Structural study of TATB under detonation-induced shock conditions

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(Dated: March 25, 2022)

We explore the response of the insensitive high explosive (IHE) 1,3,5-Triamino-2,4,6-trinitrobenzene (TATB) under detonation-induced shock conditions using in – situ synchrotron X-ray diffraction in the 100 ns time scale using either a conventional or a colliding detonation drive. In all of the detonation experiments on various sizes and morphologies of TATB, we observe an extended stability of the TATB triclinic crystal structure. As the detonation front passes through the TATB, x-ray diffraction indicates a portion of the TATB exhibits a compression up to 30+ GPa, followed subsequently by a pressure release and continued decomposition over a few hundred nanoseconds. Likewise, for colliding detonation-driven shock compression of single crystals of TATB, a significant portion of the triclinic crystal structure appears to be stable up to 60+ GPa. Conversely, in similar detonations of a LLM-105 PBX, x-ray diffraction is simply indicative of decomposition without the apparent compression and slow decomposition seen in TATB. The results indicate the surprising resilience of TATB under these high-pressure, temperature and shock conditions, providing a baseline for understanding the insensitivity of TATB that is considered the industry standard for an insensitive high explosive. The results also provide intriguing information for the extended reaction zone in TATB, and the hot-spot mechanisms for initiating and propagating detonation in this uniquely insensitive explosive.

INTRODUCTION

Energy release in detonation and insensitivity to hazards are the two most important parameters that determine the effectiveness and safety of a high explosive (HE). Given that these two characteristics are usually incompatible, 1,3,5-Triamino-2,4,6-trinitrobenzene (TATB), stands out as the optimum choice when insensitivity/safety is of utmost importance. Indeed, among similar materials with comparable explosive energy release, TATB is remarkably difficult to shock-initiative, has a low friction sensitivity, and is thermally stable at ambient pressure to approximately 615 K [1]. Thus, probing the structural/molecular evolution of TATB under detonation conditions is of key importance towards understanding the origin of its insensitivity. For these reasons, TATB has attracted extensive research effort aiming to elucidate its high-pressure structural behavior (up to and beyond detonation pressures, nominally 30-40 GPa [2]) under both static and dynamic compression.

Under static compression and according to a plethora of previous theoretical studies [3][12], TATB remains in the ambient pressure crystal structure up to at least 100 GPa. Moreover, experimental isothermal high-pressure powder and polycrystalline X-ray diffraction (XRD) studies [13][14] do not report any structural phase transition up to 70 GPa. Very recently, a subtle second order phase transition towards a monoclinic crystal structure was reported above 4 GPa [15]. Thus, the consensus in the field is that under static compression TATB retains its basic molecular/structural motif even above detonation pressures.

In contrast to the case of static compression, the structural evolution of TATB under detonation/shock conditions and the possibility of chemical reactions under these high-pressure and high-temperature conditions remains an open question. This is mainly due to the lack of in – situ X-ray diffraction (XRD) measurements under such conditions. Previous shock Hugoniot measurements of pure TATB (powder or single crystal) and TATB-based Polymer-bonded explosives (PBXs) have reported the shock Hugoniot equation of state (EOS) up to 83 GPa [16][20]. However, in these studies only the density as a function of pressure was determined under shock conditions.

To address this issue, we have performed an in – situ synchrotron XRD study of ultrafine powders of TATB (UFTATB), single crystals of TATB (SCTATB) and of a TATB-based PBX, under detonation-induced shock conditions in the 100 ns time scales. Aiming to probe larger quantities, and thus increase the confidence of the Bragg peaks assignments of TATB under shock conditions, we use detonation to shock macroscopic quantities of TATB in a geometry that X-rays are orthogonal to the shock front. This allowed us to probe the crystal structure and confirm the structural stability of the ambient-conditions.
triclinic phase of TATB under detonation-induced shock conditions up to 60+ GPa and also during pressure release towards ambient pressure. In contrast to the TATB-based specimens, identical experimental runs using a LLM-105 (2,6-diamino-3,5-dinitropyrazine-1-oxide, C₄H₄N₂O₅, Lawrence Livermore Molecule No.105) based PBX were not successful in probing a detonation induced compression of the respective ambient-conditions crystal structures.

