

Demonstration of a code coupling framework for modeling beam-collimator impacts in the advanced photon source

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The high-brightness beams being produced in current and future accelerators present new machine protection concerns with the potential for high-energy-density (HED) conditions ($> 100 \text{ J/mm}^3$) in beam-intercepting components. Simulating HED conditions in accelerators requires utilizing a suite of physics codes for particle dynamics, particle-matter interactions, and hydrodynamics. This paper describes a method of coupling the codes ELEGANT, FLUKA, and FLASH to simulate the effects of a rapid beam loss in the advanced photon source storage ring and the resulting interaction of the beam and collimators. This paper expands previous work [J. Dooling *et al.*, Collimator irradiation studies at the advanced photon source, in *Proceedings of the IBIC-2023* (2023), pp. 245–249] by introducing a definition of the evolving geometry of the collimator surface as well as providing methods for simulating the absorption of synchrotron radiation and tracking shower particles produced during beam strikes. We demonstrate this framework by simulating machine conditions of the APS ring before and after its recent upgrade. Simulation results are compared with observed damage to collimators and test samples taken from the APS ring.

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I. INTRODUCTION

Several x-ray user facilities around the globe are engaged in major upgrades to “fourth-generation” light sources [1–5], defined by significantly reduced transverse emittances. However, this creates new challenges for machine protection since increased brightness will result in higher energy density beams that can damage machine beamline components through beam loss or continuous absorption of synchrotron radiation [6].

The advanced photon source upgrade (APS-U) at Argonne National Laboratory has recently commissioned a low-emittance-lattice, fourth-generation storage ring (4GSR). The new SR contains several important machine protection system (MPS) components [7], including a decoherence kicker, a vertically-deflecting fan-out kicker (FOK), and five horizontal collimators. The APS-U SR

operates at 6 GeV with a total maximum circulating charge of 736.5 nC (200 mA), and with effective horizontal emittances (geometric emittance in the absence of dispersion) of 32/42 pm in either of its two operational modes: brightness or timing. Energy densities in potential targets could be on the order of $E_d = 10\text{--}100 \text{ J/mm}^3$; the upper end of this range defines high-energy-density (HED) conditions [8]. This represents dose levels D of 3.7–37 MGy for solid aluminum and 1.1–11 MGy for solid copper. Here $D = E_d/\rho$, where ρ is the density. In the event of sudden beam loss, the beam can strike machine components, potentially resulting in significant damage. Figure 1 shows a photo of a collimator removed from the upgraded APS storage ring in January 2025. The beam-intercepting face of the collimator is $14 \times 50 \text{ mm}$ and the depth is 20 mm.

The MPS [9] is responsible for monitoring the beam orbit and identifying when it may be lost [10]. In the event of a rapid beam loss, the main rf is muted allowing the beam to spiral inboard and strike the collimators. When a loss is indicated, the beam will also be deflected vertically using a FOK. Strong sextupoles will also cause the beam to spread out transversely so that the energy density is reduced and captured by a series of five horizontal collimators in the

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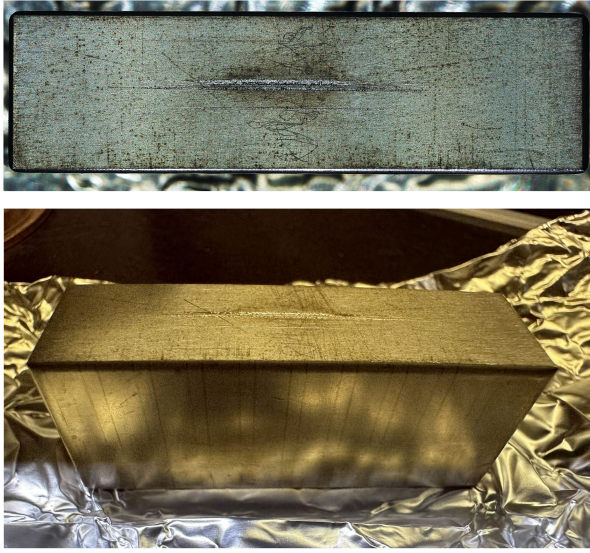


FIG. 1. Top-down view (top) and profile view (bottom) of an aluminum collimator removed from APS in January 2025 showing signs of damage from beam interactions.

ring [11]. The goal is to prevent mechanical damage to all vacuum machine components; however, the HED conditions present in the APS-U may still result in damage to the collimators over time or immediately if the FOK misfires [12]. To better understand the risks to the machine and monitor collimator health, we developed a series of computational tools to simulate these events.

There is no individual code which captures all of the physics present in these types of beam loss events. Several groups have developed methods for modeling these types of beam interactions by coupling different physics codes [13–18] to make up for multiphysics and multiscale needs. While these attempt to couple codes for studying collimator strikes in storage rings, e.g., SIXTRACK-FLUKA at CERN [19], they do not have the ability to simulate hydrodynamics and geometry evolution. Other tools like Geant4/G4beamline [20,21] produce high-fidelity simulations of particle-matter interactions and beam transmission but lack ring tracking and hydrodynamic capabilities. We take a similar approach in this study and use a series of codes to integrate multiple physical processes to modeling HED conditions in the machine protection components of APS-U. More specifically, this paper outlines a coupled framework of three physics codes, each of which captures separate physics, including ELEGANT [22] for particle dynamics, FLUKA [23] for particle-matter interaction and energy deposition, and FLASH [24] for hydrodynamics.

This manuscript is structured as follows. Section II outlines the general framework for coupling the three codes describing the scope, input, and output of each of them and the tools used to interface between them. The section also introduces the evolving geometry scheme used

to model the erosion of the collimator surface within the duration of the beam loss. Section III describes how particle dynamics are handled as the beam data is exchanged between ELEGANT and FLUKA. The particle tracking is primarily conducted in ELEGANT and the APS-U lattice is described in Sec. III A. Section III B then describes the initial FLUKA geometry, dose binning, and methods for improving dosemap quality. Section IV outlines the physics modeling considerations in FLASH, including the geometry evolution in Sec. IV A, thermal properties and conditions of phase transitions in Sec. IV B, and the 3 T capabilities of FLASH and the heat exchange between electrons and ions in solid/liquid material in Sec. IV C. In Sec. V C, we show our simulation results validated and benchmarked against two sets of observed collimator damage: (i) an earlier 2023 experiment that studied beam strikes on copper and aluminum in the APS *prior* to the upgrade and (ii) damage that occurred during commissioning and first user run of the *upgraded* storage ring. This section also describes unexpected behaviors witnessed during beam losses and attempts to characterize and model them. These simulations mimic the dynamics seen in the machine and are validated against experimental observations.

