

Characteristics of neutron beams from deuterated targets irradiated by intense sub-ps lasers

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The generation of energetic neutron beams by $d(d, n)^3\text{He}$ reactions during the interaction of an intense laser with micron-thick deuterated plastic targets is investigated through two-dimensional particle-in-cell simulations equipped with nuclear reaction formalism. The capability of modeling neutron generation along with laser-plasma interaction enables us to identify and quantify multiple distinct and competing regimes of neutron production happening concurrently at the laser irradiated target. The high-energy neutrons are seen to be produced by two different mechanisms of ion acceleration in thick targets, namely, hole boring radiation pressure occurring inside the target bulk and target normal sheath acceleration that occurs on the rear surface of the target. These two regimes contribute two distinctly different components to the final neutron spectrum. Further a narrow-band (2–3 MeV), quasi-isotropic neutron production of significant flux is also seen during the interaction due to shocklike features seeded inside the bulk target plasma by the fast expansion of contaminant species from the target's front and rear surfaces. While the peak neutron energy is found to saturate at high laser intensities, the integrated flux continues to scale favorably.

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I. INTRODUCTION

The interaction of short [subpicosecond (sub-ps)], intense ($I_0 > 10^{18} \text{ W/cm}^2$) laser pulses with micron-thick solid targets is known to be an efficient source of MeV-scale ions via the target normal sheath acceleration (TNSA) mechanism [1]. This is by far the most studied mechanism of ion acceleration using high-power lasers and produces ions with a characteristic Maxwell-Boltzmann-like exponential spectrum, with a sharp cutoff energy that scales nominally with the laser's intensity; $E_{\text{max}} \propto \sqrt{I_0}$ [2,3], where I_0 is the peak intensity of the laser pulse. Another significant mechanism taking place in these interactions is hole boring (HB) acceleration [4,5], in which the radiation pressure of the laser accelerates ions from the front surface into the target. Compared to TNSA, the HB mechanism offers a more favorable scaling of the ion energy with intensity, $E_{\text{max}} \propto I_0/\rho c^3$, where ρ is the mass density of the target and c is the speed of light in vacuum. However, this process requires low target densities in order to produce ion energies comparable to what can be achieved with TNSA for similar laser parameters. For this reason, currently available lasers ($I_0 \sim 10^{20}\text{--}10^{21} \text{ W/cm}^2$) irradiating solid-density targets produce ions via HB having only a few MeV/nucleon energies, although the spectra produced are typically more narrow band [6], as opposed to the exponentially decaying spectra exhibited by TNSA.

With TNSA producing protons with cutoffs at multiple tens of MeV energies [7,8], it has been used in the past successfully to seed nuclear reactions for the production of secondary particles, most commonly neutrons. Neutron beams are of interest in view of applications such as neutron imaging [9], nuclear transmutation [10], and boron neutron capture therapy for the treatment of tumors [11]. Typically, these neutron beams have been generated from the laser-produced protons and deuterons impinging onto a low Z converter target placed close by (in the so-called pitcher-catcher configuration). Beamed neutron fluxes of the order of 10^{10} n/sr have been measured employing this scheme in different experiments [12–15]. This configuration has also been employed, using beryllium catchers, in applications of laser-driven neutron sources for single-shot radiography and nuclear resonance spectroscopy [9,16–18]. While TNSA offers preferential acceleration of protons in typical targets containing contaminants, efficient deuteron acceleration has been shown by suppressing hydrocarbon contaminants [19] and accessing regimes of bulk acceleration in deuterated plastic (henceforth referred to as CD) targets [20,21]. In the case of the pitcher target being composed of deuterated plastic, where most hydrogen atoms are replaced by deuterium, the $d(d, n)^3\text{He}$ (D-D) reaction in the target bulk can lead to a significant neutron production [20], whereas the accelerated deuterons from the rear surface can also be deployed in pitcher-catcher scheme [21].

Generating neutrons without using secondary catcher targets works favorably toward development of a high repetition rate source for applications. In the pitcher-only scheme, neutrons are produced due to fusion reactions in the target bulk and in the surrounding plasma. With standard CD foils of several micron thickness, neutron peak energy and flux are reduced in pitcher-only mode compared to the full configuration including the catcher [12]. However, significantly high neutron fluxes (in excess of 10^9 n/sr) without using a catcher

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have been recorded recently by employing ultrathin CD foils having a few-nanometer-thick layer of high- Z material coated onto the rear surface [20]. In this work, the acceleration mechanism known as light sail (LS) radiation pressure acceleration was determined to be the dominant mechanism.

Modeling of these nuclear reactions has typically been limited to Monte Carlo simulations using a simplified seed ion distribution from the pitcher target (either from experimental data or particle-in-cell simulations) impinging onto a catcher target [16,18,21,22]. As a result of this necessary simplification, the complex and multifaceted reaction mechanisms that occur in the pitcher target have been difficult to accurately model. Recently, an algorithm was developed to incorporate nuclear fusion in to the particle-in-cell (PIC) code SMILEI [23–25], enabling simulation of both the laser interaction and the subsequent neutron generation within a single code. In this paper, we present simulations of the interaction of a subpicosecond, petawatt-scale laser pulse with micron-thick CD targets using the Smilei code [23] outfitted with a nuclear fusion algorithm. Multiple mechanisms for neutron production during and after the irradiation are identified, and their relative contributions to the final neutron spectrum are compared. Alongside the well-known roles of the HB and TNSA-driven ions, a significant portion of the total neutron yield results from a slow-moving shock wave. This shock arises within the bulk target plasma due to the rapid expansion of contaminant species from both the front and rear surfaces of the target. The integrated PIC and fusion calculations in the Smilei simulations reproduce the neutron spectrum's exponential profile and the high flux at low energies (under 2.5 MeV) typically observed in experiments. This study marks a crucial initial step toward future investigations that will elucidate the intricate physical interactions involved in laser-driven neutron sources from all types of CD targets, including the ultrathin [20] and near-critical-density [21] targets at multipetawatt facilities. Simulating the interaction for the standard CD foils in the current study indicates that at higher intensities, the neutron cutoff energy and spectrum temperature are predominantly affected by the TNSA mechanism over HB-driven in-target fusion reactions.