METHODS

High purity UFTATB, SCTATB \[21\] and a TATB-based PBX (nominally 95% TATB) of different sizes were used for all XRD experiments. Moreover, LLM-105 based PBX (nominally 96% LLM-105) specimens were also used aiming to compare with the structural stability of TATB. Diffraction experiments are limited to gram quantities due to the experimental setup, geometry, and facility. Due to these limitations, samples were boosted. UF-TATB as well as TATB and LLM-105 PBXs were generally 1/4” (6.35 mm) in diameter, and about 2.0 mm tall. Two different PBXs were used as boosters, one was hexanitrohexaaazaisowurtzitane (CL-20) based, the other pentaerythritol tetranitrate (PETN), to generate different peak pressures drive. The experiments with both boosters produced similar results with only different peak pressures. For simplicity we only present the results obtained by using CL-20 based booster. These CL-20 or PETN based boosters are each about about 0.22” (5.6 mm) tall. Single crystal samples were grown to sub-mm heights, at diameters less than the booster diameter. TATB and LLM-105 samples were either placed on top of a single PBX or sandwiched between two PBXs that have the same radius with the TATB specimens, see fig. 1. This way the peak shock pressure was controlled by both the type of HE (30-40 GPa peak pressure) and also by what we will refer to as “conventional” or “colliding”detonation. A few 3/8” (9.53 mm) diameter, 11.57 mm tall, 1.5 g UFTATB shots were also fired and boosted by a 3.9 mm tall PBX.

Time-resolved XRD measurements were performed within a Lawrence Livermore National Laboratory (LLNL) detonation tank at the Advanced Photon Source (APS), Argonne National Laboratory, at the Dynamic Compression Sector, within the special purpose hutch (35ID-B) \[16\] \[22\] \[23\] or at 32ID-B \[24\]. The explosive sample assemblies were placed within a 120L steel vacuum vessel (Teledyne RISI) and pumped down to < 200mTorr, see Fig. 1. The tank uses upstream and downstream KaptonTM (polyimide) windows to facilitate the X-ray transmission geometry required for XRD and/or radiography under low vacuum conditions. Within the vacuum vessel, LexanTM (polycarbonate) panels were used as shrapnel mitigation. The samples were detonated near the rear window to increase the angular range of the detector; a Tantalum beamstop was placed between two 2 mm polycarbonate plates, with an additional 1 mm closest to the sample. These were placed a few cm from the detonation. More details about the LLNL detonation tank and the experimental setup can be found in Refs. \[25\] and \[26\]. The sample was aligned in the beam such that the focused beam was centered horizontally and vertically on the 2.0 mm 1/4” diameter samples (1.0 mm above the booster-sample interface.) The beam was simply centered vertically, and roughly horizontally on irregularly shaped single-crystal samples. The x-ray beam was aligned 2.0 mm below the top surface of the larger 3/8” samples.

Detonation is synchronized with the APS bunch clock, thus permitting XRD from discrete 34ps rms X-ray pulses, which arrive every 153.4 ns during 24-bunch mode. The sample-detector distance was about 11cm. Scattering intensity was recorded using an array of four identical area detectors (PI-MAX4 1024i ICCD, Princeton Instruments) focused on the output of an image intensifier \[22\] \[27\] \[29\]. The image intensifier (Photek, MCP140) is equipped with a P47 phosphor and a LSO:Ce scintillator (DMI/Reading Imaging) that have decay times of 80 ns and 40 ns, respectively. Each of these cameras have “Dual Image Feature”(DIF) capability that allows for two sequential image frames spaced at least 500 ns apart. This way, a total of eight frames (noted as frames C1-C8 and separated by 153.4 ns) are recorded for each detonation event. Given that XRD images are rerecorded every 153.4 ns, \(\approx\)10% of the signal recorder in a given frame (XRD image) is expected to originate from the residual XRD image of the previously recorded frame e.g. in frame C3 a \(\approx\)10% residual intensity of frame C2 is recorded. The XRD intensity from different cameras (C1-C4) are normalized in intensity using the static

FIG. 1. Schematic diagram of the detonation tank for in-situ XRD under detonation conditions and schematic section (not to scale) of the experimental cylindrical setup showing the TATB cylinder on top of a HE cylinder. The cylindrical setup is aligned in a way that the incident X-ray beam is at the center (vertical and lateral) of the TATB cylinder and perpendicular to the shock front.
images acquired for each camera before the detonation event for each run.

