



X-Ray Diffraction Studies of L-Isoleucine Under Shocked Conditions

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Abstract

One of the most important industrial requirements is to find the materials which have the tendency to withstand harsh environments, such as high pressure, high temperature, and radiation environments, so that they will maintain high efficiency in these conditions. Such materials are greatly required for aerospace, defense, and high-temperature molecular device fabrications. In the present context, we have chosen L-isoleucine samples to assess the crystallographic phase stability under dynamic shocked conditions. The stability result has been screened by a powder x-ray diffractometer (PXRD). Based on the observed diffraction results, it is well evidenced by the cleavage planes, such as (002) (003), (004), (005), and (006), that the applied shock waves do not induce any crystallographic phase transitions and lattice deformations even at 200 shocks. The unit cell dimensions of the L-isoleucine sample were $a = 9.752 \text{ \AA}$, $b = 5.321 \text{ \AA}$, $c = 14.13 \text{ \AA}$ and $V = 728 \text{ \AA}^3$ which were found to be the same under all numbers of shocked conditions. Hence, the L-isoleucine sample is strongly suggested for device fabrication, and previous static high-pressure experimental results also support this suggestion.

Keywords Shock waves · amino acids · L-isoleucine · phase stability

Introduction

Research on materials imploded with shock waves has become nascent, and is set to revolutionize the way prominent materials are being looked at, in terms of their efficiency when it comes to harsh environments, where the materials are prone to encounter high pressure and temperature, so that highly stable materials can be obtained for the technology of today and tomorrow. As is known, organic

and inorganic materials should be studied meticulously so that a certain level of understanding about their structural and phase stabilities in high-pressure and high-temperature conditions can be accomplished. However, compared to inorganic materials, organic materials are highly sensitive to high-pressure and high-temperature conditions and hence the research on organic materials in high-pressure conditions has been highly active in recent times. Experimentation on pressure-dependent crystallographic phase stability assessments of amino acid crystals is one of the stand-out research topics, such that many investigations have been performed in the last two decades. Based on the high-pressure experimental results, it is known that a majority of amino acid materials are prone to undergo conformational changes, such as crystallographic phase changes in high-pressure regions, wherein the observed phase transitions vary with respect to the tested specimens.^{1–3} Moreover, the most familiar and technologically important amino acids, such as L-alanine and L-threonine materials, exhibit amorphization under high-pressure and high-energy irradiation conditions.^{4,5} Hence, understanding the phase stability of amino acids is crucial at high pressure, high temperature, and low temperature, as well as high-energy irradiation conditions. On the one hand, high-pressure experiments have provided key information

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about the stability profiles of materials with respect to pressure, and such kind of stability profiles are essential for the molecular crystal device engineers in order to select the right candidate for the required applications.^{6,7} On the other hand, a significant enhancement of research interest is witnessed in high-pressure amino acid materials, which is not only due to the structural stability profiles of materials but has also provided many insights into the origin of organic molecules in the universe systems.⁸ Such kinds of high-pressure experiments, like the diamond anvil cell, laser irradiation, and shock waves, result in the development of new ideas and hypotheses on structural phase transitions and novel material configurations. Nakano et al. performed femtosecond laser irradiation on L-histidine and found an enhancement in the optical absorption due to the nature of the chemical structure.⁹ In addition, such a kind of ultra-fast optical laser irradiation process can produce significant changes in the materials structures and properties.^{10–12}

In the same way, shock waves also provide many insights into understanding the properties of materials and their stability under dynamic high-pressure, as well as high-temperature, conditions which has been one of the leading research topics in recent years. Several research groups are working in this area and significant results have been found for materials on the impact of shock waves.^{13,14} Compared to the available experimental results of static high-pressure compression, the phase stability of 99% of materials and the changes occurring in the physical–chemical properties under shocked conditions are yet to be revealed. In recent years, there have been a good number of researchers who have taken up this problem and started making considerable contributions to the exploration of shock wave interaction with materials. According to the literature, studies on the impact of shock waves on hydrogen-bonded materials are less compared to pure metals and metal compounds.^{15,16} Also, there are only a very few reports available, especially on amino acid materials such as L-leucine and L-aspergene under shocked conditions utilizing the shock waves generated from a tabletop pressure-driven shock tube.^{17,18} In recent years, a few research groups have come up with a revelations of technologically important hydrogen-bonded systems, such as ammonium dihydrogen phosphate,¹⁹ potassium dihydrogen phosphate (KDP),²⁰ propyl *p*-hydroxybenzoate,²¹ and ammonium pentaborate hexahydrate single,²² with the samples examined under shocked conditions, bringing about significant changes in their physical properties, such as structural, optical, electrical, and thermal.^{19–22} It should be noted that these materials possess second harmonic generation capability so they are used in microelectronics, optoelectronics, and high-power laser applications. Moreover, under shocked conditions, amino acid materials may undergo conformational phase transitions that lead to them acquiring different functional properties. For example, L-leucine