II. COUPLED FRAMEWORK

Each of the three codes has specific formatting requirements for their respective input and output. The coupled framework is a method of automatically interfacing between each in a way that simulates the changes in the target material geometry during irradiation. This framework comprises two interacting loops as displayed in Fig. 2, including one that couples ELEGANT and FLUKA for tracking particle dynamics within the electron beam and another that couples FLUKA and FLASH for updating the target surface geometry. A series of Python and TCL scripts are used to handle the data sharing by converting the particle coordinates between the formats used by ELEGANT and FLUKA, subdividing the beam into groups of bunches, combining multiple FLUKA simulations into a single

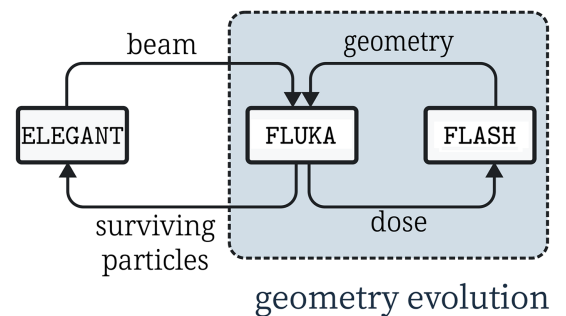


FIG. 2. Diagram of the simulation coupling. Particle dynamics through the APS/APS-U lattice are handled all at once by ELEGANT. The geometry evolution handled by FLUKA and FLASH can occur multiple times within a single pass.

dosemap, generating the FLUKA geometry using the FLASH output, and moving files between subdirectories.

The particle tracking is primarily handled within ELEGANT while FLUKA is used to simulate the interaction between the electron beam and target material. Each simulation begins in ELEGANT, tracking the beam until it starts to interact with the target. The particle coordinates are converted from the SDDS format used by ELEGANT to the source format expected by FLUKA and are read in using a custom SOURCE card. In FLUKA, the particle loss and energy deposition are computed and surviving particles return to ELEGANT to continue particle tracking through the storage ring lattice.

The FLUKA-FLASH loop models the interaction between the beam and a single target. It is possible to simulate multiple beamline targets using multiple instances of the geometry update loop. However, in these simulations, the overwhelming majority of particles are lost at a single collimator. For these collimator simulations, we simulate the full interaction of a single collimator while the rest are modeled as static apertures. The target materials that interact directly with the electrons are aluminum and copper; however, in the APS-U SR, the horizontal collimator jaws are fabricated from aluminum alloy 6061-T6511. The geometry-evolution loop models the thermodynamic behavior of the material and updates the geometry as the material changes phase. The energy deposited by the beam is calculated by FLUKA and recorded in a 3D histogram that matches the FLASH simulation grid. FLASH reads in the dosemap, deposits the energy for each bunch, and evolves the thermodynamic properties of the solid material. When a cell meets the conditions for vaporization, it is released from the solid hydrostatic state and evolves as a plasma fluid cell hydrodynamically in FLASH. The final state of the FLASH simulation step is used to generate the FLUKA geometry definition on the same simulation grid. Section IV includes a detailed description of the release conditions, thermodynamic modeling, and equations of state.

A. Comments on changes in workflow

The framework is designed to automate as much of the simulation work as possible. However, certain simulation conditions require the user to manually run and change parts of the input files. Each of the codes, ELEGANT, FLUKA, and FLASH, requires the user to specify the initial environment. In ELEGANT, these are the lattice and command files which define the accelerator lattice and control the tracking and will be defined by the machine being simulated. FLUKA and FLASH require the user to define the geometry of the impacted region relative to the ELEGANT output. Once each of the simulations is set up for the desired use case, the coupled framework interfaces between them but there are a few steps taken *by the user* prior to a fully-coupled simulation.

The simulations presented here study the effects of a vertical deflection kicker on the beam loss for a range of beam configurations. By varying the strength of the kicker, the vertical size of the impacted region changes. Other dynamics such as duration of the beam loss may be affected by the beam configuration. The first step in each simulation is to run the ELEGANT tracking without the FLUKA-FLASH loop. The loop is replaced with a static collimator element and the particle losses are recorded to a file. This file is used to determine the vertical range of lost particles as well as the pass numbers (machine turn number) on which particles impact the collimator. The vertical range is used to set the $y_{\min}/y_{\max}$ parameters in FLUKA and FLASH to minimize the volume of the simulation domain while capturing the entirety of the heat affected region. The ELEGANT loss data also give the initial turn on which particles strike the collimator. This is used to set the initial pass of the FLUKA-FLASH loop so that the loop is only called when beam will interact with the collimator material. Because a number of conditions may cause the beam to be lost earlier or later, this paper uses the term “pass number” to mean the number of machine revolutions from the start of the FLUKA-FLASH loop, i.e., when the beam first interacts with the collimator. Similarly, the grid resolution in each simulation is the same, i.e., number of voxels in each plane, but the physical boundaries are determined by the simulation requirements.

FLASH is the most computationally expensive step of the simulations. We ran a series of benchmark FLASH simulations using a single, aggregated dosemap to evaluate the scaling of node configurations. Table I lists the time (in seconds) required to run 8 depositions, or 1/6 of a turn (6.14 μ s), for a range of grid resolutions and node distributions using the Argonne Laboratory Computing Resource Center (LCRC) “Improv” cluster [25]. With the scaling shown by FLASH, we selected a grid resolution of $128 \times 128 \times 16$ for each of our simulations using $n = 16$ processes in both x/y . FLUKA and ELEGANT are both run using $n = 64$ processes for a maximum of $n = 320$ across all programs at any time. The ELEGANT beam comprises 48 bunches of 10,000 macroparticles for a total of 480,000 particles. With this distribution of resources, each pass requires $t_{\text{FLUKA}} = 24$ min, $t_{\text{FLASH}} = 44.1$ min, and $t_{\text{ELEGANT}} = < 1$ min, or (~ 68 min/pass).

TABLE I. FLASH runtime for select simulation configurations of an 8 deposition duration, with variable grid size and node distribution showing strong scaling.

Grid cells			Processes				
x	y	z	x	y	z	Total	Time (s)
128	128	16	16	16	1	256	441
			8	8	2	128	607
			8	8	1	64	853
256	256	32	16	16	1	256	2412

III. PARTICLE DYNAMICS AND MATTER INTERACTION

A. APS/APS-U lattice

The APS-U storage ring lattice is made up of 40 identical, multibend achromat sectors [26] and will contain 44 insertion devices (IDs) stationed in the straight sections between bends. Of the 40 sectors, five have no IDs but instead are dedicated to maintaining the beam, three contain the 12 main rf cavities, one is used for injection/extraction, and one contains the bunch-lengthening harmonic cavity and swap-out kickers [7]. Five sectors near the injection region of the ring (sector 1 and sectors 37–40) contain horizontal collimators designed to capture particles which receive high amplitudes from gas scattering, Touschek scattering, or nonoptimal injection. They will also act to capture particles in the event of a fast beam loss. The APS-U lattice functions and their values at the horizontal collimator location are presented in Fig. 3.

Several subsystems are responsible for monitoring the beam and initiating a fast beam abort when a beam loss is probable. During a fast beam abort, the MPS dumps the beam in a controlled manner by muting the rf power and allowing the beam to strike the collimator. Due to the small transverse beam size resulting from the APS-U lattice, rapid beam losses have the potential to vaporize the collimator material on impact. To mitigate this, the beam is first spread out using a vertically-deflecting fan-out kicker (FOK) [27], which provides a pulsed magnetic field.