Integration of powder diffraction patterns to yield scattering intensity versus 2θ diagrams and initial analysis were performed using the DIOPTAS program [30]. DIOPTAS was also used to remove/subtract the intensity contribution of the previous frame discussed above. For each frame (XRD image) the previous frame was used as the background image scaled to the point that the corresponding residual diffraction intensity disappears. A 15-20% scaling was sufficient to, almost, totally remove these diffraction spots. The slightly higher scaling, than what is expected due to the experimental setup (residual intensity), is attributed to parts of the specimens at the edge/surface of the cylinders that are at ambient conditions even under detonating-induced shock conditions [31]. Si640E (NIST standard) and CeO$_2$ were used as calibrants for the XRD sample-detector geometry. Calculated XRD patterns were produced using the POWDER CELL program [32], for the corresponding crystal structures assuming continuous Debye rings of uniform intensity. Le Bail refinements were performed using the GSAS software [33]. Indexing of XRD patterns was performed using the DICVOL program [34] as implemented in the FullProf Suite. The X-ray wavelength was $\lambda=0.52\text{Å}$.

RESULTS

Figure 2 shows integrated diffraction patterns of the TATB PBX and SCTATB at selected times after the single detonation front reaches the probing spot ($t=0$). XRD patterns with residual intensity subtraction are shown in Supporting material Fig. S1 [35]. In the case of the PBX, an almost perfect agreement can be observed between the diffraction pattern (noted as pre-shock) of TATB before the detonation front reaches the probing spot and the calculated pattern of TATB [36]. This implies that the grain size of TATB in the PBX is much smaller than the X-ray beamsize (nominally 20 μm X50 μm) and resembles a powder-like TATB specimen, this is further supported by the 2D X-ray diffraction image (see Fig. 2(c)) that exhibits apparent Debye rings of uniform intensity. On the other hand, a normally expected difference can be seen between the observed and calculated pattern in the case of SCTATB. Both the TATB PBX and SCTATB diffraction patterns exhibit a clear pressure induced shift of the most intense TATB peaks, located at 9.29° (002) and at 14.08° (convolution of TATB Bragg reflections, see Fig. S2) as a function of time. It is noteworthy that, as evident by the cake images (Fig. 2(e) and (f)), the morphology of the SCTATB is substantially altered under shock conditions, evolving towards a multigrain morphology with a more uniform diffraction intensity distribution. Interestingly, the main TATB Bragg peaks of both the PBX and the SCTATB can be also observed when the shock pressure releases at later times towards, almost, ambient pressure. Thus, part of the TATB sample remains crystalline during the whole detonation-induced shock event. The absence of any observable phase change of TATB might suggest that the triclinic structure is indeed stable [13, 14] up to molecular breakdown; however, the recently reported monoclinic HP [15] structure is indistinguishable from the triclinic structure in our data. So, TATB can not only withstand the peak pressures and temperatures created by the detonation but also remain stable during the pressure release towards the ambient conditions. This observation is probably related to the fact that TATB is remarkably difficult to shock-initiate. As it is apparent in Fig. 2(a), the intensity of the TATB Bragg peaks under shock conditions is much lower than the ones in the pre-shock pattern. A more detailed analysis, based on the relative integrated intensities of the 002 Bragg peak and the convolution of peaks at ≈14° (ambient conditions), revealed that ≈30% of crystalline TATB remains at 50 ns. It is plausible to assume that the rest 70% of the initial TATB has undergone a chemical transformation towards a non-crystalline state.
is further supported by the clear increase of the broad background (between roughly 7-17°) that resembles the XRD expected for non-crystalline materials (amorphous or liquids/gases). Thus, the recorder XRD pattern represents the superposition of TATB that has undergone a chemical reaction plus approximately 30% of crystalline TATB under pressure in areas of the specimens where TATB crystallites persist.

Figure 3 shows integrated diffraction patterns of SCTATB at selected times after the colliding detonation-driven shock front reaches the probing spot (t=0). XRD patterns without residual intensity subtraction are shown in Fig. S3. Similarly with the conventional detonation, the morphology of SCTATB evolves towards a multigrain morphology under shock conditions. The most intense TATB peaks, at ambient conditions, can be observed up to the maximum pressure achieved using the colliding setup. Thus, TATB remains a crystalline material, even far above the conventional detonation pressures (30-40 GPa).