undergoes a transition from leucine(I) to leucine(II) in the 50-shocked condition, whereas leucine(II) remains stable up to the 150-shocked condition.¹⁸ However, L-aspergene experiences only structural deformation rather than structural transitions under shocked conditions.¹⁷ Hence, the assessment of the phase stability of materials is required for molecular device fabrications and, generally, materials possessing a stable crystal structure and properties are suggested for device applications. If a material has very good nonlinear efficiency and undergoes structural deformations as well as phase transitions, the efficiency of the harmonic generation will be greatly affected. Hence, in the present context, the L-isoleucine sample has been chosen to assess shock wave-induced phase stability because it is one of the potential nonlinear optical (NLO) materials belonging to the hydrogen-bonded family.^{19–22}

Furthermore, at this point, it is worth mentioning that the information required to understand the molecule chirality of amino acids under shocked conditions has not yet been well explored. Moreover, the molecule chirality plays a major role in the physical and chemical properties of amino acids, and this chirality can be changed under shocked conditions. Note that, during static compression studies, several results have been observed involving conformational phase changes. Due to this sensitivity, several conformational phase changes and structural phases have been observed under high-pressure conditions.^{23,24} The L-isoleucine sample has several polymorphic phases, such as L-isoleucine, D-isoleucine, and D L-isoleucine,²⁵ and, furthermore, L-isoleucine crystallizes into two crystallographic phases, the monoclinic ($P2_1$) and the orthorhombic ($P222_1$).^{23,24,26,27} The monoclinic L-isoleucine is considered as the room-temperature phase. Several publications are available for the $P2_1$ phase of L-isoleucine under high-pressure and low-temperature conditions. Gorbrrz et al. demonstrated the distorted $P2_1$ phase ($P2_1$ -II) at 120 K with the lattice dimensions, $a = 9.681 \text{ \AA}$, $b = 5.301 \text{ \AA}$, $c = 13.956 \text{ \AA}$, and $V = 712 \text{ \AA}^3$.²⁸ Almeida et al. also carried out a similar experiment ranging from 17 K to 290 K and found a few conformational phase changes.²⁴ Sabino et al. performed a high-pressure phase stability experiment of $P2_1$ L-isoleucine up to 7.3 GPa and found a few slight modifications reflected in their Raman bands. However, no evidence was noticed in the signature of the crystallographic phase transitions or amorphization in high-pressure regions.²⁹ More recently, Rego et al. demonstrated the crystallographic phase stability of D L-isoleucine in a high-pressure environment up to 17.3 GPa and found two phase transitions.²³ As per the static high-pressure experiential results, the test sample is a highly deserving candidate for shock wave recovery experiments.

In this framework, we have performed an investigation on the systematic crystallographic phase stability and morphology facets stability of L-isoleucine under shocked conditions,

and the respective results have been evaluated by the x-ray diffraction (XRD) technique. Surprisingly, the test samples have not undergone any of the crystallographic phases and conformational phase changes as well as lattice deformations under shocked conditions, and the interesting aspects of the high shock resistance tendency of the L-isoleucine samples are discussed in the following sections.

Experimental

The L-isoleucine powder sample (purity, 99.99 %) was purchased commercially (Sigma Aldrich) and used for the assessment of crystallographic phase stability under shocked conditions. Prior to the loading of dynamic shock waves on the samples, the test sample was subjected to a gentle grinding process using a mortar. After the grinding process, the test samples were subdivided into five samples of equal parts and one sample was kept as the control while the remaining four samples have been exploited for the studies on crystallographic phase stability under shocked conditions. In the present investigation, shock waves of Mach number 2.2 were chosen which have a transient pressure and temperature of 2.0 MPa and 864 K, respectively, and were generated by an in-house-developed semi-automatic pressure-driven shock tube (Fig. S1). Subsequently, 50, 100, 150, and 200 shock pulses were loaded on the four test samples in a sequential order. The working methodology of the pressure-driven shock tube and shock wave-loading procedure have been discussed in our previous publications.^{30,31} After the shock wave loadings, the control and shocked samples were sent for diffraction and microscopic studies.

