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► **To cite this version:**

J. Don Jayamanne, R. Outerovitch, F. Ballanger, J. Bénier, E. Blanco, et al.. Recovering particle velocity and size distributions in ejecta with Photon Doppler Velocimetry. *Journal of Applied Physics*, 2024, 136 (8), pp.083111. 10.1063/5.0220642 . hal-04778524

HAL Id: hal-04778524

<https://hal.science/hal-04778524v1>

Submitted on 12 Nov 2024

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Recovering particle velocity and size distributions in ejecta with Photon Doppler Velocimetry

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(Dated: 12 November 2024)

When a solid metal is struck, its free surface can eject fast and fine particles. Despite the many diagnostics that have been implemented to measure the mass, size, velocity or temperature of ejecta, these efforts provide only a partial picture of this phenomenon. Ejecta characterization, especially in constrained geometries, is an inherently ill-posed problem. In this context, Photon Doppler Velocimetry (PDV) has been a valuable diagnostic, measuring reliably particles and free surface velocities in the single scattering regime. Here we present ejecta experiments in gas and how, in this context, PDV allows one to retrieve additional information on the ejecta, i.e. information on the particles' size. We explain what governs ejecta transport in gas and how it can be simulated. To account for the multiple scattering of light in these ejecta, we use the Radiative Transfer Equation (RTE) that quantitatively describes PDV spectrograms, and their dependence on the velocity but also on the size distribution of the ejecta. We remind how spectrograms can be simulated by solving numerically this RTE and we show how to do so on hydrodynamic ejecta simulation results. Finally, we use this complex machinery in different ejecta transport scenarios to simulate the corresponding spectrograms. Comparing these to experimental results, we iteratively constrain the ejecta description at an unprecedented level. This work demonstrates our ability to recover particle size information from what is initially a velocity diagnostic, but more importantly it shows how, using existing simulation of ejecta, we capture through simulation the complexity of experimental spectrograms.

I. INTRODUCTION

Probing matter's behavior under the extreme conditions of shock compression experiments allows one to better understand its properties at rest. Ejecta formation, the process through which a shocked material ejects a cloud of fast and fine particle, has been extensively studied lately¹. It has been shown that ejecta is a limiting case of Richtmyer-Meshkov instabilities^{2,3} which occurs when the initial shockwave interacts with the irregularities at the free surface of the material^{4,5}. It causes matter to partially melt, creating numerous expanding micro-jets. These micro-jets eventually fragment giving birth to the actual ejecta [see Fig. 1(b)]. One of the purpose of ejecta study is to determine the size-velocity distribution of this particle cloud.

Advances on the ejecta source model theory⁶⁻⁸ in shock compression experiments and the corresponding simulation⁹⁻¹² have permitted a better description of the distribution created by a given sample in response to a given solicitation. These simulations study the particles from their creation at the early moment of the experiment to their transport throughout the propagation medium. This simulation effort on the ejecta side was supported by the experimental development of numerous and diverse optical diagnostics which refined ejecta description to further constrained ejecta simulations. Especially, Mie scattering^{13,14} and holography diag-

nostics^{15,16} have given valuable insights on the particle size-velocity distribution. The main limitations of these diagnostics remain their difficulty of implementation and the fact that they only allow the study of elementary examples of ejecta formation, namely ejection with a few micro-jets. For now, one has no other choice than assuming that the ejection process in more complex experiments gives the same particle size-velocity distribution with no mean of verifying this claim.

Photon Doppler Velocimetry (PDV) is another optical diagnostic which was initially developed to monitor particle velocity distributions^{17,18}. With a single scattering hypothesis, the PDV response of an ejecta, its time-velocity spectrogram, can be seen as the velocity distribution of the ejecta at a given time. Recently, we have shown¹⁹ that this spectrogram is in fact the solution of a broader light transport model which is sensitive to the particle size distribution and its statistical inhomogeneities throughout the medium. Compared to Mie scattering and holography diagnostics that are based on off-axis and transmission measurements, PDV is on-axis and in reflection. A unique collimated probe is used for illumination and detection. This makes it compact, reliable and minimum invasive. These perks have made it one of the key diagnostic implemented in almost all experiments and especially the most constrained ones. Showing that it is possible to recover additional size information from a PDV spectrogram would highly impact ejecta analysis. This would enable the evaluation of particle sizes in the most complex configurations and

allow one to verify that the ejecta formation process is in fact similar to that of elementary experiments.

The purpose of this work is to showcase an experiment where, using only PDV spectrograms, we constrain the size distribution of an ejecta. To proceed, we first introduce ejecta experiments in gas, their interest for particle size study and the means available to simulate particle transport in such media. Then, we remind the working principle of PDV measurements, why they are sensitive to the ejecta size distribution and how we can compute simulated spectrograms out of simulated ejecta transport. Matching the simulated spectrograms to the experimental ones acquired for three different gas conditions, we are able to better constrain the initial size distribution of the ejecta and test its robustness. Finally, we discuss how the present work reflects on existing literature and ejecta understanding.

The paper is organized as follows. Section II is dedicated to the presentation of ejecta experiments in gas. We introduce the micro-jetting mechanism and the resulting size-velocity distribution. We explain the ways ejecta is assumed to interact with gas and how it depends on particle size. We then introduce the *Phénix* code that handles ejecta transport in gas and allows one to compute the expected ejecta description at each step of the corresponding experiment. In Sec. III, we recall the PDV instrumentation ejecta experiments receive and how, with a single scattering hypothesis, the resulting PDV spectrogram accurately estimates the velocity distribution of the ejecta. For the ejecta considered here, multiple scattering cannot be ignored. In this regime, we rewrite this spectrogram as a function of the specific intensity, a commonly used quantity in statistical optics. This quantity is the solution of a Radiative Transfer Equation (RTE) that has been modified to account for both Doppler shifts due to the particles movement and the statistical inhomogeneities of the ejecta. The PDV spectrogram can then be computed given the ejecta's size-velocity distribution in time and we do so directly on ejecta transport results obtained with the *Phénix* hydrodynamic simulation code. Our comprehensive study of particle size distribution based on simulated PDV spectrograms in different gas is reported in Sec. IV. We start in the simplest case of vacuum and then gradually increase the complexity with helium and air. Finally, Sec. V discusses the implications of this work, how it compares to existing literature and what it argues in favor of for future ejecta studies.

II. EJECTA EXPERIMENTS AND SIMULATION IN GAS

A. Ejecta creation

Typical ejecta experiments, as the ones studied in Sec. IV, are the planar shock experiments. In a tube, a sample of the material of interest, here a grooved surface of tin (Sn), is shocked by a High-Explosive (HE) driven pellet [see Fig.1(a)]. The shockwave's interaction with the surface irregularities creates liquid micro-jets of matter. These micro-jets eventually undergo fragmentation giving birth to the actual ejecta. In our experiment, the barrel's inner diameter is

$\Phi_{\text{barrel}} = 98 \text{ mm}$, the samples are tin disks with $60 \mu\text{m} \times 8 \mu\text{m}$ surface grooves. With a copper flyer hitting the tin samples at 1650 m/s , we reach a shock pressure of $P_{\text{shock}} = 29.5 \text{ GPa}$, which ensures liquid phase transition in expansion.

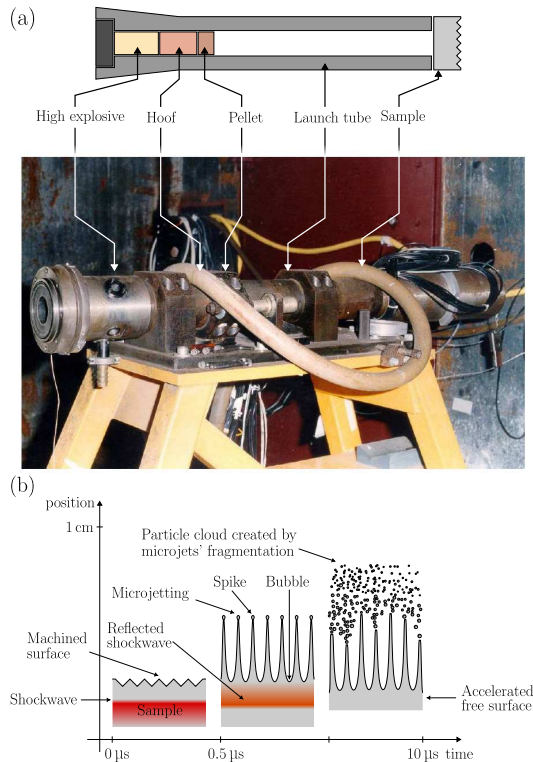


FIG. 1. (a) Typical explosive setup of a planar shock experiment. (b) Illustration of the micro-jet mechanism in a typical shock ejecta experiment. Upon reaching the machined free surface, the shock wave first comes into contact with the inwardly directed grooves. Under right angle conditions, the shock wave is reflected and the inward grooves become outward micro-jets. Due to the velocity gap between the jet-heads and the free surface, the micro-jets are stretched until surface tension is no longer sufficient to hold matter together and fragmentation begins. This results in the creation of an ejecta.