We determined the corresponding pressures as a function of time by using the known static room temperature (RT) EOSs of TATB [14, 15] i.e. by comparing the d-spacing position of the observed 002 Bragg peak (by far the most intense Bragg peak of TATB) with the expected position at a given pressure according to the previously reported isothermal RT EOSs. More details about the pressure determination are given in Fig. S2. Given that we expect elevated temperatures during the detonation-induced shock compression, the determined pressures correspond to the lower limit of the actual pressures. The results are summarized in Fig.4. In the case of conventional detonation-driven shock compression, for all TATB samples we observe practically the same peak pressure (25-27 GPa) in agreement with what is expected for a lower bound in TATB detonation pressures where the von Neumann spike is estimated to be about 34 GPa and Champman-Jouget is 25-27 GPa [2]. In our measurements t=0 is defined as the time the shock front reaches the X-ray position probing spot, that is nominally the center of the specimen. Thus, the time we observe the peak pressure is mainly defined by the corresponding height of the specimen. Nevertheless, all TATB specimens exhibit similar durations of the shock effect of ≈75-100 ns. Likewise, for colliding-driven shock compression for SCTATB a peak pressure of ≈ 60 GPa is determined with a ≈75-100 ns shock duration.

In addition to TATB-based specimens a LLM-105-based PBX was also examined under the same conditions as with the TATB, under conventional detonation conditions. Integrated diffraction patterns of the LLM-105 PBX, at selected times after the conventional detonation front reaches the probing spot (t=0), are shown in Figure 5. Good agreement can be observed between the diffraction pattern (noted as pre-shock) of this PBX before the detonation front reaches the probing spot and the calculated pattern of LLM-105 [37]. This implies that the grain size of LLM-105 in the PBX is comparable to the X-ray beamsize. In contrast to the case of the TATB PBX the 2D X-ray diffraction image, see inset of Fig.5, reveals the presence of spotty-like Debye rings of non-uniform intensity.

In contrast to the case of the TATB-based specimens, no apparent shock/pressure induced shift of the corresponding Bragg peaks can be observed in the case of
FIG. 5. X-ray diffraction patterns of the LLM-105 PBX under detonation induced, using a CL-20 based PBX, shock conditions at selected times. The calculated pattern of monoclinic LLM-105 [37] at ambient conditions is plotted with red. Times are relative to the detonation front passing through the X-ray beam. The inset 2D X-ray diffraction image in rectangular coordinates (cake) corresponds to the pre-shock pattern of the LLML PBX.

LLM-105. As it can be clearly seen in Fig. 5, at times later than t=25 ns the patterns are indicative of a superposition of the most intense Bragg peaks of LLM-105 (presumably as a residual from earlier times) and a broad feature that signals the lack of long-range order.

DISCUSSION

TATB, as opposed to LLM-105, exhibits diffraction behavior that is not consistent with prompt decomposition. We consider two scenarios to explain the difference between LLM-105 and TATB-based specimens with respect to the structural behavior under detonation conditions. First, the crystal structure of LLM-105 might not be as resilient under detonation-driven thermodynamic conditions, in contrast to TATB. This corroborates with the fact that TATB is more insensitive under shock conditions than LLM-105, although LLM-105 is also a candidate insensitive HE. The implications of the observed compressibility of TATB crystallites and associated implications are discussed further below. An alternate explanation might be due to the unique XRD pattern of TATB that is dominated by the very intense 002 peak. This peak can be easily traced under pressure given that the intensity of the Bragg peaks at higher angles than the 002 have, at least, an order of magnitude lower intensity. In contrast, the XRD pattern of LLM-105 consists of closely spaced peaks of similar intensity. In other words, in the case of LLM-105 the position under high-pressure of a given Bragg peak might coincide with the 2θ position of the next Bragg peak at ambient conditions. Due to the relatively large energy width of the incident X-ray beam, a definite conclusion about the validity of each scenario is difficult without excluding the possibility of a synergy (i.e., higher resilience of TATB over LLM-105 together with experimental limitations) between the two scenarios. Additional measurements are needed, preferably with an almost monochromatic incident X-ray beam, to completely elucidate this issue. Moreover, a more planar detonation drive would reduce the time smearing caused by the shock front curvature in our experiments.