The body of this paper is organized as follows. After an overview of the reaction kinetics associated with D-D fusion, fusion reactions simulated by the Smilei code are benchmarked against theoretical models for two test scenarios, viz., deuterons impinging on a stationary CD block and the interaction between two deuteron bunches comoving at different speeds. Thereafter, the interaction of an intense laser with CD foil is simulated using Smilei to study in detail neutron generation alongside ion acceleration. The final section before the conclusion presents the simulation results scaling neutron generation at ultrahigh laser intensities delivered at multipetawatt facilities.

II. REACTION KINEMATICS FOR COPROPAGATING DEUTERONS

The neutron emission energy and angular distribution can be derived from the reaction kinematics through the consideration of energy-momentum conservation. For the pitcher-catcher configuration, where a fast deuteron beam

collides with a stationary deuteron target, the energy of the neutrons E_n is related to their emission angle θ by the equation [12]

$$E_n = \frac{E_d}{8} \left(\sqrt{\cos^2 \theta + 2 + 6Q/E_d + \cos \theta} \right)^2, \quad (1)$$

where E_d and Q are the deuteron energy and the Q value of the reaction, respectively. For the $d(d, n)^3\text{He}$ reaction, the Q value is approximately 3.3 MeV. The limit of the above expression as $E_d \rightarrow 0$ yields the minimum neutron energy that can be emitted in the process, which is 2.45 MeV. A more general relationship can be found between two deuterons of arbitrary velocities by calculating the emission according to Eq. (1) in the rest frame of the slower deuteron and transforming the velocity components of the produced neutron back into the laboratory frame. Considering two deuterons traveling in the same direction in the laboratory frame, colliding with velocities $v_{d1} > v_{d2}$, we can choose an appropriate frame velocity where the second deuteron is at rest, $v_c = v_{d2}$. Thus, in the nonrelativistic limit we find

$$\tan \theta_{\text{lab}} = \frac{v'_n \sin \theta'}{v'_n \cos \theta' + v_c}, \quad (2)$$

$$E_{n\text{lab}} = \frac{m_n}{2} (v_n'^2 + v_c^2 + 2v'_n v_c \cos \theta'), \quad (3)$$

where v'_n and θ' are the neutron velocity and emission angles in the rest frame, calculated from Eq. (1), $E_{n\text{lab}}$ and θ_{lab} are the neutron energy and associated emission angles in the laboratory frame, and m_n is the neutron mass. Solutions to these expressions are shown in Fig. 1, where the y axis represents the energy of the first (faster) deuteron and the energy of the second (slower) deuteron is, in the laboratory frame, zero [Fig. 1(a)], one quarter that of the first deuteron [i.e., half the velocity; Fig. 1(b)], and very close to that of the first deuteron [$0.99E_{d1}$; Fig. 1(c)]. It can be seen that as the deuterons get closer in energy, the width of the neutron emission narrows. Two deuterons of identical energy and direction cannot react, as they are each stationary relative to the other; however, if we take the limit as $E_{d2} \rightarrow E_{d1}$, the kinematics expression for the maximum neutron emission energy along an angle can take on a simpler form:

$$4E_n + 2E_d - 4\sqrt{2E_d E_n} \cos \theta = 3Q, \quad (4)$$

which the plot in Fig. 1(c) closely approximates.

As a first test of SMILEI'S fusion algorithm, two simple simulations were performed. First, a short, dense bunch of monoenergetic (2 MeV) deuterons were propagated into a stationary, 1- μm -thick slab of cold deuterium plasma. The bunch was at a density of $20n_c$, where $n_c = 1.1 \times 10^{21} \text{ cm}^{-3}$ is the critical electron density of a laser with a wavelength of 1.054 μm . The target was at a density of $80n_c$, which is approximately the deuteron density contained in a 1 g/cm³ plastic target with a composition of C₂D₄. This setup is analogous to a low-energy, dense bunch of deuterons accelerated from the front surface of the target via hole boring and propagating into the target bulk.

The results of this simulation are shown in Figs. 2(a)–2(c). Deuteron density is plotted in Figs. 2(a) and 2(b) in blue at two different time points: before the

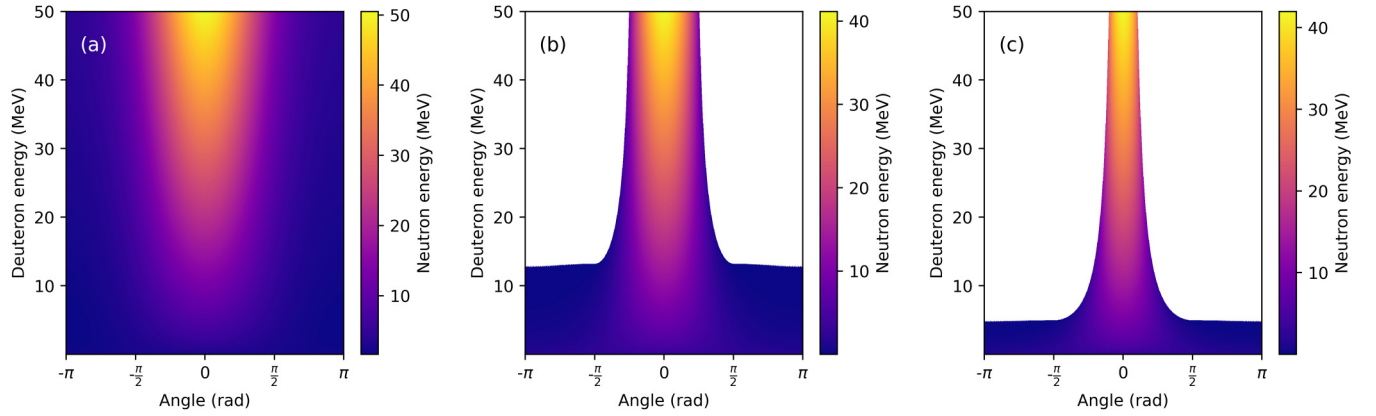


FIG. 1. Theoretical angular distributions of the neutrons emitted from D-D fusion according to the relations given in Eqs. (2) and (3) under three different scenarios. (a) Deuterons impinging on a stationary deuteron target (à la the standard pitcher-catcher arrangement). (b) Deuterons colliding with deuterons with half their velocity (i.e., one quarter of their kinetic energy, all traveling in the same direction). (c) Two deuterons colliding with similar energies and traveling in the same direction. The color scale represents the maximum neutron energy emitted along any particular angle. Note that as the deuterons get closer in energy, the neutron emission narrows for high energies. The lowest neutron energies in these plots tend toward the minimum energy of 2.45 MeV in the center of momentum frame.

collision and immediately after the moving bunch exits the rear side of the target, bringing a stop to the neutron generation. In Fig. 2(b), neutron density is plotted in red, where the neutrons propagate outward ballistically from their creation point.