To model this ejecta in gas, we need to make a few assumptions. The first one is that the ejecta is made out of spherical particles with radius a . Right after impact, it can then be described by its initial size-velocity distribution $g(a, \mathbf{v})$ normalized such that

$$\int g(a, \mathbf{v}) d a d \mathbf{v} = 1. \quad (1)$$

While recent holography imaging results^{15,16} and molecular dynamics simulations¹⁰⁻¹² suggest otherwise, this is discussed in Sec. V, our second assumption is that the initial size and velocity distributions are independent. This reads

$$g(a, \mathbf{v}) = h(a) j(\mathbf{v}), \quad (2)$$

with $h(a)$ the size distribution, $j(\mathbf{v})$ the velocity distribution

and

$$\int h(a)da = 1, \quad (3)$$

$$\int j(\mathbf{v})d\mathbf{v} = 1. \quad (4)$$

Our last assumption is that the initial size and velocity distributions do not depend on the presence nor the nature of the gas in the chamber. Once again Mie-scattering measurements have shown the limits of such an hypothesis²⁰, but as a first approximation it will prove useful.

In Sec. IV, different initial size distributions will be tested but the velocity distribution will be imposed from here on. Instead of defining it directly, we prefer using the integrated mass-velocity distribution $M(v)$ where $v = |\mathbf{v}|$. Assuming all velocities to be along the ejection direction \mathbf{u}_z , the distribution then reads

$$j(\mathbf{v}) = -\frac{1}{M_s} \frac{d}{dv} M(v) \delta\left(\frac{1}{v} \mathbf{v} - \mathbf{u}_z\right), \quad (5)$$

where M_s is the surface mass. Independent Asay foil measurements⁴ in vacuum for these experiments give

$$M(v) = \begin{cases} M_s \exp\left[-\beta\left(\frac{v}{v_s} - 1\right)\right], & \text{if } v \in [v_{\min}, v_{\max}] \\ 0, & \text{otherwise} \end{cases} \quad (6)$$

with the surface mass $M_s = 12 \text{ mg/cm}^2$, $\beta = 11.7$, $v_s = v_{\min} = 2060 \text{ m/s}$ and $v_{\max} = 3350 \text{ m/s}$.

Now that the initial properties of the ejecta have been described, we need to model its interaction with gas.

B. Ejecta transport in gas

In case of a vacuum-tight chamber, the objects are in ballistic transport and the ejecta size-velocity distribution remains the same during propagation. Now if the chamber is gas filled, the transport properties of the ejecta are altered. While we assume the same initial size-velocity distribution as in vacuum, knowing that gas interaction depends both on particle size and velocity, the size-velocity distribution will evolve with time. This discrimination is what makes ejecta experiments in gas extremely insightful. The same set of initial conditions in different gases must allow us to retrieve radically different particles transport scenarios. In other words, the robustness of a unique initial description can be tested against different gas transport conditions to see whether or not it allows one to match all experimental results. While different from a direct measurement, this technique must be seen as a powerful new way of evaluating particle size-velocity distribution with existing diagnostics and in otherwise inaccessible configurations.

In the presence of gas in front of the ejecta, the particles interact with it mainly through the drag force, which tends to drive the particle toward the gas velocity. The drag force depends on the particle radius, the gas density and the drag coefficient (based on the particle's Reynolds and Mach numbers).

We take into account the two-way coupling of the particle and the gas. The drag force is calculated using the KIVA-II formulation²¹ given by,

$$\mathbf{F}_i = -\frac{1}{2} \pi a_i^2 \rho_g (\mathbf{v}_i - \mathbf{v}_g) |\mathbf{v}_i - \mathbf{v}_g| C_{d,i}, \quad (7)$$

with ρ_g the gas density, \mathbf{v}_g its velocity, a_i the i^{th} particle's radius, \mathbf{v}_i its velocity and $C_{d,i}$ its drag coefficient. The drag coefficients are computed using a model based on Ref. 22.

A hydrodynamic break-up model, based on Ref. 23, is also introduced. The Weber number is expressed as the ratio between hydrodynamic forces and the surface tension of the particle,

$$\text{We}_i = \frac{2a_i \rho_g |\mathbf{v}_i - \mathbf{v}_g|^2}{\sigma_i}, \quad (8)$$

with σ_i the particle surface tension. If the Weber number is supercritical, the particle breaks-up. The calculation of the ratio between the initial and new radius depends on the value of We and is detailed in Ref. 23. The corresponding typical values for the critical Weber number are $\text{We}_{\text{crit}} = 10 - 20$, and current work at CEA-DAM shows that $\text{We}_{\text{crit}} = 15$ is well suited for tin.

Given an initial ejecta distribution and these two interactions, we need a simulation handling the transport of particles accordingly in time.

C. *Phénix* code for particle transport simulation

Hydrodynamic simulations have become the standard to compute matter's behavior in shock compression experiments⁹. In this work, the simulations are run with the *Phénix* code, developed at CEA-DAM which uses a multiphase particulate transport method to model two-way coupling of momentum and energy. This is based on the approach proposed by Amsden *et al.* and implemented in the KIVA-II code²¹, which has been improved from the original paper.

To perform the simulations, we have to initialize the particle cloud according to the experimental parameters to fit the other diagnostics implemented in the experimental set-up. We define the ejected mass velocity curve $M(v)$ in agreement with the Asay foil⁴ measurement under vacuum (still assuming the gas does not change the total ejected mass). For the initial size distribution, we rely on previous experiments and deal with power laws or lognormal distributions. Studying its influence on the spectrograms is one of the purpose of this article as described in Sec. IV.

For each experiment, the *Phénix* code gives the corresponding cloud description at different time steps. For each of these times, the description corresponds to a list of so-called *numerical particles*. Instead of actually simulating the transport of each individual particles, we only consider a smaller set of numerical particles. Each of them has a size, a numerical weight, i.e. the number of physical particles it represents, a position and a velocity. The number of numerical particles must be high enough to encompass the full dynamics of the ejecta

while being low enough to ensure a reasonable compute time. In practice, the typical scale of the velocity distribution introduced in Eq. (6) is v_s/β , which roughly gives 200 m/s for the case considered here. Since $v_{\max} - v_{\min} \approx 1000$ m/s and the sampling step in the velocity distribution needs to be at least ten times smaller than v_s/β , we need 50 points. Taking, the same number of points for the size distributions, which are introduced in greater details in Sec. IV A, leads to steps of $0.1 \mu\text{m}$ that are smaller than the typical scales of the size distributions that are considered. This 50×50 discretization on the size-velocity distribution gives a total of 2500 numerical particles, which is the number that will be used for the ejecta simulations in the rest of this work.

Once the ejecta is initialized, the particle transport happens as follows. On the one hand, the drag force affects the velocity and therefore the position of the numerical particles. On the other hand, the break-up process, which takes place only if the Weber number We_i is superior to the critical Weber number $We_{\text{crit}} = 15$, decreases the particle size. In practice, when a given numerical particle breaks-up, it gets associated a new size depending on its initial Weber number and its numerical weight is increased to maintain its total associated mass.

As an order of magnitude, each ejecta simulation corresponding to Sec. IV have around 2500 numerical particles, taken at 180 temporal steps each separated by $\delta t = 0.16 \mu\text{s}$. The corresponding compute time is 2 h on 1 AMD EPYC 7763 64-core CPUs clocked at 2.45 GHz.

In summary, the three main parameters that control the evolution of the particle cloud during the simulation are the initial size distribution, drag force and break-up model. In the study reported in Sec. IV, these parameters are the ones we expect to fine tune to make the ejecta robust to transport in different gases. The efficiency of such a procedure depends on the sensitivity of the chosen diagnostic to changes in ejecta transport properties. The diagnostic chosen here, PDV, is presented in Sec. III.

III. PHOTON DOPPLER VELOCIMETRY IN EJECTA

While PDV in ejecta has been shown to be deep in the multiple scattering¹⁹ regime (which will be the case for all the ejecta presented here), it is interesting to consider first the single scattering regime for which PDV was initially developed. This is the purpose of Sec. III A.

A. Photon Doppler Velocimetry in the single scattering regime

Photon Doppler Velocimetry is an interferometric technique^{17,18} where a collimated laser beam at frequency ω_0 is shined toward a cloud of moving particles and a free surface. As seen in Fig. 2, light then get scattered by this ejecta and slightly shifted in frequency before part of it is captured in reflection. The collected field interferes at the detector with a reference field at ω_0 , resulting in a beating signal $\mathcal{I}(t)$ at the

detector. This signal can be written

$$\mathcal{I}(t) = 2 \text{Re} [\bar{E}_s(\mathbf{r}, t) \bar{E}_0^*(\mathbf{r}, t)], \quad (9)$$

with $\bar{E}_s(\mathbf{r}, t)$ the analytic signal associated to the scattered field, $\bar{E}_0(\mathbf{r}, t)$ the analytic signal associated to the reference field and \mathbf{r} denotes position of the probe.