These simulations start by modeling the full APS-U storage ring in ELEGANT in a series of stages. Starting with a beam containing 48 (timing mode) or 324 (brightness mode) bunches, ELEGANT tracks macroparticles to equilibrium using a simplified linearized matrix (ILMATRIX) element. In this step, the impedance model and rf cavity feedback are slowly ramped up to full strength and the synchrotron radiation effects are computed in a single step each turn using the SREFFECTS element. When the beam, rf cavity, and impedance effects reach equilibrium, ELEGANT

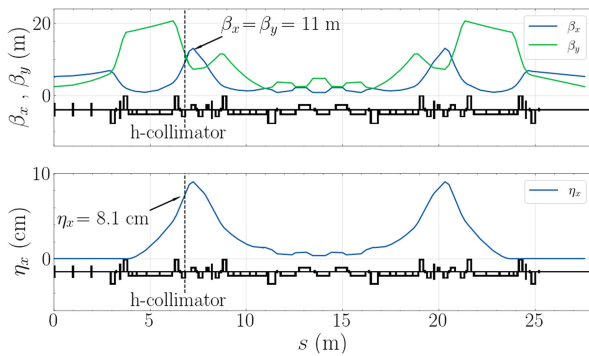


FIG. 3. Lattice functions of a single APS-U sector as well as values at the location of the horizontal collimator. The location of the horizontal collimator is shown in both by the black dashed line.

switches to full element-by-element tracking and the rf generator is muted to simulate a trip. The rf field experienced by the beam following the trip is modeled by the RFMODE element. The FOK is triggered approximately 5 μ s after the rf is muted. The BUMPER element applies a vertical kick to the beam with a maximum deflection angle and waveform defined by the user.

After $\sim 40 - 100$ turns (0.14–0.37 ms, 1 turn = $T_0 = 3.68 \mu$ s) the beam orbit begins to intersect with the collimator. At the start of the sector 38 collimator, the SCRIPT element writes the phase-space coordinates of the beam to an external file. This beam distribution is converted from the self-describing dataset (SDDS) format to a structured plain-text file and is used as the source distribution in the FLUKA step. The ELEGANT process idles until FLUKA returns the distribution of particles surviving the collimator impact.

B. Particle-matter interaction

FLUKA is used to simulate the interaction between the particle beam and collimator material. In this step, the full beam distribution is passed to FLUKA at the start of a 20 cm simulation domain (only the dose in part of the domain, matching the FLASH grid, is binned to generate the dosemap). The collimator surface geometry is initially defined by an 86.5 cm radius cylinder, with an apex at the center (10 cm) of the simulation domain and a variable offset from the beam axis (see Fig. 4). FLASH tracks the physical state of each cell, releasing material from the solid/liquid state when a cell reaches the vaporization condition. As the collimator surface is damaged during the impact, the surface geometry is updated to reflect the missing material.

FLUKA tracks the source particles through the simulation domain and computes the deposited energy and secondary particles produced when a particle enters a region containing material. The geometry and material properties of each region are defined by the user in the input file. Figure 5 shows the effect of collimator material on the shower of particles resulting from the beam strike. The geometric radiation length, $t = X_0/\rho$, where X_0 is the radiation length, is 8.9 cm for Al and 1.44 cm in Cu. The energy deposited by the beam is binned over a 3D grid that has the same size and

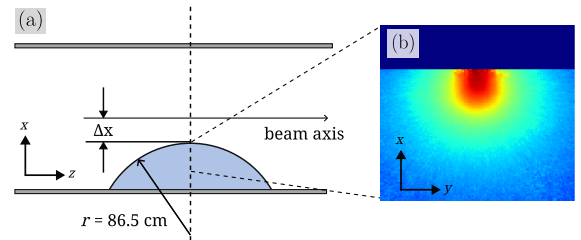


FIG. 4. Top-down view of collimator simulation geometry (a) and an example of a central cross section (b) showing the dose deposited in the collimator. The collimator is positioned Δx from the beam axis and transverse cross sections are taken at planes along the z axis.

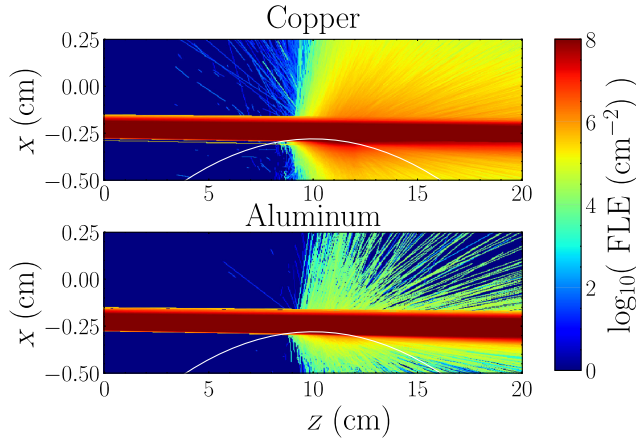


FIG. 5. Anamorphic cross section of the APS-U collimator model showing the electron flux (electron fluence: electrons per cm^2) simulated in FLUKA for copper (top) and aluminum (bottom). The copper simulation shows a greater particle shower due to the shorter radiation length.

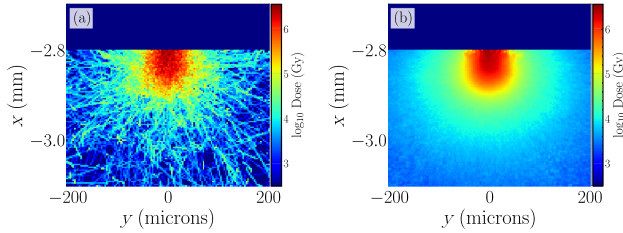


FIG. 6. Transverse cross section of a dosemap generated using a single (a) and 256 (b) trials. Increasing the number of trials reduces the noise in the dosemap showing a smoother dosemap with a maximum dose of ~ 6.5 MGy.

resolution as the FLASH simulation domain. Figure 6 shows the transverse cross section of the FLUKA-generated dosemap for a single trial (a) and the improved statistics by averaging 256 unique trials (b).

In addition to the energy deposition scoring, FLUKA tracks the source and secondary particles to the end of the simulation domain, where the coordinates are output into two files: one containing all electrons and another containing all positrons. The purpose of these files is to study the propagation and loss of shower particles in nearby sections of the beamline. For the purposes of the coupled collimator simulations, it is only necessary to return electrons with enough energy to complete another turn to ELEGANT.

IV. PHYSICS MODELING IN FLASH

We use FLASH [24,28] to simulate the evolution of the collimator surface geometry in response to the electron energy deposited to the solid collimator. Over the last decade, FLASH has been adopted in simulating state-of-the-art, multi-physics laboratory plasma experiments, rapidly growing

its user community as a primary computing tool [29–32]. For the current study, we use the official release version FLASH 4.6.2, leveraging in particular the unsplit staggered mesh (USM) solver [33,34] for (magneto)hydrodynamics, the multitemperature module for separate temperature evolutions of electrons and ions, the heat conduction module and tabulated equations of state (EoS) module for calculating the thermal properties of aluminum and copper, and the heat exchange module for capturing electron-ion equilibration using the classical Spitzer approximation of the Coulomb logarithm. The simulation domain boundaries use the Neumann boundary condition of a constant gradient to model the outflow of thermal energy.