Results and Discussion

Structural Properties

A powder x-ray diffractometer was employed for the assessment of the crystallographic phase stability of the L-isoleucine samples, since both the phases $P2_1$ and $P222_1$ have the possibility to exist in ambient conditions. For better clarification, we have compared the XRD pattern of the control L-isoleucine powder with the XRD pattern of the simulated $P2_1$ L-isoleucine (CCDC: 1207696), and the corresponding XRD patterns are presented in Fig. 1. As seen in the XRD patterns in Fig. 1, the control sample's diffraction peaks were found to be well-matched with the simulated $P2_1$. Hence, it is confirmed that the control sample has a monoclinic structure with the $P2_1$ space group symmetry.

According to the literature, the cell parameters of $P2_1$ L-isoleucine are $a = 9.75 \text{ \AA}$, $b = 5.321 \text{ \AA}$, $c = 14.12 \text{ \AA}$, $V = 728 \text{ \AA}^3$, and $\beta = 96.160^\circ$. The L-isoleucine is packed

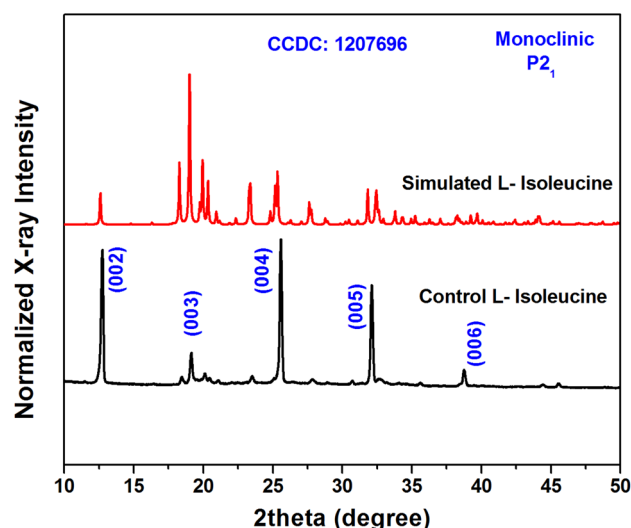


Fig. 1 XRD patterns of the control and simulated L-isoleucine samples.

with four molecules with two bimolecular asymmetric (confirmations) in the unit cell. Moreover, among the four units, two of these isoleucine molecules have one conformation angle whereas the other units have different conformation angles. Both the independent molecules in the asymmetric unit (A and B) have the ability to rotate about their two chiral centers, C_α and C_β , with gauche I (A -unit) and trans-rotation (B -unit), respectively, which results in different atomic R group positions in the unit cell, atomic bond lengths, and angle conformations. The asymmetric units of the isoleucine molecules and the respective crystal packing are presented in Fig. 2.

Figure 3 presents the control and shocked L-isoleucine's XRD patterns, from which it can be seen that the control sample has diffraction patterns of the (002), (003), (004), (005), and (006) planes, and that, from these planes, it is very clear that the test samples have prominent faces only along the c -axis which is the growth habit of the test sample.^{32,33}

In the case of the crystallographic phase stability analysis of the materials under shocked conditions or any other high-energy irradiation conditions, one can see three major changes: (1) diffraction peak shift of either lower angle or higher angle, (2) changes in XRD peak intensity, and (3) XRD peak disappearance and appearance. Changes occurring in these three parameters and their characteristics (both quantity and quality) must be taken into account prior to declaring the conclusion of the shock-resistant behavior of the test specimen. As seen in Fig. 3, these points are very clear, such that, based on this, the results of the observed XRD patterns under shocked conditions can be declared. The first point is that, as reflected in Fig. 3, none of the crystalline peaks undergo remarkable peak shifts under