Figure 2(c) shows the angular distribution of the neutrons emitted from the simulation. The solid black line indicates the analytical result from Eq. (1) for 2 MeV deuterons. As can be seen, there is very good agreement between the simulation and the theory. The somewhat broader distribution of neutron energies for each emission angle is likely due to the broadening of the deuteron beam's spectrum, primarily due to Coulomb interactions, while propagating through the target plasma.

In the second simulation two thin monoenergetic deuteron “sails” collided, one moving at 20 MeV and the other moving at 10 MeV. These sails both had a density of $1n_c$ and were set to collide at $x = 10 \mu\text{m}$. The results of this simulation are shown in Figs. 2(d)–2(f). As before, snapshots of the particle densities are shown just before and just after the collision in Figs. 2(d) and 2(e), respectively. The angular distribution of the neutrons emitted shown in Fig. 2(f), with the black line representing the analytically calculated neutron distribution from Eqs. (2) and (3). Again, the theoretical result agrees closely with the simulated neutron emission. Here, the distribution, which is across 2π in the rest frame of the 10 MeV deuteron sail, becomes much more unidirectional when back-transformed to the laboratory frame, with no neutrons emitted backward.

III. PIC RESULTS FOR NEUTRON PRODUCTION FROM LASER IRRADIATED CD FOILS

After the benchmarking simulations of the beam-fusion reaction, simulations were carried out for typical experimental setups, such as the interaction of an intense laser with CD targets. The linearly polarized laser had a wavelength of $1.054 \mu\text{m}$, a Gaussian temporal profile with a duration of 500 fs full width at half maximum (FWHM), and a peak

intensity of $2 \times 10^{20} \text{ W/cm}^2$. It was focused into a Gaussian spot $5 \mu\text{m}$ FWHM onto the front surface of a $4\text{-}\mu\text{m}$ -thick CD target at normal incidence. The target was set at a density of 1 g/cm^3 and was composed of carbon and deuterium in the ratio CD_2 . The bulk deuterium was given a hydrogen impurity of 1%. Hydrocarbon contaminants in the ratio CH_2 were initialized on both the front and rear surfaces, with an electron density of $80n_c$ and thickness of 10 nm. Dynamic ionization was implemented in all simulations. In an effort to reduce the computational load, the effects of laser contrast and the resulting preplasma formation were not considered.

The simulation box was $90 \mu\text{m}$ in x and $40 \mu\text{m}$ in y , with grid cell sizes of 10 and 20 nm, respectively. The simulation was initialized with 40 macroparticles per cell of deuterons and 10 particles each per cell of carbon and protons. This gave the simulation, after ionization, $>10^8$ total macroparticles.

Figure 3 shows the deuteron and neutron beam properties from this simulation. Figures 3(a) and 3(b) show the angular distribution of forward-directed deuterons and neutrons at the end of the simulation, respectively. The angular distribution of the deuterons is somewhat typical of a TNSA-dominated interaction, i.e., no significant spectral peaks and a declining particle number toward the sharp cutoff energy at around 25 MeV/nucleon. The neutron angular distribution largely reflects that of the deuterons; however, the number of neutrons at lower energies ($<5 \text{ MeV}$) is orders of magnitude higher than that of the energies above 5 MeV and appears to reflect two different distributions: a high-density, lower-energy semi-isotropic distribution (in orange and yellow) atop a low-density, higher-energy, forward-directed distribution with a small divergence angle (in purple). Additionally, the neutron spectrum is observed to have a wider divergence than that of the deuterons. The reason for this difference arises from the emission of neutrons from the D-D reaction being isotropic in the center of momentum frame. This results in the beam of neutrons, after transforming back to the laboratory frame, to be broader by some amount. This effect is also evident from the simulations in Fig. 2, which show a broad divergence of