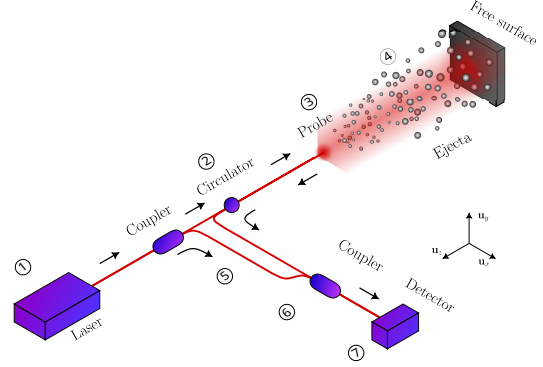


FIG. 2. Schematic representation of a typical shock-loaded experiment with a PDV setup. The probe illuminates the ejecta and the free surface with a highly collimated laser beam (numerical aperture of 4.2 mrad and pupil size $\phi_p = 1.3 \mu\text{m}$). The backscattered field is collected by the probe acting as the measuring arm and interferes with the reference arm at the detector. The beating signal is registered with a high bandwidth oscilloscope before being analyzed.

In post-treatment a Short-Term Fourier Transform (STFT) is applied defining the spectrogram $S(t, \omega)$ as

$$S(t, \omega) = \left| \int \mathcal{I}(\tau) w(\tau - t) \exp(i\omega\tau) d\tau \right|^2 \quad (10)$$

where $w(t)$ is a gate function of typical width T_w such that $\int w(t) dt = T_w$.

With a single scattering hypothesis, the scattered field is the sum of the fields scattered by each particle. We consider scalar fields, since our focus in this work will be in the multiple scattering regime, where the field can be considered unpolarized, since depolarization is known to occur on scales of the order of the scattering mean free path²⁴. For a number of particle $N(t)$, and assuming a detection in the far field, the scattered field then reads

$$\bar{E}_s(\mathbf{r}, t) = \frac{e^{ik_0 r}}{r} \sum_{j=1}^{N(t)} \mathcal{A}_j(\mathbf{u}, \mathbf{u}_0, t) \times \exp\{-i[\omega_0 + k_0(\mathbf{u} - \mathbf{u}_0) \cdot \mathbf{v}_j(t)]t\}, \quad (11)$$

where $r = |\mathbf{r}|$, $k_0 = \omega_0/c$ with c the light velocity in vacuum, \mathbf{u}_0 is the unit vector defining the direction of illumination, $\mathbf{u} = \mathbf{r}/r$ defines the direction of observation, $\mathcal{A}_j(\mathbf{u}, \mathbf{u}_0, t)$ is the amplitude of the field scattered by particle j and $\mathbf{v}_j(t)$ its velocity. Using Eq. (11) and for an observation direction

$\mathbf{u} = -\mathbf{u}_0$, the spectrogram given in Eq. (10) becomes

$$S(t, \omega) = \frac{\pi^2 |\mathcal{A}_0|^2}{r^2} \int \sum_{j=1}^{N(t)} |\mathcal{A}_j(-\mathbf{u}_0, \mathbf{u}_0, t)|^2 \times \left\{ \left| \delta \left[\omega + \frac{4\pi}{\lambda} v_j(t) \right] \right|^2 + \left| \delta \left[\omega - \frac{4\pi}{\lambda} v_j(t) \right] \right|^2 \right\} d\mathbf{r}, \quad (12)$$

where \mathcal{A}_0 is the amplitude of the reference field and δ the Dirac delta function. This simple expression allows one to convert the frequency appearing in PDV spectrograms directly into a velocity using $v = \omega/(4\pi)\lambda$. In this regime, as shown in Fig. 4(a), the spectrogram gives an accurate estimation of the velocity distribution in the ejecta.

B. Photon Doppler Velocimetry beyond single scattering

With z denoting the depth along the ejection direction, the single scattering hypothesis holds as long as the optical thickness $b \ll 1$. The optical thickness is defined as

$$b = \int \frac{1}{\ell_s(z)} dz \quad (13)$$

where $\ell_s(z)$, the photon scattering mean-free path, will be introduced in greater details in this section. We have shown that in ejecta experiments b can far exceed unity, for example $b = 42$ in the study by Shi *et al.*²⁵ In these conditions, Eq. (11) does not hold and the spectrogram expression must be enriched to account for multiple scattering. This was the purpose of a previous work¹⁹ where we explain in great details and with the relevant hypothesis how the PDV spectrogram expression given in Eq. (12) can be extended to the multiple scattering regime. The purpose of this section is to recall the most important results of this previous work that will be useful to perform spectrogram simulation in Sec. IV.

The quantity of interest in the multiple scattering regime is the specific intensity $I(\mathbf{r}, \mathbf{u}, t, \omega)$ ^{26–29}. This radiometric quantity can be interpreted as a radiative flux at position \mathbf{r} , in direction \mathbf{u} , at time t and at frequency ω . In this sense, we can show that the specific intensity satisfies the Radiative Transfer Equation (RTE) which will be presented in detail below. The specific intensity can also be related to the wave field via the Fourier transform of its correlation function. This definition allows one to connect the specific intensity to the spectrogram by the relation

$$S(t, \omega) = \delta(k - k_r) T_w S_p^2 |\mathcal{A}_0|^2 \times \int_{\Omega} [I_s(\mathbf{r}, \mathbf{u}, t, \omega_0 + \omega) + I_s(\mathbf{r}, \mathbf{u}, t, \omega_0 - \omega)] \times \left[\left(\frac{k_r}{2} \mathbf{u} + \frac{k_0}{2} \mathbf{n} \right) \cdot \mathbf{n} \right]^2 k_r d\mathbf{u}. \quad (14)$$

where S_p is the surface of the probe, $k_r = n_r \omega_0/c$, n_r being the real part of n_{eff} the effective refractive index of the medium as defined in Ref. 19, Ω is the angular aperture of the probe, \mathbf{u}

corresponds to integration over the solid angle, and \mathbf{n} is the unit vector normal to the probe surface.

The RTE governing the evolution of the specific intensity takes the form¹⁹

$$\left[\frac{1}{v_E(\mathbf{r}, t, \omega)} \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla_{\mathbf{r}} + \frac{1}{\ell_e(\mathbf{r}, t, \omega)} \right] I(\mathbf{r}, \mathbf{u}, t, \omega) = \frac{1}{\ell_s(\mathbf{r}, t, \omega)} \int p(\mathbf{r}, \mathbf{u}, \mathbf{u}', t, \omega, \omega') I(\mathbf{r}, \mathbf{u}', t, \omega') d\mathbf{u}' \frac{d\omega'}{2\pi}, \quad (15)$$

with v_E the energy velocity, ℓ_e the extinction mean-free path and p the phase function. Equation (15) is a generalized form of RTE that takes into account the inhomogeneities of the particle cloud (under a quasi-homogeneous approximation^{30,31}). This equation that naturally accounts for multiple scattering can be understood as an energy balance. The two derivatives of the specific intensity in the left-hand side of Eq. (15) corresponds to the spatio-temporal evolution of this quantity. This evolution is governed by both losses and gains. Losses are caused by absorption and scattering as described by the extinction mean-free path ℓ_e . It is worth pointing out that these losses happen at the same frequency ω . The gains, also caused by scattering, are handled by the phase function in the right-hand side of Eq. (15). The scattering process being inelastic, it allows a conversion from a frequency ω' to ω . The extinction mean-free path ℓ_e is defined as

$$\frac{1}{\ell_e(\mathbf{r}, t, \omega)} = \int \rho(\mathbf{r}, t) \sigma_e(a, \omega) h(\mathbf{r}, t, a) da, \quad (16)$$

where $\sigma_e(a, \omega)$ is the extinction cross-section of a particle with radius a at frequency ω and $h(\mathbf{r}, t, a)$ is the size distribution at position \mathbf{r} and time t . In our case $h(\mathbf{r}, t_0, a) = h(a)$ as introduced in Sec. II, with t_0 the ejecta creation time. The scattering mean-free path ℓ_s and the phase function p are defined as

$$\frac{1}{\ell_s(\mathbf{r}, t, \omega)} p(\mathbf{r}, \mathbf{u}, \mathbf{u}', t, \omega, \omega') = \int \rho(\mathbf{r}, t) \frac{d\sigma_s(a, \mathbf{u} \cdot \mathbf{u}', \omega)}{d\mathbf{u}} \times 2\pi \delta[\omega' - \omega - k_R(\mathbf{u}' - \mathbf{u}) \cdot \mathbf{v}] g(\mathbf{r}, t, a, \mathbf{v}) d\mathbf{a} d\mathbf{v}, \quad (17)$$

where $\sigma_s(a, \omega)$ is the scattering cross-section of a particle with radius a and $g(\mathbf{r}, t, a, \mathbf{v})$ is the size-velocity distribution at position \mathbf{r} and time t . Again, in our case, $g(\mathbf{r}, t_0, a, \mathbf{v}) = h(a)j(\mathbf{v})$ as introduced in Sec. II. With this definition, the phase function is normalized as

$$\int p(\mathbf{r}, \mathbf{u}, \mathbf{u}', t, \omega, \omega') d\mathbf{u}' \frac{d\omega'}{2\pi} = 1, \quad (18)$$

and, integrating Eq. (17) over \mathbf{u} , the scattering mean free-path reads

$$\frac{1}{\ell_s(\mathbf{r}, t, \omega)} = \int \rho(\mathbf{r}, t) \sigma_s(a, \omega) h(\mathbf{r}, t, a) da. \quad (19)$$

We define the absorption mean-free path $\ell_a(\mathbf{r}, t)$ as

$$\frac{1}{\ell_a(\mathbf{r}, t)} = \frac{1}{\ell_e(\mathbf{r}, t)} - \frac{1}{\ell_s(\mathbf{r}, t)}. \quad (20)$$

Finally, since we have nonresonant scattering, the energy velocity v_E is given by $v_E = c/n_{\text{eff}}$.