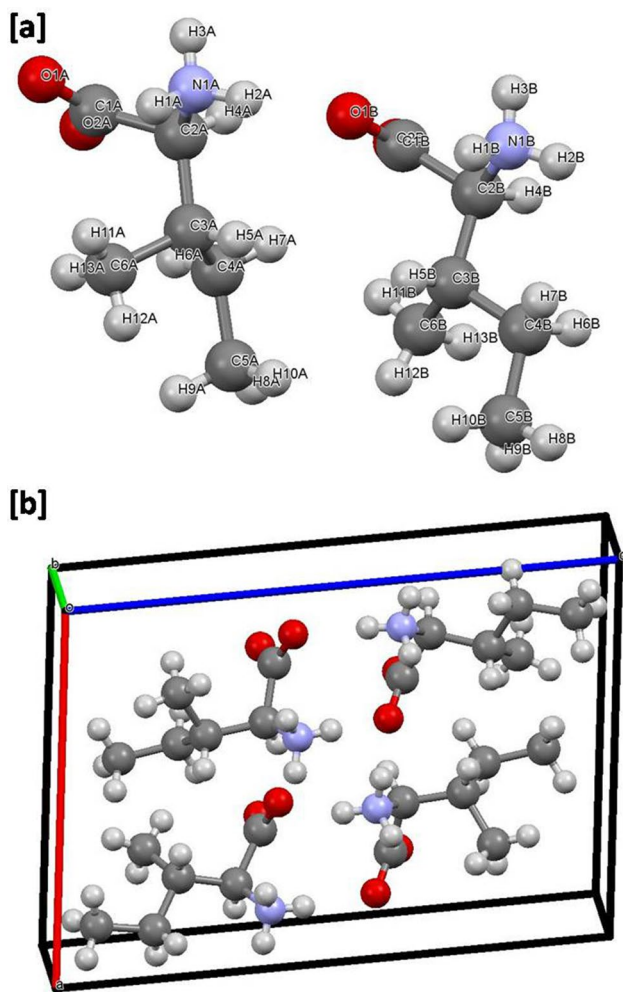


Fig. 2 (a) Asymmetric units and (b) crystal packing of L-isoleucine molecules.

shocked conditions. The second point is that none of the diffraction peaks loses its original x-ray intensity even at the 200-shocked condition. All the diffraction peaks, such as the (002), (003), (004), (005), and (006), hold the original diffraction positions and original intensity under shocked conditions. The third point is that none of the diffraction peaks disappear, nor do new peaks appear, while under shocked conditions. These three points are quite sufficient to declare the high-stability performance of the test samples against the impact of shock waves. As seen by the naked eye, no significant changes in terms of diffraction peak shift, peak intensity and peak appearance and disappearance are observed. It is thus suggested that the L-isoleucine sample is one of the highly shock-resistant materials among hydrogen-bonded materials. In order to justify the implication, the XRD patterns of the control and shocked KDP samples are provided in Fig. 3b, from which it can be seen that the three changes are highly visible at just 100 shocks. In the case of the KDP sample, several diffraction peaks disappear and reappear under shocked conditions, while the XRD peak intensity is significantly altered with respect to the number of shock pulses.³⁴ Hence, it is authentically evidenced that the L-isoleucine has a high shock-resistant behavior compared to the most important technological NLO material of the KDP samples.³⁴ For better clarification of the claim, the zoomed-in versions of the XRD patterns are displayed in Figs. 4 and 5. As seen in Fig. 4a and b, diffraction patterns of the control and shocked samples are presented, i.e., the (002) and (003) planes, respectively.

Even in the zoomed-in versions, no significant change is observed in the diffraction peak profiles, unlike in the KDP samples. In the case of 150 shocks, the (002) plane shows a slight peak broadening compared to the other shock-loaded