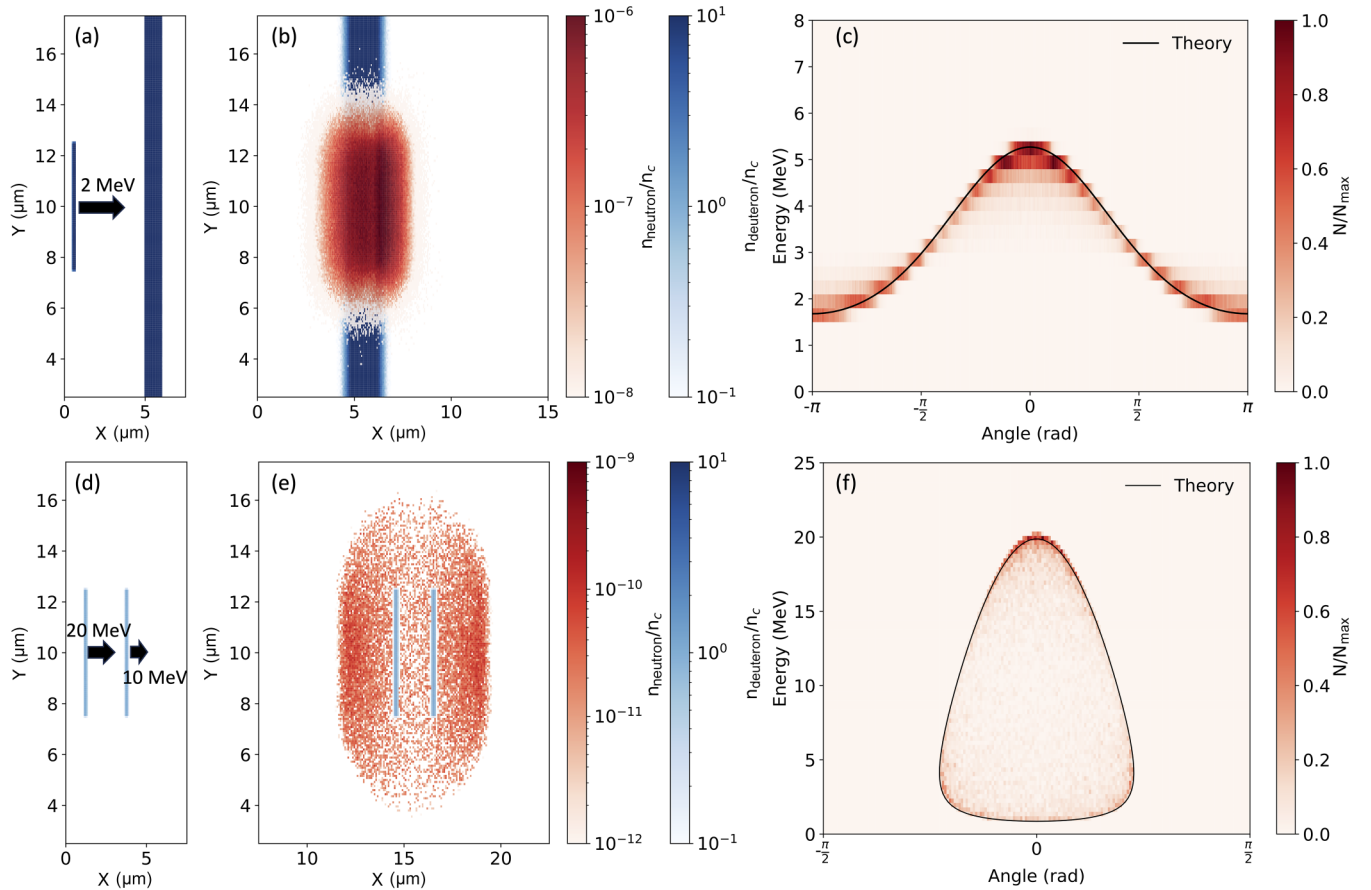


FIG. 2. PIC simulations comparing Smilei's nuclear reaction kinematics with theoretical predictions. (a)–(c) A simple beam-fusion reaction is modeled, where a deuteron bunch of 2 MeV energy impinges into a stationary, 1- μm -thick cold deuteron slab. Snapshots of the density are shown (a) at an early time before the collision and (b) just before the deuteron sail breaks out from the rear of the slab, after which the fusion process is terminated. Deuteron and neutron densities are shown by the blue and red color bars, respectively. (c) The angular distribution of the emitted neutrons. The solid black line corresponds to the analytical results given by Eq. (1) for a 2 MeV deuteron beam. (d)–(f) Two deuteron sails, one with an energy of 10 MeV and another at 20 MeV, collide at $x = 10 \mu\text{m}$. The snapshots of the particle densities just before and just after the collision are shown in (d) and (e), respectively. (f) The angular distribution of the emitted neutrons in this simulation. The solid black line corresponds to the analytical distribution given by Eqs. (2) and (3). All neutrons in this scenario are emitted in the forward direction in the laboratory frame.

neutrons arising from zero divergence deuterons. This effect was discussed in detail previously by Alejo *et al.* [26].

Figure 3(c) shows the x - p_x phase space of deuterons, taken approximately 200 fs after the interaction of the laser pulse peak with the target. The unperturbed target is situated in the region $x = 30$ – $34 \mu\text{m}$. Evident from the deuteron phase space is the occurrence of two distinct regions of forward-accelerating deuterons: the high-energy tail originating from TNSA at the target's rear surface and a bunch of lower-energy deuterons that appear to be originating from the front surface of the target—these are the ions accelerated via the hole boring mechanism [4]. As the plastic target is relatively high density ($\sim 320n_c$), the peak energy of these ions reaches only ~ 1.25 MeV, which is the energy represented by the pink dotted line. The inset in Fig. 3(c) shows a zoomed-in view of the target bulk, highlighting the HB driven deuterons. The red box highlights a backward-propagating component to the deuterons phase space, accelerated via reflection off a

collisionless shock front seeded from the rear surface (discussed further below).

Figure 3(d) represents the x - E phase space of all neutrons produced during the simulation. Since the neutrons propagate only ballistically once created, the x positions on this plot represent the point at which neutrons were created, meaning the color scale corresponds to the relative number of fusion events throughout the simulation when the statistical weight of each macroparticle was taken into account. What is evident from Fig. 3(d) is the presence of two lobes of the highest fusion events, which are aligned with the position of the target bulk, at the energy corresponding to the minimum neutron energy that can be produced in the center of momentum frame (2.45 MeV, red dashed lines). These events are mainly due to thermonuclear fusion between the low-energy (sub-MeV) deuterons residing in the hot, dense plasma of the target, resulting in an isotropic, quasimonoeenergetic emission. Also of note is the void of zero fusion