Given that TATB and LLM-105 exhibit, practically, the same elastic parameters \( B_0 = 15 \text{ GPa}, \quad B' = 9 \) for LLM-105 [38] and \( B_0 = 17 \text{ GPa}, \quad B' = 8 \) for TATB [13] the higher insensitivity of TATB over LLM-105 could not be attribute to a difference in compressibilities. On the other hand, TATB adopts a layered 2D graphite-like crystal structure as opposed to, at some extent, a 3D one in case of LLM-105 or other HEs. For this reason, under static compression, TATB exhibits low intralayer incompressibility \((a \text{ and } b \text{ axes})\) while the interlayer compressibility is large, resembling the one of graphite [14, 15, 39]. According to our study, the lattice parameters of TATB under detonation-induced shock conditions follow the same trend, see Fig. S2, with the case of static compression [39]. Thus, a plausible explanation for the insensitivity of TATB is that pressure cannot effectively affect the distance of the molecules inside the layers (and thus, trigger chemical reactions) while the pressure can be “absorbed” by the decrease of the interlayer distance that does not substantially affect the intermolecular distance in the short range order level.

As mentioned in the results section, in the case of the TATB PBX only \( \approx 30\% \) of crystalline TATB is observed under detonation-induced shock conditions. This could be attributed to a highly heterogeneous shock reactivity in the TATB PBX that proceeds according to the “hot spot” mechanism [40, 42], where behind the leading edge of the shock, shrinking compressed crystalline TATB regions would coexist with growing regions of reaction products. This is what normally one would expect in a polycrystalline, see 2D images in Fig. 2(a), polymer bonded material. As discussed in the experimental section, persistence in the scintillators of detector system may be responsible for the ambient peaks that persist; we cannot discount the possibility that a small contribution to this ambient set of peaks arises at the cylinder edges, were a discontinuity in pressure exists, and the detonation may be releasing a small amount of undetonated
material on these timescales. (See also Figs. S1 and S3.) It is noteworthy, that the evolution of SCTATB, in both conventional and colliding detonation setup, under shock conditions from single crystal to a multigrain morphology is also consistent with heterogenous reactivity.

Interestingly, the observation of the 30% remaining TATB under shock conditions is also in agreement with the basic principle of the Zel’dovitch-von Neumann-Doering (ZND) theory for detonation \[43\]. In this context, the 30% of the observed TATB under pressure could represent the material at and immediately behind the thin von Neumann spike shock wave that compresses the explosive to a high pressure yet instantaneously, much of the explosive remains unreacted. The measurement might then be the first direct measurement of decomposing TATB crystallites, sufficient to exhibit compressed 002 diffraction peak, that persist in the long reaction zone relative to other explosives \[2, 44\]. Given that in our experimental setup the incident X-rays are orthogonal to the curved shock front \[25, 26\], we do simultaneously probe a superposition of various states through the thin shock front and the reaction zone, but also note that we observe pressure decreasing as the TATB continues to decompose (Fig. 2) and essentially complete decomposition at very late times (Fig. 6). The remaining 70% of the TATB that does not contribute to the pressurized 002 peak is material that has decomposed and/or rubberized sufficiently small to no longer produce meaningful diffraction.

Now we turn our attention to the broad feature observed in the patterns of both TATB and LLM-105 that signals the lack of long-range order. Although a detailed analysis on the origin and the characteristics (e.g. structural factor) of this feature is beyond the scope of this paper, it is plausible to attribute this broad feature to XRD originating from non-crystalline states. This is probably formed from the HE that has undergone a shock-induced chemical transformation under detonation-like conditions towards non-crystalline detonation reaction products. Fig. 6 shows XRD pattern of the TATB and LLM-105 PBX specimens at later times than the ones considered for detonation-induced shock compression. It is noteworthy that for both the TATB and LLM-105 the $2\theta$ position of the maximum of this feature shifts towards lower angles (higher $d$-spacings) with time. This is probably due to the pressure release and the consequent increase of the interatomic/intermolecular distances. In the case of LLM-105, the absence of a crystalline XRD pattern at earlier times than TATB, under basically identical shock conditions, suggests a faster reactivity and is consistent with a shorter reaction zone in LLM-105.