The quasi-homogeneous approximation used in this form of the RTE, which amounts here to the \mathbf{r} and t dependencies of the ejecta description, makes it perfectly suited here to evaluate the effects of inhomogeneities caused by ejecta experiments in gas. Moreover, the dependence of the mean-free paths and phase function on the size-velocity distribution of the ejecta $g(\mathbf{r}, t, a, \mathbf{v})$ makes PDV a good candidate for indirect size-velocity measurement we aim to perform. While the idea of ejecta experiments in gas to evaluate particle size-velocity distribution is not new^{20,32}, the novelty of this work resides in connecting historic ejecta simulation schemes directly to a light transport model for PDV. The intricacies of this link is the subject of Sec. III C.

C. Photon Doppler Velocimetry spectrogram simulation

The RTE given in Eq. (15) can be rewritten in an integral form which is naturally suited for a Monte Carlo simulation scheme. Such a process can be seen as a random walk for energy quanta (behaving as classical particles), where each step is sampled in statistical distributions for step length, scattering direction, and frequency. While the expression of these statistical distributions and the details of the random walk procedure are available in Ref. 19, what is relevant in the scope of this paper is that they only require the mean-free paths and phase function defined in Eqs. (16) and (17) on a time scale small enough to capture the temporal evolution of the ejecta and on a spatial scale small enough to capture its statistical inhomogeneities. The challenge here is to connect the ejecta description, i.e. the numerical particles, computed by the *Phénix* code to the aforementioned quantities of interest.

Firstly, the value of δt , the time step introduced in Sec. II chosen for the *Phénix* code, is well below the typical value of $1 \mu\text{s}$ for the ejecta evolution time scale. Same goes for the spatial scale where the typical number of numerical particles of 2500 mentioned in Sec. II provides a good sampling of the ejecta on position, velocities and size. Now, at a given step of the hydrodynamic simulation, here is how the resulting ejecta description, i.e. the numerical particles and their attributes, allow to compute the corresponding mean-free paths and phase function. The numerical particles are given in the launch tube geometry. This ejecta is then discretized spatially into several layers depending on the space variations of the ejecta's statistical properties. In each layer the integration over size a and velocity \mathbf{v} appearing in Eqs. (16) and (17) is replaced by a discrete sum over the numerical particle. In these discrete sums, the product $\rho(\mathbf{r}, t)h(\mathbf{r}, t, a)$ and $\rho(\mathbf{r}, t)g(\mathbf{r}, t, a, \mathbf{v})$ is replaced by the particle number density $w_i/\delta V$ where w_i corresponds to the numerical weight of the i^{th} numerical particle and δV the volume of the layer in the ejecta geometry. The regular and differential cross-sections are computed using the routine given in Ref. 33. An example of this entire procedure is depicted in Fig. 3 for computing the extinction mean-free path. As an order of magnitude, the compute time for each simulated spectrogram presented in Sec. IV is around 1 h 20 min on

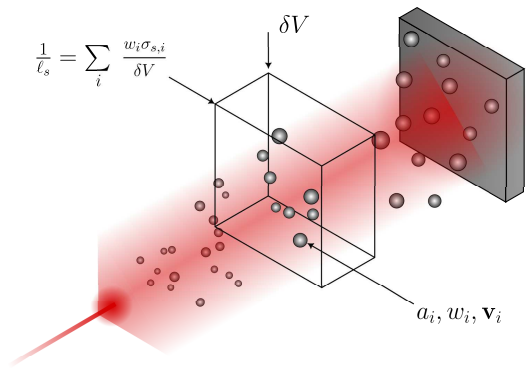


FIG. 3. Illustration of how to use hydrodynamic simulation results as input data for PDV spectrogram simulation. The medium is sliced in layers of equal thickness and each of them intersects part of the ejecta. For each layer, the numerical particles concerned are then used to compute the local mean-free paths and phase functions.

80 AMD EPYC 7763 64-core CPUs clocked at 2.45 GHz for 5.12×10^9 Monte Carlo draws, at 180 different times, with 2500 numerical particles arranged in 100 effective layers.

After presenting the simulation tools permitting to describe the path from the solicitation on the sample to the spectrogram, the aim of Sec. IV is to do a comprehensive study to constrain ejecta description using simulated PDV spectrograms.

IV. EJECTA BEHAVIOR RECOVERY BASED ON PDV SPECTROGRAMS ANALYSIS

In the remainder of this article, we propose to study a complex set of ejection experiments in gas. We consider three experiments, differing only by the gas present in the chamber. The experimental setup is the one presented in Sec. II A and pictured in Fig. 1. Ejecta travels, respectively, in $P_{\text{vacuum}} = 1 \text{ Pa}$ vacuum, $P_{\text{helium}} = 500 \text{ kPa}$ helium and $P_{\text{air}} = 100 \text{ kPa}$ air.

We start by simulating a spectrogram in vacuum to define a size-velocity distribution baseline. Next, in order to see if this baseline holds in helium, we focus on the induced drag forces. Finally in air, we explore the additional effect of hydrodynamic break-up.

A. Ejecta's initial size distribution in vacuum

For this first simulation in vacuum, we choose a standard power law distribution of the particle size, in the form¹⁴

$$h(a) = \begin{cases} \frac{\alpha - 1}{a_{\min}^{-\alpha+1} - a_{\max}^{-\alpha+1}} a^{-\alpha}, & \text{if } a \in [a_{\min}, a_{\max}] \\ 0, & \text{otherwise} \end{cases}, \quad (21)$$

with $\alpha = 5$, $a_{\min} = 1 \mu\text{m}$ and $a_{\max} = 6 \mu\text{m}$. With these input parameters, the *Phénix* code handles the particle transport during the entire simulation, from $t = 0$ to $t = 27 \mu\text{s}$. This data is then given as input data in the Monte Carlo simulation to compute

the corresponding expected spectrogram for the experimental setup characteristics.

On the one hand, for the experimental spectrogram, we do not directly have access to $\mathcal{S}(t)$ as introduced in Eq. (9). In practice, the time frequency analysis is performed on the signal in volts recorded at the photodiode which gives $S_{\text{exp}}(t, \omega)$. Instead of directly representing the spectrogram, the preferred quantity is $P_{\text{exp}}(t, \nu)$, defined as

$$P_{\text{exp}}(t, \nu) = 10 \log \left[\frac{1}{K_{\text{ph}}^2 T_w^2 P_0 P_{\text{ref}}} S_{\text{exp}} \left(t, \frac{4\pi}{\lambda} \nu \right) \right] \quad (22)$$

where K_{ph} is the efficiency of the photodiode, P_0 is the optical power of the reference arm and P_{ref} is a reference power. For this set of experiments, we have $K_{\text{ph}} = 10^4 \text{ V/W}$ and choose $P_{0,\text{exp}} = 1 \text{ mW}$, such that $P_{\text{exp}}(t, \nu)$ is expressed in dBm. On the other hand, we represent the simulated spectrogram with $P_{\text{sim}}(t, \nu)$ defined as

$$P_{\text{sim}}(t, \nu) = 10 \log \left[\frac{4}{(k_r + k_0)^2 T_w^2 |\mathcal{A}_0|^2 S_p^2 F_{0,\text{sim}}} S \left(t, \frac{4\pi}{\lambda} \nu \right) \right] \quad (23)$$

where \mathcal{A}_0 is the amplitude of the reference field, S_p is the surface of the detector and the reference flux $F_{0,\text{sim}} = 1 \text{ V}^{-2} \text{ s}^{-2}$. Even in the presence of the multiple scattering regime, for both spectrograms frequencies are converted to *apparent* velocities using the single scattering relation $\nu = \omega / (4\pi) \lambda$. One has to keep in mind that the apparent velocity correspond to the actual velocity of particles only in the single scattering regime. Given these definitions, it is meaningful to compare the dynamic range rather than the absolute value.

Figure 4 displays the comparison between the experimental spectrogram in vacuum [Fig. 4(a)] and the first simulated spectrogram of this study [Fig. 4(b)]. The first interesting observation is that, while the levels differ, the dynamic ranges of both spectrograms are similar - around 50 dB. Secondly, we see that the dynamic of velocities as expected between $\nu = 2000 \text{ m/s}$ and $\nu = 3000 \text{ m/s}$ and that from $t = 4$ to $t = 23 \mu\text{s}$, the spectrogram does not depend much on time. We only see a slight decrease on velocity readings as displayed for example for $\nu = 2100 \text{ m/s}$ in Fig. 4(c). To understand this second observation, we have to consider the behavior of particles in vacuum.