FLASH takes as an input the dosemap created from the ELEGANT-FLUKA loop to evolve four major physical properties (see below) of the collimator configured on a 3D computational domain. The computational domain is resolved on a uniform grid of size $128 \times 128 \times 32$ parallelized on multiple compute nodes using FLASH’s MPI-based domain decomposition. The physical boundaries of each simulation are determined by the dynamics of each loss case to minimize the volume of the simulated region while capturing the entire heat-affected geometry. For this reason, the simulations do not share a common domain but the boundaries are noted in each figure.

A. Geometry evolution

The evolving geometry is a vital component of the coupled simulation framework and is best understood from the perspective of the FLASH simulation domain, where FLASH tracks the hydrodynamical and thermodynamical properties of cells on a Cartesian grid.

We begin each simulation with an initial condition, including setting up an initial temperature, density, and material phase using the variables TELE (electron temperature), DENS (density), and BDRY (boundary), respectively. As a grid-based shock-capturing fluid code, FLASH’s USM solver cannot model multiphase evolutions of the solid collimator cells to liquid/plasma states. As a workaround, we utilize the “BDRY” variable to tag each individual cell with three different values, $\text{BDRY} = 1$ (solid), 0.5 (pseudoliquid), or -1 (gas/plasma). In the “pseudoliquid” state FLASH uses certain thermodynamic properties of liquid material (density and thermal conductivity) but does not evolve the material hydrodynamically. In this way, the liquid phase better accounts for heat diffusion but does not currently model liquid flow. The simulation domain shares the dimensions of the 3D histogram described in Sec. III B and the initial BDRY value is set to 1 for each cell containing solid material. Energy is deposited in the FLASH simulation using the dosemaps produced in FLUKA by directly injecting the energy dose to electron energy. During the simulation, the BDRY value on each cell changes when the melting and vaporization conditions (as described in Sec. IV B) are met.

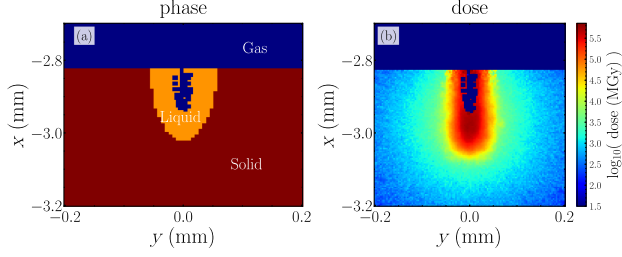


FIG. 7. (a) Value of the BDRY variable at the horizontal center ($z = 100$ mm) of the collimator and (b) the resulting dose of a beam strike partially through a beam strike event.

FLASH simulates the thermal evolution of the material for the entire duration of a number of depositions defined by the user. At the end of the simulation step, FLASH writes all cell properties to an HDF5 formatted checkpoint file. This file is also used to restart FLASH after the next dosemap is produced and to create the geometry input for FLUKA. A Python script reads in the checkpoint file and writes a geometry definition, which can be interpreted by FLUKA. The script does this by generating “voxels,” which are either solid material ($\text{BDRY} > 0$) or vacuum ($\text{BDRY} = -1$) and creates regions using FLUKA’s combinatorial geometry. An example of the geometry used by FLUKA is shown in Fig. 7.

In our previous studies, the dose calculations had been conducted using a “static” beam loss distribution generated by placing a flat aperture at a point in the storage ring lattice [35]. This approach did not include several important dynamics that are captured by the current “dynamic” approach with code-coupled, geometry-evolving simulations. The evolving geometry enables the transmission of more of the source particles through vaporized regions, leading to a protracted beam loss with a lower average dose per turn. Additionally, the dosemap computation will only produce interactions in regions where there is material in the FLASH simulation. This accounts for energy that was lost in the former static approach, which did not have self-consistent geometry.

B. Thermal properties and phase conditions

The BDRY variable represents the phase of each cell and determines how the cell evolves at each time step. In the states with $\text{BDRY} = 0.5$ or 1 (liquid or solid), the material is held stationary (i.e., no advection) and its state is evolved thermodynamically only, while when $\text{BDRY} = -1$ (gas), the material in each cell is advanced using FLASH’s (magneto)hydrodynamics USM solver. The thermal properties of the material are treated differently depending on if the material is a solid, liquid, or gas. While in the gas phase, those fluid cells are hydrodynamically evolved following the governing PDEs using a tabulated EoS to relate state variables like density, pressure, and energy. In the temperature range corresponding to liquid phase, we do not have access to a tabulated EoS and therefore we use a temperature dependent model for density. A temperature

TABLE II. Models used for aluminum and copper in each temperature range for ρ (density) and κ (thermal conductivity).

Temperature range	BDRY	$\rho(T)$ model	$\kappa(T)$ model
$T \leq T_{\text{melt}}$	1	Constant	Other [36].
$T_{\text{melt}} < T \leq T_{\text{vap}}$	0.5	Al: linear [37] Cu: linear [38]	Quadratic [37] Linear [39]
$T_{\text{vap}} < T \leq 1.5 T_{\text{vap}}$	0.5	Al: linear [37] Cu: linear [38]	Spitzer Spitzer
$1.5 T_{\text{vap}} < T$	-1	FLASH hydro	Spitzer

dependent model for density is not used for the solid cells ($\text{BDRY} = 1$), and instead the density is simply held constant. We do, however, use a temperature dependent model for thermal conductivity in both the solid and liquid phases.

A cell will change its state from solid to liquid, or liquid to gas, when a set threshold temperature is reached. This approach, while simple to implement, ignores latent heat during a phase change. For this reason, the temperature at which a cell is changed from liquid to gas is set to 1.5 times the actual vaporization temperature of the material. This is done in an attempt to emulate the latent heat of melting and vaporization since FLASH does not currently have the ability to model latent heat in phase changes. The temperature at which a cell is changed from solid to liquid is kept at the actual melting temperature.

The temperatures that define the different phases along with the models used for density and thermal conductivity in those temperature ranges are shown in Table II for aluminum and copper. The values of the melting temperatures and vaporization temperatures used for copper and aluminum are given in table Table III.

The type of model used (constant, linear, quadratic, other) is specified in Table II along with the source of the model (if applicable). See the Appendix for more details. The model being specified as Spitzer means that FLASH uses its built-in Spitzer model of conductivity, and FLASH hydro means that the density is being handled via FLASH’s (magneto)hydrodynamics USM solver.

C. Electron-ion heat exchange

FLASH uses a three-temperature (3T) set of hydrodynamics equations, which considers electron, ion, and radiation temperature independently. We only use separate

TABLE III. Melting temperatures (T_{melt}) and vaporization temperatures (T_{vap}) for aluminum and copper. Vaporization temperatures are given for 1-atmosphere of pressure [40].