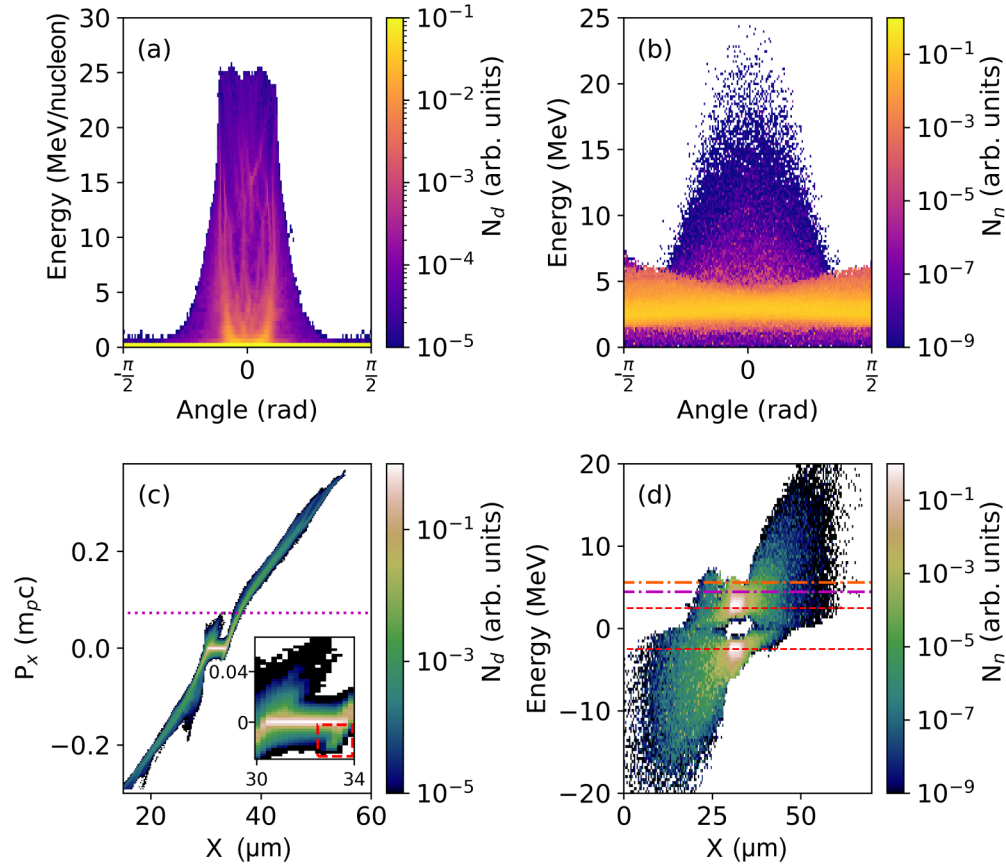


FIG. 3. Results from 2D PIC simulation showing deuteron and neutron distributions from the interaction of a laser pulse with a CD target. (a) Forward-directed deuteron's angular distribution toward the end of the simulation, showing a peak energy of ~ 25 MeV/nucleon. (b) The same plot, for neutrons. (c) A snapshot of the x - p_x phase space of deuterons taken at ~ 200 fs after the pulse peak interaction. The laser impedes on the target from the left. The dashed pink line indicates 1.25 MeV—the maximum deuteron energy achieved through the hole boring mechanism. The inset shows a zoomed-in section of the target bulk, showing the hole boring-accelerated ions, as well as those deuterons accelerated due to a backward-propagating shock front (highlighted by the red box). (d) The time-integrated x - E phase space for all neutrons created in the simulation. Negative energies correspond to a propagation in the $-x$ direction. The red dashed lines indicate the minimum neutron energy that is created in the center of momentum frame (2.45 MeV). The pink and orange dash-dotted lines indicate the maximum energy that can be created from deuterons of 1.25 MeV energy, according to Eqs. (1) (pink) and (4) (orange). The x position corresponds to the point at which each neutron is created; thus, the color scale is a representation of the number of fusion events at that point. The colorbars shows deuteron and neutron densities in arbitrary units.

events at very low energy, again indicative of the 2.45 MeV minimum.

Observed energies lower than 2.45 MeV (e.g., either side of the aforementioned void) are a result of transforming neutron velocities from the center of momentum frame to the laboratory frame, where neutron energies can become lower than what kinematics suggest is possible [e.g., Fig. 2(f)]. The peak neutron energy generated inside the bulk target region is, in fact, higher than this minimum energy. This is mainly due to the hole boring of deuterons through the target. As seen in Fig. 3(c), the peak energy reached by these deuterons is ~ 1.25 MeV. The pink and orange dashed-dot lines in Fig. 3(d) represent the maximum energy attained by neutrons reacting with 1.25 MeV deuterons according to Eqs. (1) (4.5 MeV, pink) and (4) (5.6 MeV, orange). Since the two primary mechanisms of D-D fusion inside the target mentioned so far, namely, thermonuclear and hole boring mediated fusion, are occurring inside a high-density plasma, they necessarily create significantly larger numbers of neutrons compared to

the fusion processes outside the bulk target region. This is the reason for the appearance of the sharp boundary at ~ 5 MeV between the two distributions seen in Fig. 3(b).

Further analysis concerning the fusion is shown in Fig. 4. Figure 4(a) shows the (time-integrated) summation of all fusion events that occur throughout the simulation boundary. The interaction point at (30, 20) μm is clearly identifiable, having a fusion rate orders of magnitude greater than the plasma outside of the target bulk. Figure 4(b) shows a similar plot, but the color scale indicates the average energy of fusion neutrons generated at each grid point. As already highlighted in Fig. 3, the most energetic neutrons are not generated inside the target, but rather outside the target bulk in the region of plasma dominated by the TNSA interaction. Figure 4(c) shows the time-resolved streak of fusion events along the x direction. From this, the sources of neutron generation are again clearly discernible. Labeled in the plot is the beginning of neutron generation via hole boring (“HB”), as well as the neutron generation via TNSA. The TNSA-generated neutrons

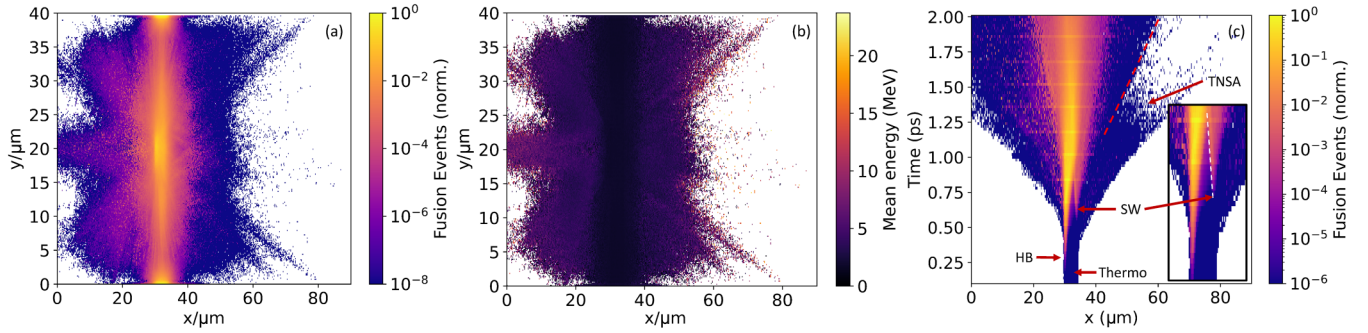


FIG. 4. Plots showing the normalized number of fusion events that occur throughout the simulation. (a) The number of fusion events that occur throughout the simulation, integrated over the full duration. Most fusion events occur inside the target bulk, close to the laser interaction point. The laser impinges from the left, centered on $y = 20 \mu\text{m}$. The initial unperturbed target resides between $x = 30$ and $34 \mu\text{m}$. (b) The average energy of the neutrons created at each point in space. The highest energies are created outside the bounds of the target bulk. (c) A time-resolved streak of the fusion events created along the x direction, integrated along a $15\text{-}\mu\text{m}$ -thick slice centered on $y = 20 \mu\text{m}$. The laser pulse peak interaction occurs at ~ 0.7 ps. The neutrons originating from the hole boring mechanism is labeled “HB” in the plot. Likewise, backward-accelerating neutrons originating from a shock front generated from the target’s rear is labeled “SW,” the neutrons from TNSA-accelerated deuterons are labeled “TNSA,” and those from thermonuclear fusion are labeled “Thermo.” The red dashed line in the top right corresponds to a deuteron energy of 2 MeV/nucleon . The inset shows a zoomed-in view of the origin of HB and SW neutron generation, with the white dashed line indicating the gradient (i.e., velocity) of the shock structure.