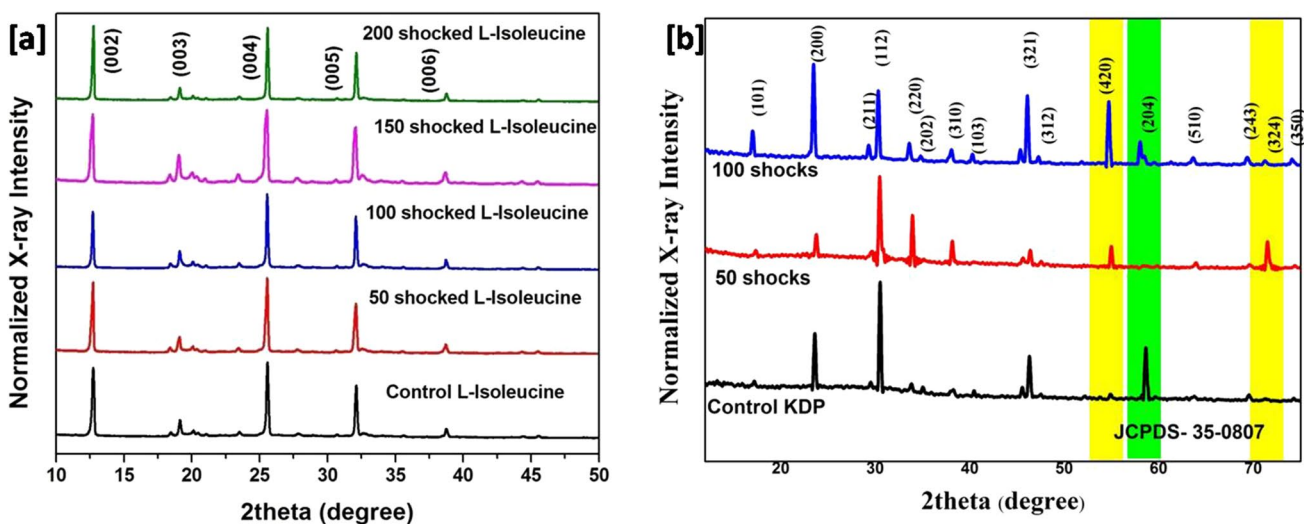


Fig. 3 (a) PXRD patterns of the control and shocked L-isoleucine samples; (b) XRD pattern of potassium dihydrogen phosphate (KDP) sample adopted with permission from Ref. 34.

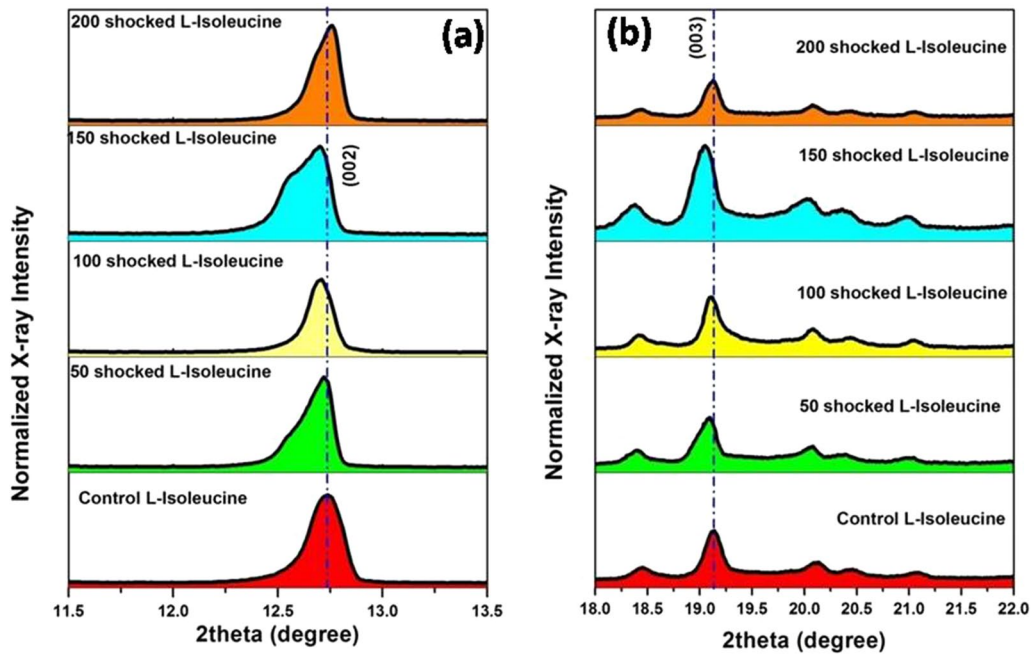


Fig. 4 Zoomed-in PXRD patterns of the control and shocked L-isoleucine samples: (a) 11.5–13.5°, and (b) 18–22°.