Material	T_{melt} (K)	T_{vap} (K)	$1.5 T_{\text{vap}}$ (K)
Aluminum	933	2740	4115
Copper	1358	2835	4253

temperatures for electrons and ions in our study, as contributions to radiation temperature are negligible under the expected conditions. The energy deposited by the electron beam is added to the electron temperature of each cell. FLASH uses the Spitzer model of conductivity to equilibrate the energy between the electron and ion temperatures. However, the rate of conduction between electrons and ions in solid/liquid copper and aluminum is approximately an order of magnitude faster than in the Spitzer (plasma) model. To remedy this, we scale the Spitzer equilibration time in the solid/liquid cells by a factor of 0.1.

D. Wakefield heating

In addition to the energy deposited during beam strikes, the collimator material is continuously heated by the wakefields emitted by the circulating beam. The power on the collimator surface due to beam depends on the peak current, I , and distance between the beam and collimator, d , where $T_0 \propto I^2/d$ [41]. While the wakefield heating is relatively low power, it can raise the temperature of the collimator by ~ 100 K above the environment. To account for this effect, the initial temperature of the collimator is set to 450 K.

V. DEMONSTRATION AND BENCHMARKING

A. Geometry-evolution loop

To demonstrate the effects of an evolving geometry, we simulated the loss of a beam for both the APS and APS-U lattices first using the SPEEDBUMP element, then including the geometry-evolution loop with FLUKA and FLASH. In both cases, the beam current is 200 mA (4420 J), using a 48 bunch fill pattern (92.08 J/bunch), and excluding the FOK deflection to allow for the maximum damage. The cumulative maximum dose and maximum temperature of the aluminum cells during the simulation are shown in Fig. 8. The maximum temperature increases with dose until the cells reach the release condition of $1.5 T_{\text{vap}}$ (~ 4115 K in aluminum) at which point they are vaporized and evolve according to the hydrodynamic equations. Vaporization is first seen when the cumulative dose reaches ~ 40 – 50 MGy.

Cross sections of the final collimator geometry are shown in the panels (a)–(c) in Fig. 9 for three turns during the period of highest energy deposition. The bunch-by-bunch loss for the static and evolving cases are shown in Fig. 9(d). The losses are nearly identical for approximately the first 4 turns. The lower rate of loss in the “evolving” case can be explained by the inclusion of scattered particles. Once the material begins to vaporize (turn 24 for APS and turn 35 for APS-U, in both cases referenced to the time after rf muting), the rates diverge as more particles are transmitted (and survive for the next turn) through the eroded collimator region in the evolving geometry case; otherwise, those particles would be lost, bringing about a higher loss as in the static case. These differences result in a

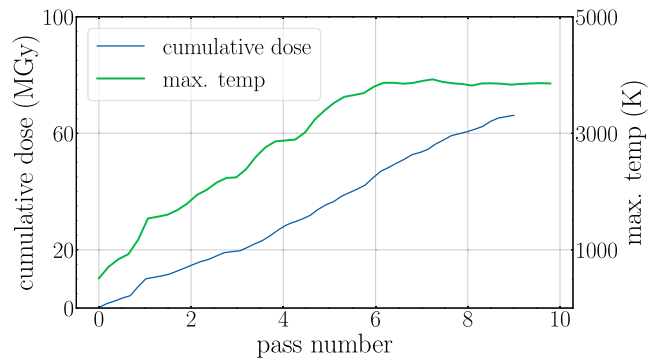


FIG. 8. Cumulative maximum dose (blue) and maximum temperature (green) of aluminum collimator during a beam strike at 200 mA. The maximum temperature plateaus around ~ 4100 K corresponding to the release condition of $1.5 T_{\text{vap}}$ when cells are vaporized.

protracted beam loss and lower average dose per turn with the evolving geometry. The curves shown in Fig. 9(d) only include the particles lost at the sector 38 collimator. Because FLUKA also simulates particle scattering, some particles returned to ELEGANT are lost to other elements in the ring before completing another full turn. This reduces the percentage of the total beam lost at sector 38. Tracking simulations have shown that these other losses primarily occur at the additional three downstream collimators.

The effects of the evolving geometry can further be seen in cases where the fan-out kicker creates a vertical oscillation in the beam motion, as shown in Fig. 10. Here, the losses are again similar for the first couple of

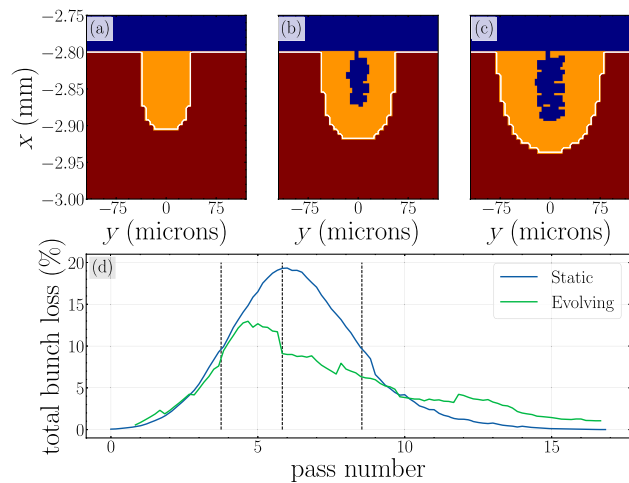


FIG. 9. (a)–(c) Cross section of material phase during the period of highest energy deposition. The regions of the solid (red), liquid (orange), and gas (blue) are shown for each. (d) Percent loss of total bunch charge per turn during a beam loss for the static (blue) and evolving (green) geometry. The material starts to vaporize around pass 4, leading to a relative decrease in the beam loss. The geometry shown in (a)–(c) corresponds to the dashed lines in (d).

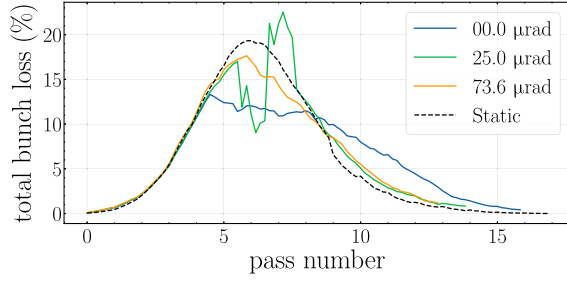


FIG. 10. Beam loss for increasing strengths of FOK deflection compared to the static geometry.

turns until the surface is damaged. Around turn 4, the material begins to vaporize and the characteristic decrease in the loss signal appears. However, the following turn shows a larger loss than in the static case. This can be explained by the vertical motion of the beam. The damaged collimator surface allows a higher transmission of electrons. Then in the next turn, the beam strikes a different vertical region of the collimator, which has not yet been eroded by the beam. Therefore the number of particles which intersect with the collimator geometry is larger than in the same turn of the static case.