feature a sharp drop off in the reaction rate at around 1.25 ps (approximately 550 fs after pulse peak interaction). This is due to the decompression of the deuteron plasma as it expands longitudinally into the vacuum, and since the neutron yield is proportional to the square of the plasma density [27]. As the deuteron-rich plasma sheath expands, fusion reactions will occur up to the point at which the plasma has expanded sufficiently that the fusion rate is suppressed, while the deuterons continue to gain energy through the TNSA mechanism. Indeed, the fusion reactions are seen in Fig. 4 to sharply stop before $x \simeq 60 \mu\text{m}$. In Fig. 4(c), it can also be seen that there continue to be some fusion reactions from forward-propagating deuterons until the end of the simulation after fusion events from the TNSA beam have ceased. Taking the gradient of this front (red dashed line in the plot) indicates an energy of $\sim 2 \text{ MeV/nucleon}$, suggesting they are most likely due to the fastest HB deuterons breaking through the target’s rear surface, where they gain some energy from the remaining sheath fields and react with low-velocity deuterons left behind in the ambient plasma sheath.

Additionally, Fig. 4(c) has another source of fusion reactions (“SW”), bounded by a front that appears to be propagating backward into the bulk plasma, toward the laser interaction. It is likely related to a shock front that is seeded on the target’s rear surface due to the fast plasma expansion by TNSA. Shock-wave-like structures arising inside targets have been described before for short pulses interacting with thin foils [28–30]; however, in these cases the shocks were seeded by the ablation during the nanosecond-duration laser pedestal that typically precedes the main pulse. In this work the shocks have been seeded on a sub-ps timescale by the expanding TNSA fronts. The deuterons reflected by the shock are also indicated by the red box in the inset in Fig. 3(c). The shock also occurs on the front surface of the target, but this is clouded by the much more dominant HB interaction. These shocks have a very low peak velocity, $\beta \simeq 0.01$ [this velocity is shown as the white dashed line in the inset in Fig. 4(c)] and

hence contribute only low-energy neutrons around 2.5 MeV to the total yield. Considering the logarithmic color scale on the plot, the fusion rate of this mechanism appears to surpass that of thermonuclear effects by several orders of magnitude. However, as the thermonuclear mechanism occurs over a larger volume and for a longer time, it is likely that the total integrated thermonuclear-driven neutrons exceed those from the shock mechanism.

Figure 5(a) shows ion density plots to highlight these shocklike features, roughly 100 fs before the pulse peak interaction. The density spike due to the hole boring front is clearly visible, originating from the front surface (labeled “HB”), while outside the focal spot area the shocklike features appear in the form of narrower density spikes (labeled “SW”) that propagate from the target edges in, toward the target bulk. The rear surface density spike is destroyed close to the laser focus, possibly due to the much hotter electron current and stronger plasma expansion in this region overcoming any counterpropagating density spikes that may arise. These features are made more apparent in the lineouts, shown in the inset, taken close to the focal spot center (dotted lines) and $8 \mu\text{m}$ off-center (solid lines). The regions where these lineouts are taken are indicated in the main panel by the boxes. The inward-propagating nature of the waves is further highlighted by considering the green dashed lines in the inset, which indicate the positions of the unperturbed target’s front and rear surfaces. The maximum energy of these shock deuterons can be obtained from the x - p_x phase space [see the red box in the inset in Fig. 3(c)]. The peak x momentum of the deuterons in this feature, in units of $m_p c$, is -0.025 , converting to energy that corresponds to $\sim 0.375 \text{ MeV}$, or $\beta \simeq 0.02$. This, being double the shock velocity, is what is predicted according to models of ion acceleration by reflection off a collisionless shock [31,32].

As the neutrons from these shock structure interactions could not be isolated from those originating from thermonuclear/HB mechanisms in the main simulation, a second