In vacuum, the size-velocity distribution of the particles remains constant due to ballistic transport. The velocity difference between the front and the back particles will therefore stretch the ejecta along the z -axis linearly over time. Since the size-velocity distribution does not change, this stretch does not impact the local phase function but nonetheless it causes the particle number density to decrease as $1/t$ and therefore the mean-free paths to increase linearly with t . To predict the impact on the specific intensity measured by the PDV probe, it is instructive to stick to the random walk picture. On the one hand, since the mean-free paths expand at the same rate as the medium, all the random walks will expand accordingly, i.e. the light propagation in the ejecta is homothetic with time. If we consider the transverse profile of the specific intensity

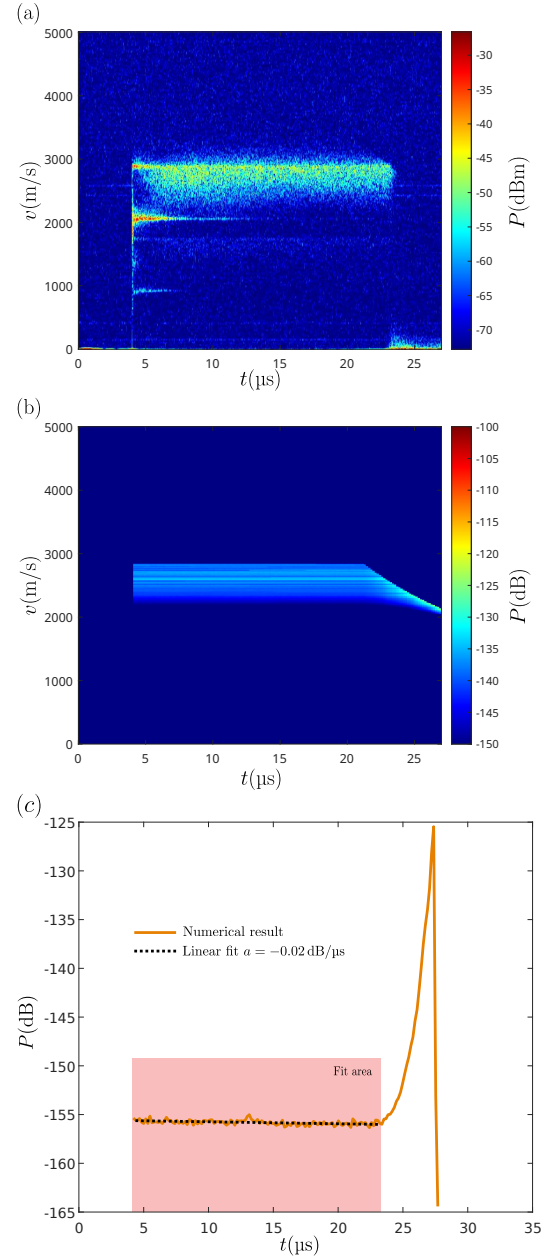


FIG. 4. (a) Experimental spectrogram in vacuum. The setup characteristics are given in Sec. II A. The shock pressure is $P_{\text{shock}} = 29.5 \text{ GPa}$ and vacuum residual pressure was $P_{\text{vacuum}} = 1 \text{ Pa}$. The ejecta is created at $t = 4 \mu\text{s}$, it travels in ballistic expansion before reaching the probe at $t = 23 \mu\text{s}$. (b) Simulated spectrogram in vacuum with a power law size distribution of parameter $\alpha = 5$. (c) Extraction of the simulated spectrogram at $\nu = 2100 \text{ m/s}$ which illustrates the expected signal small decrease from $t = 4$ to $t = 23 \mu\text{s}$.

distribution at the front of the ejecta, it spreads and therefore decreases quadratically with time t in the xy -plan. On the other hand, considering its narrow aperture of 4.2 mrad , the collection from the PDV probe mostly happens in a cylinder of diameter ϕ_p which does not change with time. The combination of both these phenomena results in a decrease with time of the PDV signal. In practice, considering that the

particle are mostly forward scattering, the light spread at the front of the ejecta remains small and the decrease is subtle as seen in Fig. 4(c). While obvious in the single scattering regime, this observation is here extended to multiple scattering. A formal explanation of this phenomena based on the RTE is provided in App. A. Finally, the fastest particles reach the probe at $t = 23 \mu\text{s}$ in both the experimental and simulated spectrograms. In the experimental case, this causes a particle accretion on the probe and an almost immediate loss of return signal. In the simulation, we do not account for this effect. The particles are simply removed for the medium and we eventually recover the free surface at $t = 27 \mu\text{s}$.

The key difference in the experimental spectrogram is that the free surface is visible almost over the full duration of the experiment, while it does not appear in the simulation. This observation suggests that the ejecta has a too large optical thickness b for the free surface to be seen. Indeed, we find $b = 16$ from $t = 4$ to $t = 23 \mu\text{s}$. To investigate this, we break down the scattering mean-free path contributions of each numerical particle compared to its corresponding particle size, i.e. we plot the integrand of Eq. (19). We observe in Fig. 5(a) that, while they do not contribute much to the mass of the ejecta, a group of numerical particles with a small associated size have the leading contribution to the scattering mean-free path. This ought to be the main reason why the free surface remains hidden in the simulated spectrogram compared to the experimental one. This result argues in favour of a size distribution with a lesser density at small particle sizes.

Beyond the standard power law distributions, lognormal size distributions have been proposed lately¹⁴. Since they tend to 0 when a tends to 0, they precisely address the divergence issue of power laws at small particle sizes. Therefore, we propose to change $h(a)$ to a lognormal distribution which reads

$$h(a) = \begin{cases} \frac{K}{a\sigma\sqrt{2\pi}} \exp\left[-\frac{\ln^2(a/a_0)}{2\sigma^2}\right], & \text{if } a \in [a_{\min}, a_{\max}] \\ 0, & \text{otherwise} \end{cases} \quad (24)$$

with $\sigma = 0.5$, $a_0 = 2.25 \mu\text{m}$, $a_{\min} = 1 \mu\text{m}$, $a_{\max} = 6 \mu\text{m}$ and $K = 2 / \left\{ \text{erf}\left[\ln(a_{\max}/a_0) / (\sigma\sqrt{2})\right] - \text{erf}\left[\ln(a_{\min}/a_0) / (\sigma\sqrt{2})\right] \right\}$ where erf is the Gauss error function. In Fig. 5(a), we see that for the same surface mass, the lognormal distribution tends to attenuate the contribution of the numerical particles having a small associated size. This results in a drastic decrease of the optical thickness to $b = 6$ and should allow to recover the free surface in the simulated spectrogram.

Figure 5(b) represents the simulated spectrogram in vacuum for this corrected size distribution. As expected, it allows one to recover the free surface in the spectrogram while keeping all the already present and desired characteristics of the simulated spectrogram.

A residual defect is that free surface response seems to fade away quicker in the experimental spectrogram than in the simulated one. We assume this effect is due the modelling of the free surface as a loss-less specular reflector instead of properly accounting for the deformation induced by micro-jetting. This tends to overestimate its contribution to the spec-

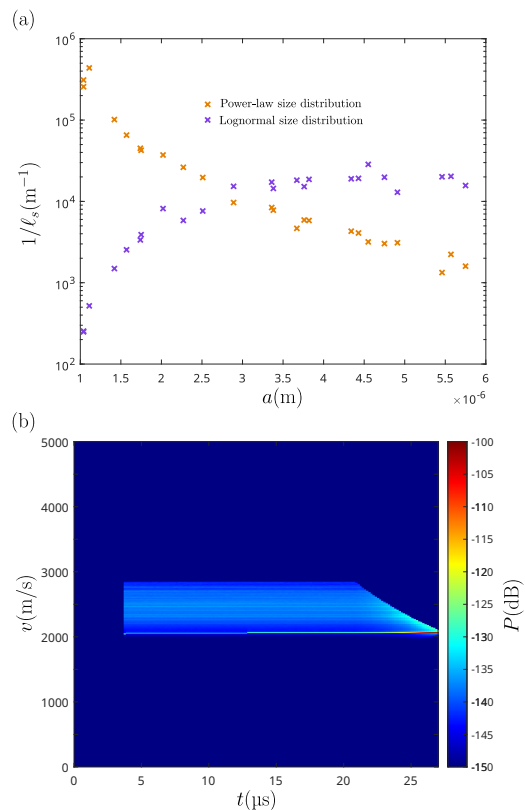


FIG. 5. (a) Scattering mean-free path contributions over size for power law and lognormal initial particle size distribution. (b) Simulated spectrogram in vacuum with a lognormal size distribution of parameters $\sigma = 0.5$ and $a_0 = 2.25 \mu\text{m}$.

trogram. Moreover, it is known experimentally and confirmed by molecular dynamics simulations^{10–12} that an intermediate regime exists right after breakout and before the transverse homogenization of the ejecta. In this time window, between $4 \mu\text{s}$ and $7 \mu\text{s}$ in Fig. 4 (a), the microjets' structure causes only the spike velocity at high values and the bubble velocity at values around the free surface to be visible in the early moment for the ejecta³⁴ [see Fig. 1 (b)]. This effect is indeed not rendered in the current simulation where we assume the ejecta creation to happen instantly at the breakout. Additionally, we also assume the ejecta to be translationally invariant right after breakout, which again takes a few microseconds experimentally. These phenomena explain the remaining discrepancies between the experimental and simulated spectrograms.