B. Comparison with experimental data

Observations of beam strikes on copper and aluminum samples were made prior to the decommissioning of the APS storage ring in 2023 [42]. These studies involved modifying the lattice parameters to mimic the reduced vertical beam size of the APS-U ring and allowing the beam to strike the samples while varying the strength of the fan-out kicker. A vertical bump was introduced to the beam orbit at the collimator location in order to distinguish the beam strikes on the two sample pieces. In order to validate the three simulation codes, we modeled this experiment using the coupled framework. Specific simulation parameters are listed in Table IV.

Damage was seen in each case in the copper sample and all but the strongest deflection in the aluminum sample.

TABLE IV. Vertical offset and maximum deflection angle used in each of the cases during the collimator impact study.

Material	Vertical offset (mm)	FOK voltage (kV)	Deflection angle (μrad)	SN
Copper	+3.0	0.0	0.0	1
	+2.0	3.0	367.5	2
	+1.5	2.0	245.0	3
Aluminum	−1.5	2.0	245.0	4
	−2.0	1.0	122.5	5
	−3.0	0.0	0.0	6

Photographs of the samples are shown in Fig. 11. As was done in previous studies [12], the samples were analyzed using an Olympus BX51M Metallurgical microscope system to characterize the width and depth of each damaged region.

Each of the six cases was simulated using the evolving geometry framework described above. Four cases corresponding to 0/2 kV in Al and Cu are shown in Fig. 12, displaying the transverse cross section at the collimator. These results show a similar trend to the observed damage. The damage is greater in copper than in aluminum for the same deflection due to the shorter radiation length of copper. Additionally, the damage is reduced as the deflection angle increases, indicating that the FOK is helpful in mitigating damage.

These experimental data serve as an important benchmark for validating our coupled simulation code capability. Cross sections of the simulated copper geometry are shown in Fig. 13 and compared against surface profile measurements taken of the damaged copper sample. The simulated cross sections are each presented at different longitudinal positions along the beam path and combined with the three measured cases into a single figure.

The size of the damaged regions shows some agreement but discrepancies exist; these can be explained by limitations of the current model. In the simulated 3-kV (367.5 μrad) case, no vaporization is seen but a melt region

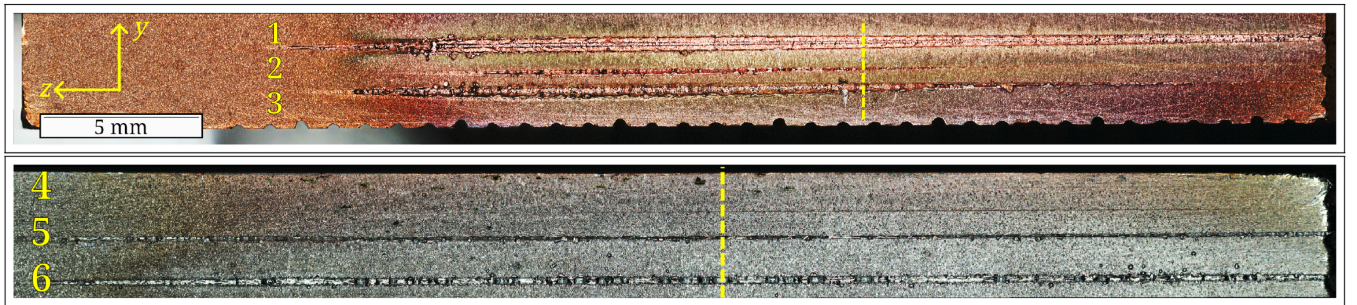


FIG. 11. Damage to copper (top) and aluminum (bottom) samples in the 2023 APS experiment. Fiducial markings indicating 1-mm spacings are visible on the lower edge of the copper and right-hand (upstream) end of the aluminum. Figure placement matches the real orientation with the beam moving in the $+z$ direction and the serial numbers (1–6) match those listed in Table IV. The yellow dashed line indicated the apex of each sample ($z = 10.0$ cm in Figs. 4 and 5).

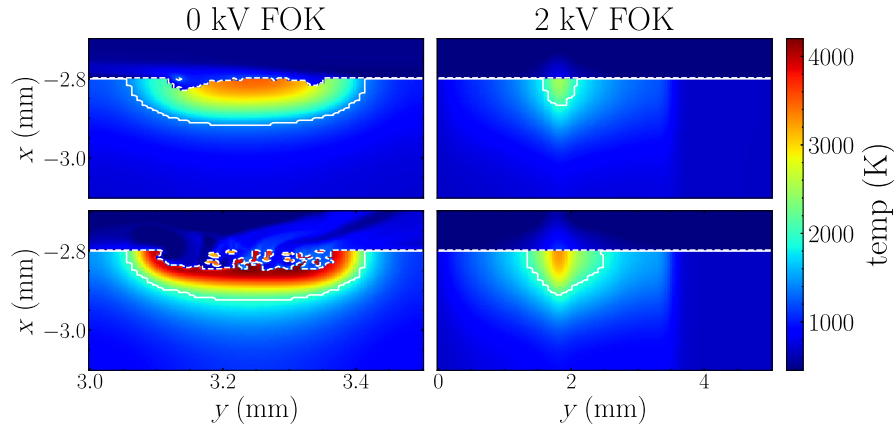


FIG. 12. Top: final simulated temperature at the central cross section of aluminum samples and bottom copper samples. The white contours represent the boundaries between the solid/liquid (solid line) and liquid/gas (dashed line) regions of material. Note that the y scales differ in the first and second columns.

(orange) appears in the downstream cross sections. This may be explained by the lack of a dynamic liquid state in FLASH. Figure 14 shows the cross sections of beam damage to an aluminum sample from a 2020 experiment.

The material which melted and resolidified can be seen in the green highlighted regions. This is evidence that liquid material may flow into or be driven out of the damaged region, changing the final geometry. Because liquid cells are currently held static, liquid flow cannot be captured by

the model and may be a source of the damage observed in the experiment sample. Additionally, in both FOK cases, the vertical size of the simulation domain is $y = [0, 5]$ mm, while the damaged region is only hundreds of microns across. The large vertical size is required to capture the range of intercepted particles but reduces the effective resolution in the region of interest. This may be the cause of the large melted region seen in the 2 kV case; while the vaporized region has a similar width to the measured damage, the liquid dynamics likely contribute to some of the surface geometry changes. Future work will improve on the liquid phase modeling in order to fully understand this effect.