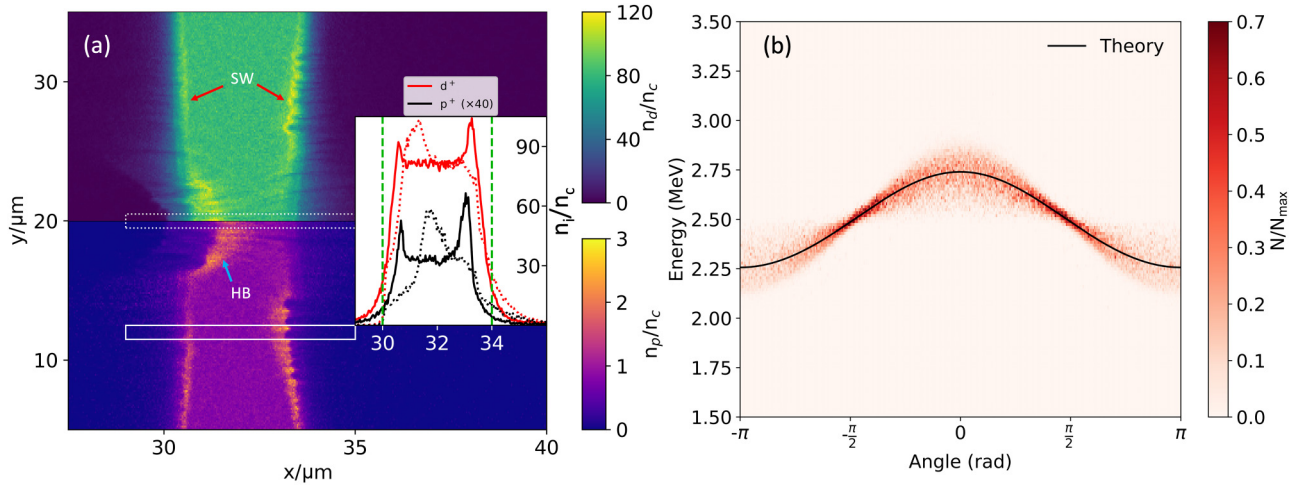


FIG. 5. (a) Snapshot of the deuteron (top) and proton (bottom) density distributions (in units of the critical density n_c) at ~ 100 fs before the pulse peak interaction. The hole boring front and shocklike features are labeled “HB” and “SW,” respectively. The inset shows ion density lineouts centered on the laser focal spot (i.e., the hole boring front, dotted lines) and off-center, close to where the SW amplitude is strongest (solid lines). Regions where the lineouts were taken are indicated in the main panel by the corresponding boxes. Proton density has been scaled by a factor of 40 to ease viewing. The green dashed lines indicate the positions of the unperturbed target front and rear surfaces, highlighting that the shock features have propagated from their original position toward the target bulk. (b) Neutron angular distribution arising from a separate simulation of a deuteron sail of $\beta = 0.01$ impinging on a cold deuteron target. The black line indicates the theoretical distribution for purely monoenergetic deuterons from Eq. (1).

beam-target simulation was run, similar to the one performed in Figs. 2(a) and 2(b). This time, the deuteron sail was initialized with a velocity of $0.01c$ (~ 0.1 MeV), similar to that measured for the shock front in Fig. 4(c). The neutron distribution from this simulation is shown in Fig. 5(b). The theoretically predicted neutron energies from Eq. (1) are shown by the black line. Due to spectral broadening of the initially monoenergetic deuteron bunch from (primarily) Coulomb interactions inside the target, there is also a resultant broadening of the neutron distribution about the theoretically predicted values. The angular distribution is almost isotropic, with only slightly higher energies in the forward direction compared to backward one. In the PIC simulation in Figs. 3, 4, and 5(a), the shock fronts are mostly directed backward with respect to the laser. In this scenario, the distribution energies in Fig. 5 will be reversed. Overall, however, the described shock mechanism is shown to be a quasi-isotropic source of narrow-band neutrons between 2 and 3 MeV and is a significant contributor to the overall neutron flux in that energy range, potentially surpassing the yield from thermonuclear fusion in the target bulk.

Figures 6(a) and 6(b) show the final spectra of deuterons and neutrons, respectively, directed within a half-cone angle of 1° along the 0° , 30° , and 90° directions with respect to the laser axis. The neutron spectrum along 90° gives an indication of the component of the neutron spectrum generated inside the target bulk ($x = 30\text{--}34 \mu\text{m}$). The clear distinction between in-target fusion neutrons and higher-energy neutrons generated in the TNSA sheath is once again clearly visible. The neutrons from the three in-target mechanisms (HB, shock, and thermonuclear) exhibit a very high flux, with a narrow-band spectral distribution peaking at ~ 2.5 MeV, and have a sharp cutoff at around 5–7 MeV, as predicted from the reaction kinematics for observed HB deuteron energies (see Fig. 3). Such

peaked spectral features were also observed in experiments on D-D fusion in bulk CD targets in the past [33].

On the other hand, the TNSA-generated neutrons show a thermal (exponentially decaying) spectrum, much like the thermal spectrum exhibited by the deuterons, at fluxes orders of magnitude lower than the 2.5 MeV peak. Fitting functions of the form $e^{-E/kT}$ to these distributions, where E is energy and kT is a characteristic temperature, shows that the neutron spectrum is significantly cooler, at 1.7 MeV, than the deuteron spectrum, which has a temperature of ~ 6 MeV. This is reconciled by the fact that the fusion reactions in the TNSA postplasma terminate prematurely compared to the duration of the acceleration process due to plasma decompression, as discussed above and shown in Fig. 4(c). Some qualitative comparisons can be made between the temperatures mentioned above and empirically measured temperatures from Kar *et al.* [12]. The deuteron and (on-axis) neutron temperatures from that work were extracted and were measured to be 2 and 0.7 MeV, respectively. These values are lower than what is observed in the simulations here; however, their ratios are comparable. The higher temperatures seen in the simulation can be understood when we consider the lower dimensionality, which has been shown to exaggerate particle energies compared to three dimensions [34–37].

IV. SCALING AT HIGHER INTENSITIES

As seen in the simulations, there are multiple sources of neutrons from a single-target interaction. The same simulation parameters were run again, but with different peak intensities, ranging from 5×10^{19} up to 10^{21} W/cm², to examine how these neutron energies scale with increasing intensity. The results of these simulations are shown in Fig. 7.