This study of ejecta in vacuum is conclusive and gives us a first draft of ejecta description. Comparing different simulated spectrograms to the experimental one allowed us to clearly favor one distribution over the other only based on a PDV spectrogram. Before, a choice would have been harder to justify. The next step is a more complex particle transport scenario - ejecta in helium - and the aim is to see if the description established in vacuum holds.

B. Drag coefficient effect study for ejecta in helium

We now consider an ejecta in helium at $P_{\text{helium}} = 500 \text{ kPa}$. We assume the same initial size distribution as in vacuum, the lognormal distribution given in Eq. (24), but now the presence of gas will change the transport of particles as stated in Sec.II B. In case of helium, the shockwave in gas, with a velocity $v = 3084 \text{ m/s}$, travels ahead of most of the ejecta. Therefore, particles travel in shocked gas resulting in low particle-gas velocity differences. The Weber number We_i given by Eq. (8) remaining subcritical, the ejecta interacts with the gas mostly through drag forces. Figure 6(a) represents the experimental spectrogram in helium. The interaction with gas can be seen in the slowing down of the fastest particles, typically from 3000 m/s to 2500 m/s . Since the drag force \mathbf{F}_i scales with particle size as a_i^2 , the slowing down of particles scales in a_i^{-1} . Recovering the slowing down slope in simulated spectrograms would further confirm the choice of the size distribution. To have a comparison point for the simulations, we compute a numerical fit of the experimental spectrogram's upper boundary. It appears as a red overlay in Fig. 6.

As for vacuum in Sec. IV A, we use the *Phénix* code to compute the ejecta description throughout transport in helium. We then use this output data to simulate the expected spectrogram in Fig. 6(b) and compare it with the experimental one. We see in Fig.6(b) that we kept the desired characteristics obtained in the vacuum case, but this first spectrogram in helium does not fit the slowing down curve of the experimental spectrogram. The slowing down of particles is underestimated, suggesting that the current drag force \mathbf{F}_i is undervalued. Considering the expression of \mathbf{F}_i in Eq. (7), to increase drag forces we can either shift back the particle size distribution towards smaller particles or increase the drag coefficients C_d . Since we need to change the slowing down slope of the spectrogram while keeping the current optical thickness, we have chosen to modify the drag coefficients C_d to fit the experimental spectrogram. Indeed, in a context where drag models in turbulent flows are still under debate^{35,36}, we use this case in helium to experimentally tune the drag coefficient model for our ejecta thanks to the comparison allowed by simulated spectrograms. After such a correction, the drag coefficient are roughly multiplied by a factor of 5 compared to their initial values and we obtain another spectrogram in helium which is shown in Fig. 6(c). This time, the slowing-down nicely fits the experimental upper boundary. A down side remains the overvaluation of the free surface which remains visible in the simulated spectrogram while it disappears at $t = 8 \mu\text{s}$ in the experimental one. This bias of the model was already discussed in Sec. IV A.

Now that we have a size distribution tested in the presence of a drag force, the next step is to see how it holds up in a configuration with an additional interaction, i.e. hydrodynamic break-up.

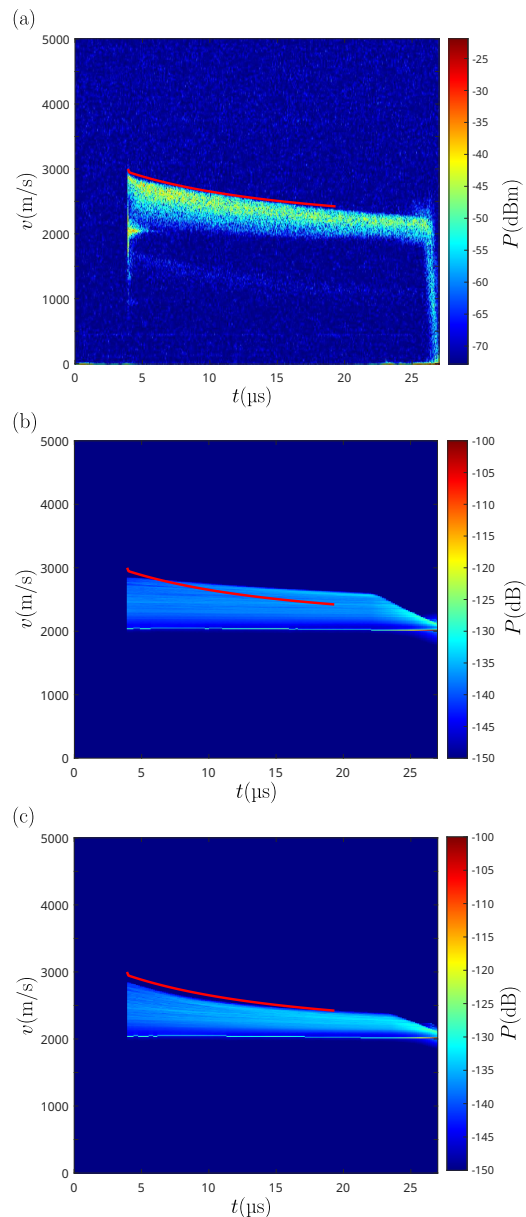


FIG. 6. (a) Experimental spectrogram in helium. The setup characteristics are given in Sec. II A. The shock pressure is $P_{\text{shock}} = 29.5 \text{ GPa}$ and helium pressure was $P_{\text{helium}} = 500 \text{ kPa}$. The ejecta is created at $t = 4 \mu\text{s}$, it travels in helium before reaching the probe at $t = 26 \mu\text{s}$. The spectrogram is overlaid with an analytic fit of its upper boundary (red line). (b) Simulated spectrogram in helium for a lognormal size distribution of parameters $\sigma = 0.5$ and $a_0 = 2.25 \mu\text{m}$, overlaid with an analytic fit of the upper boundary of the experimental spectrogram (red line). (c) Simulated spectrogram in helium for a lognormal size distribution of parameters $\sigma = 0.5$ and $a_0 = 2.25 \mu\text{m}$, corrected drag force coefficients and overlaid with an analytic fit of the upper boundary of the experimental spectrogram (red line).

C. Ejecta break-up model in air

We now consider the final and most complicated case, ejecta transport in air. We keep the same size distribution as in helium, the lognormal distribution given by Eq. (24), and check its relevance in this new scenario. In air, the initial shockwave travels at $v = 2520\text{m/s}$. This means that while the slowest particles travel in shocked air and, as in helium, interact with the gas mostly through drag forces, the fastest particles travel in unshocked air. For the latter, if they are rather small, they slow down rapidly through drag forces before being caught-up by the shockwave and eventually reaccelerated in shocked air. If they are rather big, their Weber number We_i is supercritical and they additionally experience break-up. They may first slow down with a gentle slope but as soon as they break up, their reduced size makes them slow down much faster before being caught by the shock wave and reaccelerated in the shocked air. In Fig. 7(a), displaying the experimental spectrogram in air, we can observe both phenomena. Between 4 and $7\mu\text{s}$, we can see a plateau around 2800m/s corresponding to the fast particles before break-up. After break up, around $8\mu\text{s}$, the free surface gets screened and the slowing down is much more substantial. In the meantime, between 10 and $15\mu\text{s}$, we see around 1800m/s the reacceleration of the slowest particles. We aim to capture these two phenomena in the simulated spectrogram.

Figure 7(b) represents the simulated spectrogram in air. The expected key features are clearly observed. Firstly, we observe that high velocity particles remain visible between $t = 4$ and $t = 6\mu\text{s}$ before disappearing, which matches very well the experimental spectrogram. Secondly, some particles are heavily slowed down and then reaccelerated by the shocked air between $t = 7$ and $t = 10\mu\text{s}$. While this behavior is expected, it happens a bit too early, we do not expect to see the reacceleration before $t = 10\mu\text{s}$. Thirdly, we keep the free surface velocity in the early moment of the spectrogram before break-up screens it. Finally, the main issue is the long term velocity distribution. While in the experiment, all velocities tend to the gas velocity of $v = 2060\text{m/s}$, in the simulation a spreading between $v = 2000\text{m/s}$ and $v = 2400\text{m/s}$ remains. We believe that the inability to perfectly match the experimental spectrogram puts forward the limit of validity of the hypothesis made in Sec. II A on the initial size-velocity distribution. Namely, this observation argues in favor of a correlated size-velocity distribution. This question is discussed in Sec. V.

V. DISCUSSION

A certain number of observations have been made in this study and it is worth discussing their implications, and to compare them to results reported in the existing literature.