C. Simulations and observations of APS-U

The APS-U storage ring began commissioning in April 2024 and entered its first user run in August 2024. Aluminum serves as the collimator material for the upgraded machine due to the reduced damage seen in the 2023 experiment. The APS-U operated in two

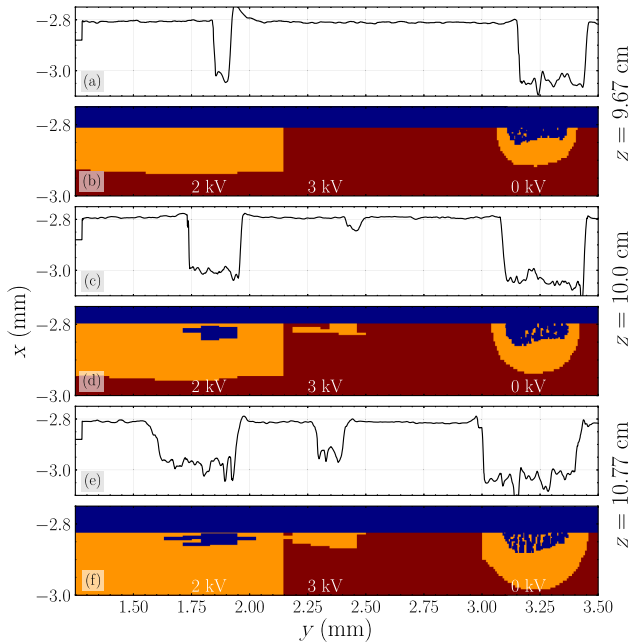


FIG. 13. Panels in (a), (c), and (e) are the measured damage at three locations observed along the z axis on the 2023 Cu sample. Panels in (b), (d), and (f) show cross sections of the Cu target simulated geometry at these three locations immediately after the final deposition with the material phase being represented by the color scale solid (red), liquid (orange), and gas (blue).

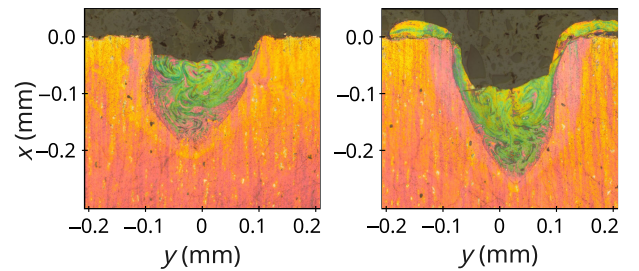


FIG. 14. Cross section of damage to an aluminum target in a 2020 experiment showing the effects of a single beam strike (left) and double beam strike (right). The highlighted green region shows the material that melted and resolidified following the strike. Strikes were carried out at 200 mA with a 972-bunch fill pattern (charge in every 3 of 4 rf buckets).

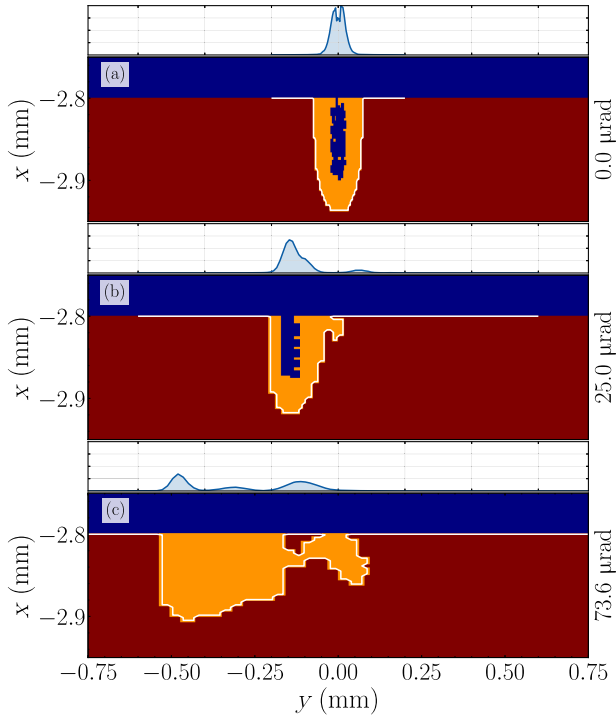


FIG. 15. Final transverse cross section showing the simulated damage to the aluminum collimator at the apex for a maximum deflection angle of (a) $0.0 \mu\text{rad}$ (no FOK), (b) $25.0 \mu\text{rad}$, and (c) $73.6 \mu\text{rad}$. The color scale shows the solid (red), liquid (orange), and gas (blue) phases of material. The distribution of the cumulative dose for each FOK strength is shown above each figure.

experimental configurations in 2024: (i) a 162 bunch fill pattern up to 160 mA and (ii) a 48 bunch fill pattern up to 114 mA. Some high-charge machine studies were conducted in December up to 170 mA. During these runs, a number of beam loss events occurred with and without the FOK and three of the five collimators were accessed during operational shutdowns. The sector 1 (S01) collimator jaw was observed during the first shutdown and showed signs of beam-strike damage. During the January 2025 shutdown, the collimators in sectors 37 (S37) and 38 (S38) were accessed and damage was only observed on the S38 collimator jaw. Damage to the sector 1 jaw was considered minor and it was not removed; however, the beam effects on the S38 jaw were more significant and it was replaced. Further details on the S38 collimator jaw are given below.

Several dedicated machine studies as well as beam losses that occurred during operations provide data about the beam position during losses. Some observations also indicate the FOK may not provide the desired vertical deflection to prevent damage to the collimators. This is further supported by the location of the damage observed during the accesses. The infrequent access to the collimators and limited diagnostic tools make it challenging to determine which set of beam parameters have resulted (and will result) in damage.

To match operational conditions, we simulated the loss of a 48-bunch, 114 mA beam for a range of FOK deflection

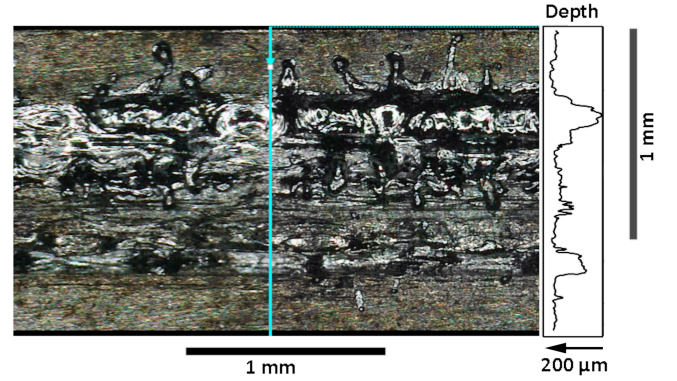


FIG. 16. Microscopy image of the S38 aluminum collimator near its apex showing damage from beam loss. The depth of the damage along the vertical line is indicated on the right-hand plot.

angles. These studies simulated the full interaction of a single collimator (sector 38) while the rest are modeled as static apertures in ELEGANT. The deflection values were chosen to be $73.6 \mu\text{rad}$, the estimated nominal FOK deflection angle, $25.0 \mu\text{rad}$, corresponding to a reduced deflection, and $0.0 \mu\text{rad}$ for cases where the FOK fails to fire. These deflection angles are lower than those presented in Table IV due to the choice of the FOK vacuum chamber material. In APS, a ceramic chamber was used, whereas in APS-U, the vacuum chamber is fabricated from stainless steel. Eddy currents in the APS-U SS chamber reduce the amplitude and extend the duration of the FOK pulse. A cross section of the final geometry of each case is shown in Fig. 15. As the deflection angle increases, the damaged region grows vertically (in y direction) but the amount of vaporized material decreases. This suggests that the FOK works as intended to mitigate damage to the collimator surface but that there is likely still significant damage under current operational conditions. During the January 2025 maintenance period, examination of the S38 collimator jaw revealed damage to the surface near its apex. Microscopy indicated a relatively broad, vertical region of damage $\sim 850 \mu\text{m}$ in extent. Figure 16 shows this damaged region near the S38 apex; the depth of the damage, evaluated along the vertical line, is indicated on the right-hand plot.