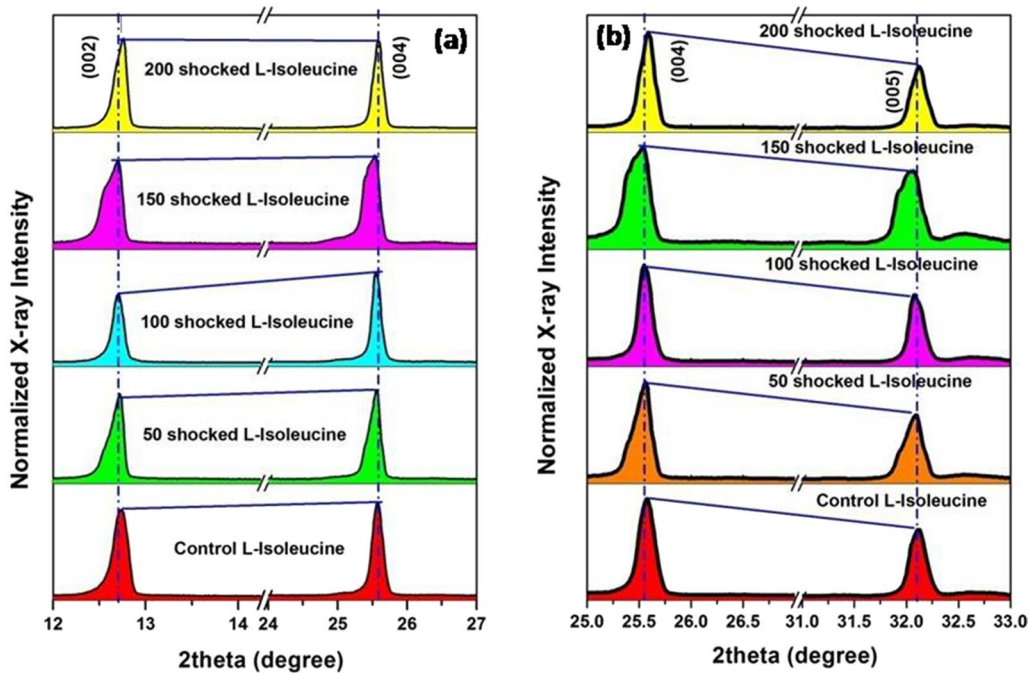


Fig. 5 Zoomed-in PXRD patterns of the control and shocked L-isoleucine samples: (a) 12–27°, and (b) 25–33° (Color figure online).

conditions. On the other hand, in the case of the (003) plane at 150 shocks, the x-ray peak intensity has slightly increased compared to the other shocked conditions. However, other than these slight changes, a few minute changes are observed which is quite common under shocked conditions.

Furthermore, the diffraction peak profiles of the (004) and (005) in shocked conditions are portrayed in Fig. 5a and b. There is no change observed, such as peak shifting, peak disappearance, and intensity changes, even at the 200-shocks condition. Furthermore, it is imperative to

provide one more important aspect to substantiate the high shock-resistant behavior of the test sample under shocked conditions. In Fig. 5, the comparison of the x-ray peak intensity is made between the two diffraction planes of (002) and (004) as well as (004) and (005). In Fig. 5a and b, the blue line connects the two diffraction peak top edges on which the line length and line angle do not significantly vary under shocked conditions. In Fig. 5a, at 100 shocks, a slight bending is observed for the line. However, it is identified to be not worthy enough to be considered as a significant change under shocked conditions. Figure 5b also shows no change in the line length and line angle connecting the two diffraction peak edges for the control and shocked conditions. It is one of the non-debatable proofs for considering the claims in the present experiment.

The L-isoleucine (002) and the KDP (200) samples have the most prominent crystal faces as the prismatic facets. Hence, the XRD patterns of the L-isoleucine as well as the KDP samples are provided, and the zoomed-in prismatic facet diffraction peak profiles are depicted in Fig. 6 for the control and shocked conditions. As seen in Fig. 6a, the nature of the (002) diffraction peak in terms of peak shifting and peak intensity is not much altered. However in the case of the KDP samples, peak shifting and peak intensity changes are observed with respect to the number of shock pulses. Moreover, even at the exposure of 100 shocks, the KDP samples exhibit significant changes in their crystal lattice and the changes are highly

visible. However, in the case of L-isoleucine, such kinds of changes are not observed even at the 200-shocks condition.