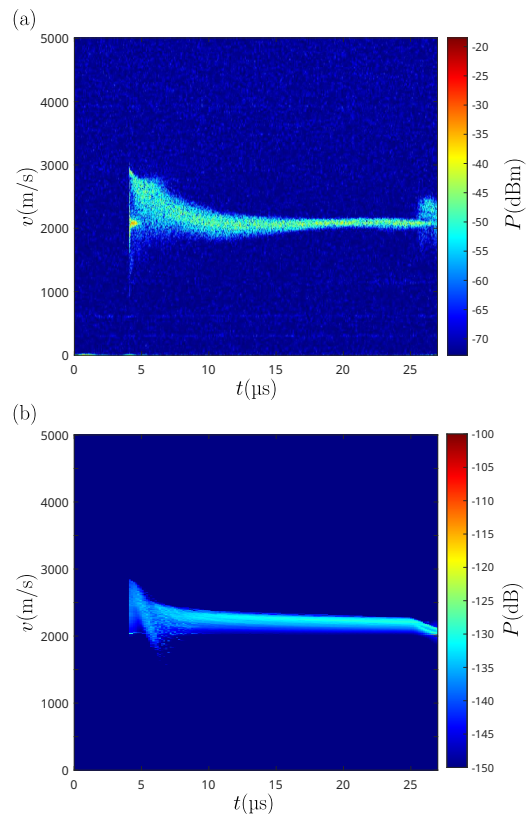


FIG. 7. (a) Experimental spectrogram in air. The setup characteristics are given in Sec. II A. The shock pressure is $P_{\text{shock}} = 29.5\text{GPa}$ and air pressure is $P_{\text{air}} = 100\text{kPa}$. The ejecta is created at $t = 4\mu\text{s}$. The ejecta front is heavily slowed down and experience break-up in unshocked air until $t = 10\mu\text{s}$. From $t = 10$ up to $t = 20\mu\text{s}$ the slowest particles fall back in shocked air and are reaccelerated. From $t = 20$ to $t = 27\mu\text{s}$, all particles seem at free surface velocity. (b) Simulated spectrogram in air for a lognormal size distribution of parameters $\sigma = 0.5$ and $a_0 = 2.25\mu\text{m}$.

A. Effect of particle break-up on the scattering mean-free path

In Sec. IV A, we showed that small particles between $1\mu\text{m}$ and $3\mu\text{m}$ had the leading contribution to the scattering mean-free path. This observation was confirmed by the free surface disappearance for ejecta in air in Sec. IV C. We attributed this phenomenon to an increase in the optical thickness due to the break-up of initially large particles into numerous smaller ones. To check this hypothesis, we have used the simulation results of the *Phénix* code and Eq. (13) to compute the optical thickness during each simulation reported in Sec. IV. The results are reported in Fig. 8. We see that for all three simulations, the initial optical thickness is around $b = 6$, since all simulations have the same initial size-velocity distribution. In the vacuum and helium cases, this optical thickness remains constant until $t = 23\mu\text{s}$ where the ejecta gets shaved down from reaching the probe. It eventually decreases back to zero by $t = 27\mu\text{s}$. In the case of air, we see that because of fragmentation the optical thickness increases up to $b = 9$ from $t = 4$ to

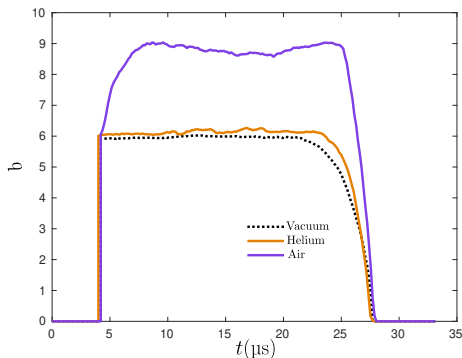


FIG. 8. Optical thickness evolution during the simulation for each gas configuration. Using the simulation results from *Phénix* code and Eq. (13), the optical thickness is computed during the time corresponding to the experiments. The three ejecta simulations for a lognormal size distribution of parameters $\sigma = 0.5$ and $a_0 = 2.25 \mu\text{m}$ seen in Sec. IV are represented: vacuum (dotted black line), helium with corrected drag coefficients (solid orange line) and air (solid magenta line)

$t = 7 \mu\text{s}$.

Buttler *et al.*²⁰ investigate ejecta in gas as well but consider a reactive break-up scenario. In their study, a cerium ejecta is created and travels in deuterium gas. Through an hydriding reaction between the metal and the gas, the initial particles also break up into multiple smaller ones. This mechanism is similar to the hydrodynamic break-up in air we consider but interestingly Buttler *et al.* report opposite observations. In their experiment, they assume that the fragmentation of the ejecta's front in smaller particles makes it invisible to the PDV wavelength, allowing to see particles that up to that point had been hidden in the back of the ejecta. A key point to understand this difference is to consider the size limit reached by each break-up mechanism. In the case of tin ejecta in shocked air we reach an average size of $a = 1 \mu\text{m}$ while Buttler *et al.* assume the average size of particles to be on the order of $a = 100 \text{nm}$. For a mono-disperse ejecta of homogeneous particle number density, the initial scattering mean-free path is $\ell_{s,0} = 1/[\rho(a_0)\sigma_s(a_0)]$ with a_0 the initial particle size and $\rho(a_0)$ the corresponding initial particle number density. If this ejecta were to break up into smaller particles of size a with mass conservation, the particle number density would scale as $\rho(a)/\rho(a_0) = (a_0/a)^3$, leading to

$$\ell_s(a) = \frac{a^3}{a_0^3 \rho(a_0) \sigma_s(a)}. \quad (25)$$

We have studied the scattering-mean free path given in Eq. (25) for a tin ejecta of an initial size $a_0 = 10 \mu\text{m}$ and $\rho(a_0) = 10^{14} \text{m}^{-3}$ and used Mie theory^{37,38} to compute the scattering cross-sections σ_s . In Fig. 9, we report its variation from $10 \mu\text{m}$ down to 10nm . We observe that, upon break-up and down to $a = 250 \text{nm}$, the scattering mean-free path first decreases. This is consistent with the phenomenon we observed for hydrodynamic break-up. It corresponds to

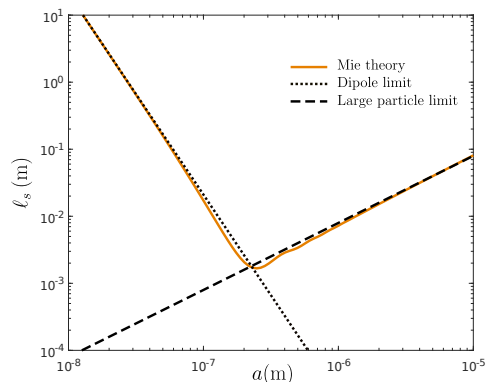


FIG. 9. Scattering mean-free path for a size mono-disperse ejecta of tin in air experiencing fragmentation. The exact scattering mean-free paths is computed tanks to Mie theory (orange solid line). For comparison, we display the dipole limit case (black dotted line) and the large particle limit case (dashed solid). Mie theory allows one to describe the scattering mean-free path evolution over this large break-up window and recover limit cases at each end of it.

the limit case of particles much bigger than the wavelength. The scattering cross-section scales as $\sigma_s(a) \sim a^2$ and therefore the scattering mean-free path as $\ell_s(a) \sim a$. Now, if we were to reach smaller particle sizes, for example due to reactive break-up as in the study of Buttler *et al.*, we see that the scattering mean-free path would increase again - even exceeding its initial value below $a = 60 \text{nm}$. We have reached here the limit case of dipole approximation where the scattering cross-section scales as $\sigma_s(a) \sim a^6$ and therefore the scattering mean-free path as $\ell_s(a) \sim a^{-3}$. Both limit cases are represented in Fig. 9. We believe that this mechanism explains the phenomenon observed by Buttler *et al.* after multiple break-up cycles for cerium in deuterium. Break-up first decreased the scattering mean-free path, as in our case, followed by an increase large enough to uncover particles initially hidden.

The effects of reactive break-up were not opposite to the ones of hydrodynamic break-up, they were in fact exceeding them. Going past the initial decrease in the scattering mean-free path, the increase for small particle was enough to exceed the initial mean-free path.

B. Introducing size and velocity dependencies

As mentioned in Sec. IV C, the main issues in the simulated spectrogram show up at the end of the experiment and in its early moments. At the end of the simulation, the spread in velocity is broader than the one observed experimentally. We believe this is due to large particles, that sit right before the shockwave in gas. These particles only travel in shocked air, therefore their velocity differential to the gas is low and they do not break-up. In the meantime, they are too big to slow down only through drag force to the free surface velocity and by the $20 \mu\text{s}$ mark. The velocity curve of such a particle with radius $a = 4.15 \mu\text{m}$ taken from the ejecta dynamics simulation

is overlaid in red on the simulated spectrogram in Fig. 10. This observation argues in favor of a size velocity distribution with bigger particles at low velocities and smaller particles at higher velocities. This is in agreement with observations made by holographic measurements¹⁵ and the ejecta mechanism suggested by molecular dynamics simulations^{10–12}.