FIG. 6. XRD patterns of TATB and LLM-105 under detonation induced, using a CL-20 based PBX, shock conditions at selected times. Times are relative to the detonation front passing through the X-ray beam.

**CONCLUSION**

The structural evolution of TATB was studied under detonation-induced shock conditions using in-situ synchrotron X-ray diffraction in the 100 ns timescale up to 60+ GPa. The results indicate that a portion of the TATB remains stable up to the highest pressure of this study. Moreover, under moderate shock pressure (<35 GPa) the crystal structure of TATB also remains stable during pressure release. In contrast to the TATB, in the case of LLM-105 a similar structural behavior was not observed and this can be attributed either to the vast insensitivity of TATB and/or to experimental limitations relevant to the energy width of the incident X-ray beam and the characteristics of the corresponding XRD patterns. Our findings highlight differences between TATB and other explosives (LLM-105 presented herein) may give insight into the extreme insensitivity
TATB, under detonation conditions, exhibits diffraction peak shifting which may indicate a relatively unique response.

This work was performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Security, LLC under Contract DE-AC52-07NA27344. We gratefully acknowledge the LLNL LDRD program for funding support of this project under 18-SI-004. We thank Ben Yancey for the Laue measurements on the SC TATB samples. The Dynamic Compression Section at the Advanced Photon Source is managed by Washington State University and funded by the National Nuclear Security Administration of the U.S. Department of Energy under Cooperative Agreement No. DE-NA0002442. Supporting experiments and data were also performed at 32-ID-B at APS. This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

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Supplemental Material for “Structural study of TATB under detonation-induced shock conditions”
FIG. S1. X-ray diffraction patterns, after residual intensity subtraction, of a) the TATB PBX and b) SCTATB under detonation-induced shock compression, using a CL-20 based PBX booster, at selected times. The calculated pattern of triclinic TATB at ambient conditions is plotted with red. The vertical dashed line indicates the position of the most intense 002 Bragg peak of TATB at ambient conditions. The static patterns in a) and b) are scaled by /5 and X5, respectively for clarity. Times are relative to the detonation front passing through the X-ray beam. The X-ray wavelength is $\lambda = 0.52\text{Å}$. 2D X-ray diffraction images in rectangular coordinates (cake) below the patterns correspond to the static (left) and under shocked condition (right) diffraction patterns of the TATB PBX and SCTATB, respectively.
FIG. S2. X-ray diffraction pattern of the TATB PBX at 50ns (black) in comparison to the calculated pattern of TATB at 21 GPa (red) using the published EOS in Refs. [14] and [15]. The procedure for pressure determination is as follows: from the most intense Bragg peak of the experimental pattern (002 of TATB) the value of the c-axis of TATB is determined. The pressure is determined as the pressure in which the same value of the c-axis was reported under RT static compression as reported in previous DAC studies [14, 15]. The broad feature at \( \approx 15^\circ \) (\( \approx 14^\circ \) at ambient conditions) is the convolution of 6 Bragg peaks (noted in the figure) of similar intensity (9-10.5% of the 002). Thus, the pressure can not be unequivocally determined from this peak. However, using the corresponding lattice parameters at the pressure determined through the 002 peak, the calculated/expected position of this feature is in agreement with the observed position. Thus, it is plausible to suggest that the pressure evolution of the lattice parameters of TATB under detonation-induced shock conditions, follows the same trend with the one under static compression.
FIG. S3. X-ray diffraction patterns of SCTATB, after residual intensity subtraction, under detonation-induced shock compression, using a CL-20 based PBX in colliding arrangement, at selected times. The calculated pattern of triclinic TATB at ambient conditions is plotted with red. The vertical dashed line indicates the position of the most intense 002 Bragg peak of TATB at ambient conditions. The static pattern is scaled by X5 for clarity. Times are relative to the detonation front passing through the X-ray beam. The X-ray wavelength is $\lambda=0.52 \text{Å}$. 2D X-ray diffraction images in rectangular coordinates (cake) at the right of the patterns correspond to the static and under shocked condition diffraction patterns SC-TATB, respectively.