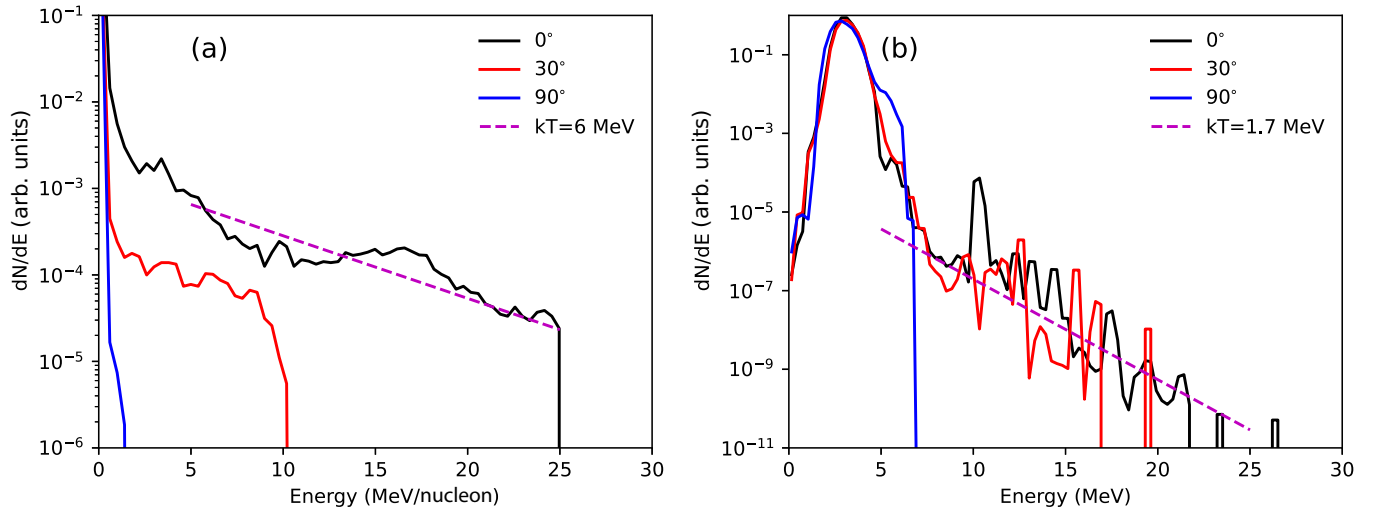


FIG. 6. (a) Results from the 2D PIC simulation showing the deuteron ion spectra along three different angles at the end of the simulation. The spectra are taken for half-cone angles of 1° about 0° , 30° , and 90° with respect to the laser axis. The dashed line shows a fit of the form $e^{-E/kT}$, where kT is a characteristic spectrum temperature, here determined to be 6 MeV. (b) The complementary spectra for neutrons along the same angles. The 90° spectrum serves as an indicator of the spectrum generated inside the target bulk ($30\text{--}34\text{ }\mu\text{m}$), highlighting the two distinct aforementioned distributions. A similar temperature fitting was performed on the high-energy portion of the spectrum, yielding a temperature of 1.7 MeV. The y-axis in both plots shows dN/dE in arbitrary units.

Figure 7(a) compares the maximum recorded deuteron energy to the maximum neutron energy. As can be seen, there is a plateau in the peak neutron energies observed as laser intensity increases, despite deuteron energies continuing to increase, contrary to what the reaction kinematics formulas predict should happen. This is again due to the premature termination of the TNSA-driven fusion processes by the rapid plasma decompression. However, when we examine the neutron flux variation [Fig. 7(b)], we see that there is still a clear upward trend, with no plateau in flux. The flux scales approximately with the square of the peak laser intensity, as evidenced by the fit line in Fig. 7.

These results suggest that the primary factors driving the flux measurements are the in-target mechanisms (HB, shock, and thermonuclear processes), while peak energy is determined by the TNSA mechanism. However, without a secondary target in place to act as a catcher, the peak neutron energy is not likely to increase as rapidly as the deuteron energies when laser intensity is increased. In scenarios where we may prefer to limit the peak neutron energy while maximizing flux, utilizing a very thick target to suppress the TNSA interaction and favor the HB mechanism could be preferable, in particular with modern multipetawatt laser facilities that are now becoming available.

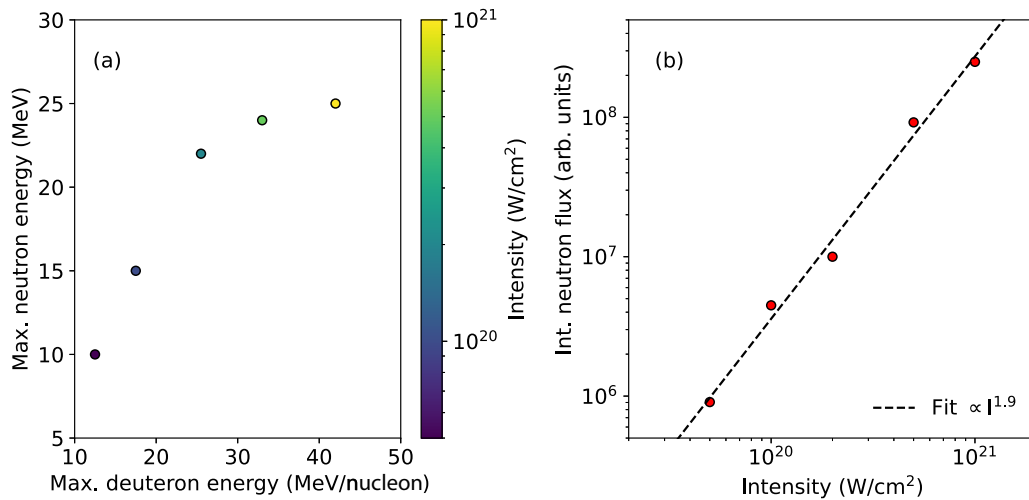


FIG. 7. Results from 2D PIC simulations showing the scaling of neutron beam properties. (a) The relationship between the maximum deuteron energy and the maximum neutron energy. The color scale represents the peak intensity of the laser pulse used in each simulation. (b) The variation in total neutron flux contained in a $0^\circ \pm 2^\circ$ cone with laser intensity. The neutron flux along the y-axis is in arbitrary units. While neutron maximum energy saturates, the total flux of the neutrons continues to rise with the square of the intensity.

V. CONCLUSION

In conclusion, the neutrons generated in a target via the $d(d,n)^3\text{He}$ reaction during a high-power laser interaction were simulated using the fusion algorithm implemented in the Smilei PIC code. Multiple mechanisms of deuteron acceleration were identified from the simulations which directly lead to neutron generation, each contributing uniquely to the final neutron distribution. The simulations show that the HB mechanism is the most favorable as laser intensity increases, evident from the large increase in flux. However, the neutron cutoff energy and spectrum temperature, which are most heavily influenced by the TNSA mechanism, saturate quickly. Using thick targets to suppress TNSA could enable the generation of high-flux, but relatively low-energy, neutron beams without the need for a secondary catcher target, simplifying the experimental setup requirements and favoring high-repetition operation. In addition, multilayer or microstructured targets may be designed with a view to maximizing the shock effect for the production of an isotropic narrow-band neutron source. However, it is likely that the successful seeding of shock fronts will require very high contrast lasers, as preionization of the front and rear surfaces and long scale-length preplasmas could inhibit their

formation, which requires rapid ablation of plasma from the surface. These novel target schemes could be favorable in applications where high neutron beam energies are not required, in particular for configurations using a moderator to slow neutrons to thermal/epithermal (MeV–keV) energies, which are typically the relevant energy ranges for a broad range of neutron applications.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [38].

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