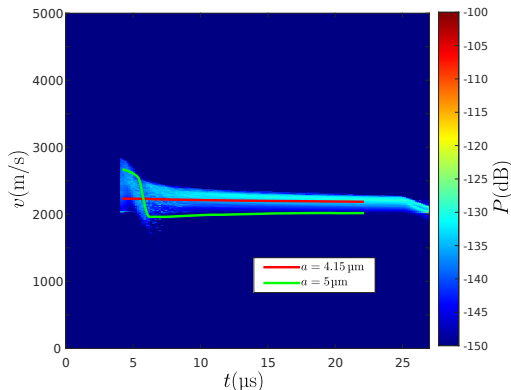


FIG. 10. Simulated spectrogram in air for a lognormal size distribution of parameters $\sigma = 0.5$ and $a_0 = 2.25 \mu\text{m}$. The simulated spectrogram is overlaid with the velocity curves of two interesting numerical particles extracted from the corresponding *Phénix* simulation: a particle of radius $a = 4.15 \mu\text{m}$ with an initial velocity of $v = 2234 \text{ m/s}$ (red solid line) and a particle of radius $a = 5 \mu\text{m}$ with an initial velocity of $v = 2670 \text{ m/s}$ (green solid line)

Nonetheless, in the early moments, particles at the front of the ejecta must correspond to the high-velocity plateau between $t = 4$ and $t = 6 \mu\text{s}$. These particles need to be big enough so that despite of heavy drag forces in non shocked air they do not slow down immediately. When eventually they break-up and slow down, they also allow to recover the re-acceleration slope below the free surface velocity between $t = 7$ and $t = 10 \mu\text{s}$. An example of such a particle of radius $a = 5 \mu\text{m}$ taken from our simulation is overlaid in green on the simulated spectrogram in Fig. 10.

We believe this observation balances the previous one and illustrates the need of a more complex size velocity distribution. Overall, we need big particles at the back of the ejecta and small particles at the front to achieve the long term velocity profile. This distribution must then be completed with a few big particles typically for the ejecta head, to observe the desired plateau in the early moments. While investigating such correlations is beyond the scope of this article, this is an insightful observation. The ability to simulate spectrograms has not only allowed to constrain size-velocity distributions to experimental spectrograms, but also to confirm that the actual size velocity distributions of ejecta ought to be correlated distributions.

VI. CONCLUSION

In summary, we have shown that PDV measurements could be used to retrieve additional information on the size distri-

bution of ejecta particles in shock compression experiments. Based on an exact relationship between the specific intensity and the measured signal in PDV experiments and a rigorous RTE model for PDV experiments in the multiple scattering regime, we have shown the influence of particle size distribution in PDV spectrograms. To exploit this sensitivity, we implemented a simulation scheme allowing to use directly the results of ejecta hydrodynamic simulations to compute simulated spectrograms. This opens up the possibility of indirect size-velocity distribution evaluation thanks to different particle transport conditions accounting for drag forces and particle break-up models. Finally, a comprehensive study on a real-conditions experiment showed how, through an iterative process, spectrogram simulation allowed to better our ejecta description. We are not aware of any technique that can describe in detail the partition of mass below the resolution limit of that diagnostic. Indeed, we observed the effect of particles down to $a = 60 \text{ nm}$ while still working at $\lambda = 1.55 \mu\text{m}$.

From a more general point of view, this work is a proof of concept of a simulation chain aiming to mimic PDV measurement in ejecta experiments. It shows that with a clear implementation of the direct problem including the full path from an ejecta to its expected spectrogram, the comparison with experimental spectrogram already allows one to have insightful ideas for the inverse problem of reconstructing this ejecta (or at least its statistical properties). In the case of size-velocity distribution studies, this work argues in favor of correlated size-velocity distributions, for the early moments of the experiment, corresponding to the phenomenology captured by molecular dynamics simulations. The current simulation chain, including particle transport and spectrogram simulation, would remain identical. Coupled with a better treatment of light scattering close the free surface, typically around the micro-jets, we believe this would allow to recover experimental spectrograms even in very complex cases as in air. This kind of indirect measurements could be applied to many other ejecta scenarios, especially those with no analytical expression of the size-velocity distribution throughout the experiment. For example, the transport of reactive ejecta in gas. In addition, this opens the possibility of sensitivity studies on other parameters such as shock pressure, illumination wavelength or material type. In this work, the fact that the simulated spectrograms give semi-quantitative results, i.e., that spectrograms have the right dynamics even if their absolute values are shifted from the experimental ones, allowed one to compare them to their experimental counterpart. Either by the presence of the free surface or the shape of slowing down slope of the fastest particles, being able to visually compare spectrograms have proven plenty useful in this study. For future work, this difference would need to be measured by global and local metrics that allow quantifying the distance between spectrograms, either experimental or simulated. These are potential lines to be followed in further investigations.

ACKNOWLEDGMENTS

This work has received support under the program “Investissements d’Avenir” launched by the French Government.

DATA AVAILABILITY STATEMENT

The data that supports the findings of this study are available within the article.

Appendix A: Spectrogram invariance for single shock ejecta in vacuum

In the ejecta geometry where the mean-free path and the phase function depend only on depth, and in the quasi-static approximation (slow cloud dynamics compared to the light travel time in the ejecta), the RTE given in Eq. (15) becomes

$$\begin{aligned} & \left[\mathbf{u} \cdot \nabla_{\mathbf{r}} + \frac{1}{\ell_e(\mathbf{r} \cdot \mathbf{u}_z, t, \omega)} \right] I(\mathbf{r}, \mathbf{u}, t, \omega) \\ &= \frac{1}{\ell_s(\mathbf{r} \cdot \mathbf{u}_z, t, \omega)} \int p(\mathbf{r} \cdot \mathbf{u}_z, \mathbf{u}, \mathbf{u}', t, \omega, \omega') I(\mathbf{r}, \mathbf{u}', t, \omega') d\mathbf{u}' \frac{d\omega'}{2\pi}. \end{aligned} \quad (\text{A1})$$

Equation (A1) taken at $\mathbf{r}(1 + \Delta t/t)$ and $t + \Delta t$ reads

$$\begin{aligned} & \left\{ \mathbf{u} \cdot \nabla_{\mathbf{r}} + \frac{1}{\ell_e[\mathbf{r}(1 + \Delta t/t) \cdot \mathbf{u}_z, t + \Delta t, \omega]} \right\} \\ & \quad \times I[\mathbf{r}(1 + \Delta t/t), \mathbf{u}, t + \Delta t, \omega] \\ &= \frac{1}{\ell_s[\mathbf{r}(1 + \Delta t/t) \cdot \mathbf{u}_z, t + \Delta t, \omega]} \\ & \quad \times \int p[\mathbf{r}(1 + \Delta t/t) \cdot \mathbf{u}_z, \mathbf{u}, \mathbf{u}', t + \Delta t, \omega, \omega'] \\ & \quad \times I[\mathbf{r}(1 + \Delta t/t), \mathbf{u}', t + \Delta t, \omega'] d\mathbf{u}' \frac{d\omega'}{2\pi}. \end{aligned} \quad (\text{A2})$$

In a single shock experiment in vacuum, the particles at the depth $\mathbf{r} \cdot \mathbf{u}_z$ at time t are the one that will be at the depth $\mathbf{r}(1 + \Delta t/t) \cdot \mathbf{u}_z$ at time $t + \Delta t$. Therefore the mean-free path and phase function obey the following conservation law

$$p\left[\mathbf{r}\left(1 + \frac{\Delta t}{t}\right) \cdot \mathbf{u}_z, \mathbf{u}, \mathbf{u}', t + \Delta t, \omega, \omega'\right] = p(\mathbf{r} \cdot \mathbf{u}_z, \mathbf{u}, \mathbf{u}', t, \omega, \omega'), \quad (\text{A3})$$

$$\ell_{s,e}\left[\mathbf{r}\left(1 + \frac{\Delta t}{t}\right) \cdot \mathbf{u}_z, t + \Delta t, \omega\right] = \ell_{s,e}(\mathbf{r} \cdot \mathbf{u}_z, t, \omega) \left(1 + \frac{\Delta t}{t}\right). \quad (\text{A4})$$

While the phase function remains constant, for the mean-free paths the $(1 + \Delta t/t)$ factor accounts for the decrease in particle density caused by the homothetic stretch of the ejecta along the z -axis. Using this property, Eq. (A2) multiplied by

$(1 + \Delta t/t)$ reads

$$\begin{aligned} & \left[\mathbf{u} \cdot \nabla_{\mathbf{r}} (1 + \Delta t/t) + \frac{1}{\ell_e(\mathbf{r}, t, \omega)} \right] I[\mathbf{r}(1 + \Delta t/t), \mathbf{u}, t + \Delta t, \omega] \\ &= \frac{1}{\ell_s(\mathbf{r} \cdot \mathbf{u}_z, t, \omega)} \int p(\mathbf{r} \cdot \mathbf{u}_z, \mathbf{u}, \mathbf{u}', t, \omega, \omega') \\ & \quad \times I[\mathbf{r}(1 + \Delta t/t), \mathbf{u}', t + \Delta t, \omega'] d\mathbf{u}' \frac{d\omega'}{2\pi}. \end{aligned} \quad (\text{A5})$$

Comparing Eqs. (A1) and (A5) shows that at t and $t + \delta t$ the specific intensity obeys to the same equation except that in the latter configuration all distances are to be scaled up by a factor $1 + \Delta t/t$, which formally proves the claim of Sec. IV A.

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