMX energetic material (Fig. 18). These results will be generalized and used for PTs between multiple carbon phases.

One of the main goals of the project is to develop and verify macroscale models and FEM to coupled plastic flow and PTs in a sample compressed in traditional diamond anvil cell (DAC) and compressed and sheared in rotational diamond anvil cell (RDAC). This is important in order to describe experiments in DAC and RDAC performed by TTU group, plan new experiments, extract material parameters from heterogeneous fields, and find ways to control PTs and search for new phases. The following breakthrough results are obtained in these directions.

4. Pressure self-focusing effect and novel methods for increasing the maximum pressure in traditional and rotational diamond anvil cells [8]

The highest possible static pressure is currently produced by compressing a thin sample/gasket by two diamond anvils in DAC. One of the goals in high pressure research is to reach the highest possible pressure to explore material behaviors and find new phases at such extreme conditions.
Another objective is to achieve medium-high pressure but for multiple times, without breaking diamonds.

The main principles of producing a region near the center of a sample, compressed in DAC, with a very high pressure gradient (which is called here the pressure self-focusing effect) and, consequently, with high pressure are predicted theoretically. Initial analytical predictions utilized generalization of a simplified equilibrium equation. Then, the results are refined using our advanced model for elastoplastic material under high pressures in FEM simulations. The main points in producing the pressure self-focusing effect are in using beveled anvils and reaching a very thin sample thickness at the center. It is found that the superposition of torsion in a RDAC offers drastic enhancement of the pressure self-focusing effect and allows one to reach the same pressure under a much lower force and deformation of anvils in Fig. 19. Consequently, a novel method for achieving record pressures is related to using torsion under fixed applied force in RDAC with beveled anvils and reaching a small sample thickness.

Fig. 19. Distribution of the pressure $p$ in the sample (a) and at contact surface (b) under a fixed applied normal stress $\sigma_n = 1.1$ GPa with the growing rotation angle $\varphi$: 0, 0.4, 0.8, 1.2 and 1.6 (in radians). The zoomed central part of a sample is shown above the sample for each rotation angle. For comparison, curve 6 in (b) is shown for compression in DAC to the same pressure at the center.

5. Effects of gasket on coupled plastic flow and strain-induced phase transformations under high pressure and large torsion in a rotational diamond anvil cell [9]

Coupled strain-induced PT and plastic flow in the sample within a gasket under high pressure and large torsion in RDAC are studied in detail. In comparison with compression in DAC, PT rate is much faster in RDAC under the same maximum pressure in the sample (Fig. 20), in accordance with experiments. This may lead to a misinterpretation that plastic shear promotes PTs in comparison with uniaxial compression. It is shown that this statement does not refer to material physical and mechanical properties, but it is a consequence of a behavior of the sample-gasket-loading system. Indeed, PT kinetics is independent of the mode of stresses and strains. For any mode of plastic straining, the PT can be driven and completed at pressure as low as the critical minimum pressure for direct PT. The difference between results in DAC and RDAC is because of heterogeneity of the stress and strain fields required to produce high pressure and
large plastic strain in the sample under different loading programs. For DAC, plastic flow is generated by increasing the axial force, which causes a fast growth in pressure in the sample, even while pressure increase is not required for PT. However, for RDAC, the plastic straining can be produced by rotation of an anvil under a fixed axial force with minor changes in pressure. A correct statement of the promotion of PT by plastic straining should be in comparison with pressure- or stress-induced PTs under hydrostatic or quasi-hydrostatic loading without plastic straining. Still, advantages of RDAC in comparison with DAC demonstrate a possibility to search new phases at lower pressure, to obtain a transformed sample under lower pressure without breaking a diamond, and to scale up the process for large volumes using anvils from strong metals or hard alloys, like in high-pressure torsion. Stronger gaskets and longer gaskets reduce plastic deformation and pressure gradient in the sample as well as PT rate. The effect of gasket thickness on PTs and plastic flow is not pronounced, excluding initial stages of rotation of an anvil. Multiple experimental results are qualitatively reproduced and interpreted. Obtained results are useful for the design of experiments searching new high-pressure phases, controlling homogeneity of all fields in the sample and transforming volume, optimizing loading programs, as well as for extracting kinetic properties from an experiment with heterogeneous fields.

Fig. 20. Variations of maximum pressure $p$ in the sample versus the concentration of the high-pressure phase $c_0$ averaged over the entire sample for compression without torsion and torsion under a fixed axial force $F=6.19$ and different ratios of the yield strengths of high and low pressure phases, $\sigma_{y1}/\sigma_{y2}$. Torsion in RDAC allows to obtain the same concentration of high pressure phase under much lower pressure.

References:


This work was leveraged by the support from DARPA, ARO, ONR, and PI’s endowment.
Presentations

Conference Presentations (Talks and Proceedings Abstracts)

1. V. I. Levitas. Effect of two nanoscale size parameters on the macroscopic transformation behavior within phase field approach. 52nd Annual Meeting Society of Engineering Science, College Station, TX, 10/25/15-10/28/15.


Seminars given by the PI


Organization of Symposia

PI’s Honors

- Who's Who in America, 2016
- ISU Award for Outstanding Achievement in Research for 2016
- Symposium on Structural Changes in Materials in honor of Prof. Valery Levitas at Plasticity’17 International Symposium, Puerto Vallarta, Mexico, 3/1/17-9/1/17.

Both these symposia were and are devoted to the interdisciplinary interaction between theoretician, computational researchers, and experimentalists, in a spirit of MGI philosophy.

Student Award

*Kasra Momeni*, PhD student

2016 Zaffarano Prize Honorable Mention for excellent graduate research at ISU.