However, now the interesting questions are why L-isoleucine has a higher shock-resistant behavior than that of the KDP sample, and what are the special characteristics of L-isoleucine that lead to such a high shock-resistance tendency? When the possible reasons are analyzed for this behavior of L-isoleucine under shocked conditions, in fact, as per the crystal lattice configuration of the L-isoleucine, the *c*-axis is much higher than the other two axes, and is highly favorable for achieving the lattice compression which could be seen in the diffraction peak shifts. However, there is no such significant change observed in the L-isoleucine lattice configurations even in the 200-shock pulse-loaded condition. Furthermore, the values of the lattice parameters have been calculated using the UNITCELL program and the obtained values are presented in Fig. 7. The values clearly show that the initial axis lengths are not altered under shocked conditions, which provides a good justification for the generalization. In the case of L-isoleucine, the existence of strong interactions between the amino group (NH_3^+) and the carboxylic group COO^- is very well established.

In Fig. 8, the hydrogen bond network of the L-isoleucine unit cell is presented to draw more convincing reasons behind the high shock-resistant behavior. L-isoleucine contains 2A and 2B molecules in the unit cell, both of which are present in the zwitterionic form, and each isoleucine molecule has different torsion angles. As mentioned earlier, molecule A has a gauche configuration around $\text{C}\alpha\text{-C}\beta$ and

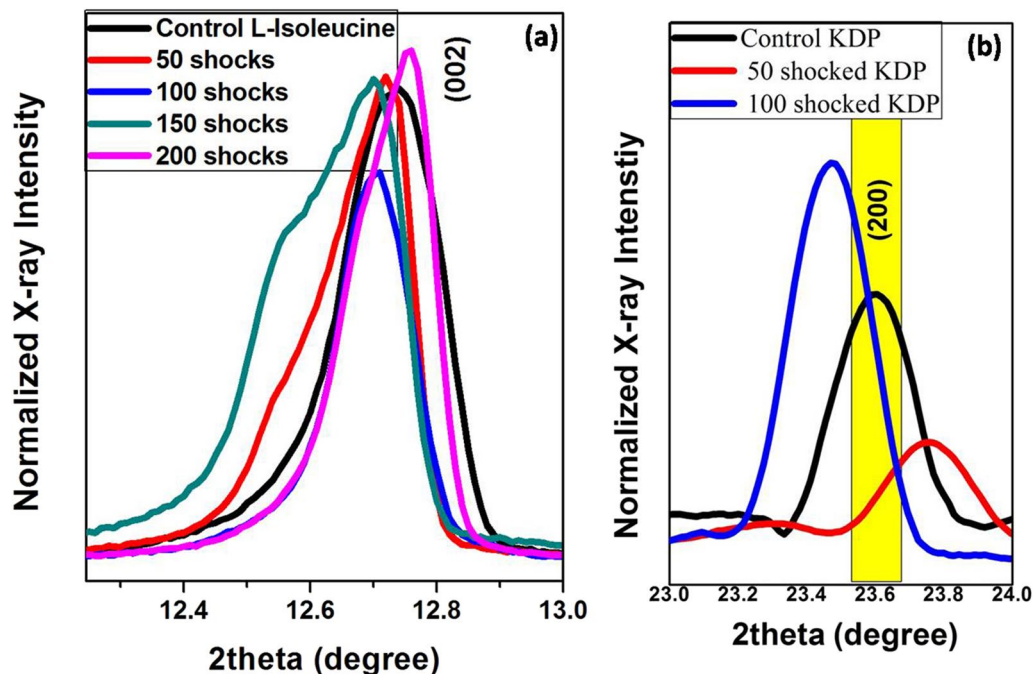


Fig. 6 The zoomed-in prismatic face XRD patterns of the control and shocked samples: (a) L-isoleucine, (b) KDP.

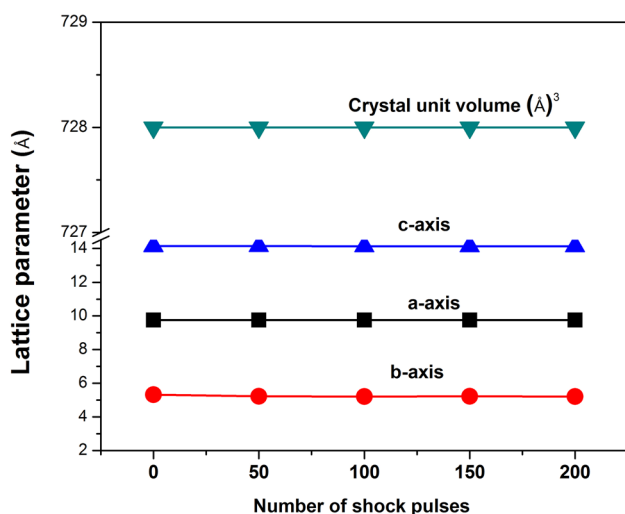


Fig. 7 Lattice parameter values of the control and shocked L-isoleucine samples.

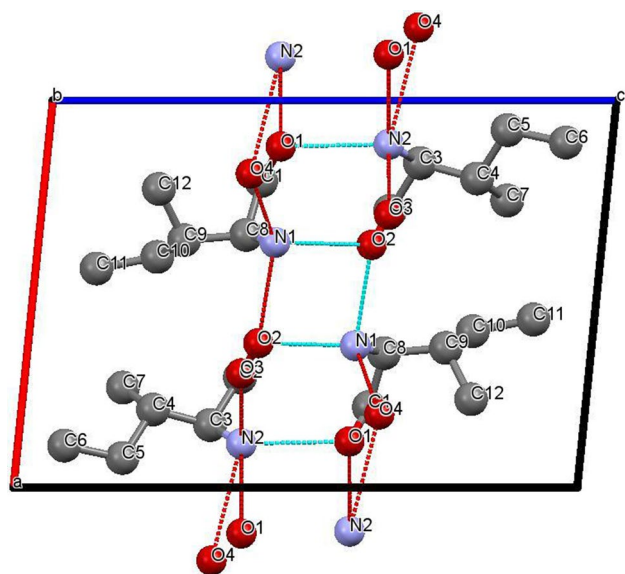


Fig. 8 Hydrogen bond pattern of L-isoleucine unit cell (projection along *c*-axis).

molecule *B* has the *trans* configuration. As seen in Fig. 8, the *A* and *B* isoleucine molecules are interlinked by $N\cdots H\cdots O$ along the *a*-axis, which raises the double layers of molecules, while the molecules are connected along the *c*-axis by weak van der Waals forces.

As seen in Fig. 8, the unit cell has four strong hydrogen bonds along the *c*-axis in which only two strong hydrogen bonds are found to be linked with the unit cells along the *a*-axis. Moreover, the growth rate of the *a*-axis is more rapid than that of the *c*-axis. Hence, the crystal structure of L-isoleucine has a large (001) face with some elongation

along the *a*-axis.^{32,33} Hence, the primary crystal growth direction is the *c*-axis, and this is the prime reason for receiving only the (002), (003), (004), (005) and (006) diffraction planes in the XRD pattern. The formation of hydrogen bonds leads to the strongest intermolecular forces as well as the most efficient atomic packing in the unit cell along the *c*-axis, since the presence of hydrogen bonds along the *a*-axis is much stronger than the van der Waals forces found along the *c*-axis. Hence, the hydrogen bonds present in the *c*- and *a*-axes hold the fulcrum to maintain the entire crystallographic structural stability of L-isoleucine under shocked conditions, which may be the prime reason for the existence of such a high shock-resistant behavior of the L-isoleucine. Due to the outstanding crystallographic phase stability of the L-isoleucine, it is highly deserved for device fabrication applications which are well consistent with the previous studies on high pressure, as well as the results obtained from shock-loaded conditions.³⁴

Conclusion

In summary, systematic investigation of the crystallographic phase stability and morphological facet stability of L-isoleucine under a wide variety of shocked conditions has been established, and the results have been screened by the XRD technique. Interestingly, the recorded XRD results demonstrate a high shock-resistant behavior even at the 200-shock-loaded condition. The unchangeable diffraction peak intensity, peak position, and quality of the facet under shocked conditions is one of the non-debatable proofs for the claims which corroborate the previous results of high-pressure experiments, that also support the present experiment's conclusion. The hydrogen bonds of *c*- and *a*-axes are the major contributors to the existence of such the high shock-resistant behavior which has been found to be greater than the KDP samples, which are highly prominent for device fabrications involving microelectronic and optoelectronic applications.

Supplementary Information The online version contains supplementary material available at <https://doi.org/10.1007/s11664-023-10873-1>.

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Data Availability The data that support the findings of this study are available from the corresponding author upon reasonable request.

Declarations

Conflict of interest The authors declare that they have no conflict of interest.

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