VI. CONCLUSION

The coupled simulation framework presented here demonstrates powerful capabilities for designing and understanding accelerator systems where high-energy-density conditions are present. By including particle dynamics, particle-matter interaction, and thermodynamic evolution tools, it is possible to simulate the complex behaviors seen in beam strike events. With minor adjustments, it is also possible to simulate other events relevant to machine protection, namely the production and absorption of synchrotron radiation and the propagation of shower particles following a beam strike.

By evolving the simulation geometry in this way, we show that the model is much better at capturing the dynamics of a beam loss than the previous static version of the model [12]. The automatic interfacing between codes reduces the need for user involvement when setting up and running these simulations. Future work will need to incorporate (magneto) hydrodynamics into the FLASH simulations.

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DATA AVAILABILITY

The data are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX: TEMPERATURE DEPENDENT DENSITY AND THERMAL CONDUCTIVITY MODELS IN FLASH

1. Thermal conductivity of solid material

For both solid copper and solid aluminum, we use the following model from Hust and Lankford [36] to model thermal conductivity as a function of temperature,

$$\kappa_{\text{solid}}(T) = (w_0 + w_i + w_{i0})^{-1}, \quad (\text{A1})$$

where w_0 , w_i , and w_{i0} are temperature dependent terms that are different depending on whether copper or aluminum is being modeled. The values are given by

$$\begin{aligned} w_0 &= \frac{\rho_i(273)}{(\text{RRR} - 1)L_0 T} \\ w_i &= \frac{P_1 T^{P_2}}{1 + P_1 P_3 T^{(P_2 + P_4)} \exp(-(P_5/T)^{P_6})} + w_c(T), \\ w_{i0} &= \frac{P_7 w_i w_0}{w_i + w_0} \end{aligned} \quad (\text{A2})$$

where $\rho_i(273)$ is the intrinsic resistivity of the metal at $T = 273$ K ($\rho_i(273) = 15.4 \times 10^{-9} \Omega \text{ m}$ for copper and $\rho_i(273) = 24.8 \times 10^{-9} \Omega \text{ m}$ for aluminum), RRR is the residual resistivity ratio¹ (RRR = 300 is used in FLASH),

¹The residual resistivity ratio is frequently used to characterize the purity of a metal (high RRR corresponds to high purity) and is a dimensionless constant. This value has a very small effect above 100 K.

TABLE V. Parameters in the thermal conductivity model for solid copper and aluminum from Hust and Lankford [36] used in the thermal conductivity implementation in FLASH. A value of RRR = 300 was used in P_7 for copper.

Parameter	Copper	Aluminum
P_1	1.754×10^{-8}	4.716×10^{-8}
P_2	2.763	2.446
P_3	1102	623.6
P_4	-0.165	-0.16
P_5	70	130.9
P_6	1.765	2.5
P_7	$0.235(\text{RRR} - 1)^{0.1661}$	0.8168
a_1	-1.2×10^{-4}	-0.5×10^{-3}
a_2	-1.6×10^{-4}	-1.3×10^{-3}
a_3	-0.2×10^{-4}	0
b_1	420	330
b_2	73	110
b_3	18	
c_1	470	380
c_2	87	94
c_3	21	
d_1	0.7	0.6
d_2	0.45	0.5
d_3	0.5	

$L_0 = 2.443 \times 10^{-8} \text{ V}^2 \text{ K}^{-2}$ is the Lorenz number used to relate thermal conductivity and electrical conductivity in the Wiedemann-Franz law, the P_i are parameters determined by a nonlinear least squares fit of experimental data for each metal, and $w_c(T)$ is a correction term in the least squares fit that is also specific to each metal. The functional form of $w_c(T)$ for both copper and aluminum is

$$\begin{aligned} w_c(T) &= a_1 \ln\left(\frac{T}{b_1}\right) \exp\left[-\left(\frac{\ln(T/c_1)}{d_1}\right)^2\right] \\ &+ k a_2 \ln\left(\frac{T}{b_2}\right) \exp\left[-\left(\frac{\ln(T/c_2)}{d_2}\right)^2\right] \\ &+ a_3 \ln\left(\frac{T}{b_3}\right) \exp\left[-\left(\frac{\ln(T/c_3)}{d_3}\right)^2\right]. \end{aligned} \quad (\text{A3})$$

Table V contains the values for the remaining quantities that have not been specified thus far for both copper and aluminum.

2. Thermal conductivity of liquid material

For liquid aluminum, a model from Leitner *et al.* [37] is implemented. The model is a quadratic fit to thermal conductivity data in the temperature range of 933.47 to 1491 K and is given by

$$\kappa_{\text{liquid,Al}}(T) = a + bT + cT^2, \quad (\text{A4})$$

where $a = 33.9 \text{ W m}^{-1} \text{ K}^{-1}$, $b = 7.892 \times 10^{-2} \text{ W m}^{-1} \text{ K}^{-2}$, and $c = -2.099 \times 10^{-5} \text{ W m}^{-1} \text{ K}^{-3}$. Equation (A4) is used

in FLASH from the melting temperature of aluminum from $T_{\text{melt,Al}} = 933.47$ to 1491 K. This model for thermal conductivity starts to decrease before the boiling temperature, $T_{\text{vap,Al}} = 2743$ K, and is therefore physically unsuitable for modeling thermal conductivity in the entire range of temperatures from 1491 K to $T_{\text{vap,Al}}$. In the absence of a thermal conductivity model in this range, we extrapolate Eq. (A4) into $1491 \leq T \leq T_{\text{vap,Al}}$ using a linear approximation at $T = 1491$ K which is given by

$$\kappa(T) = a' + b'T, \quad (\text{A5})$$

where $a' = 80.562 \text{ W m}^{-1} \text{ K}^{-1}$ and $b' = 0.016327 \text{ W m}^{-1} \text{ K}^{-2}$.

For liquid copper, we use the following model from Assael *et al.* [39],

$$\kappa_{\text{liquid,Cu}}(T) = c_1 + c_2(T - T_{m,\text{Cu}}), \quad (\text{A6})$$

where $c_1 = 150.49 \text{ W m}^{-1} \text{ K}^{-1}$, $c_2 = 0.070410 \text{ W m}^{-1} \text{ K}^{-2}$, and $T_{m,\text{Cu}} = 1357.77 \text{ K}$ is the melting temperature of copper. This model was determined by a linear fit on thermal conductivity data in the temperature range of 1358 to 1700 K. However, Eq. (A6) is used in FLASH to model the thermal conductivity of liquid copper from the melting temperature to the vaporization temperature of copper.

3. Density of solid material

The density of solid aluminum/copper is held constant in the simulations. The value for aluminum is

$$\rho_{\text{solid,Al}} = 2.7 \text{ g cm}^{-3} \quad (\text{A7})$$

and the value used for copper is

$$\rho_{\text{solid,Cu}} = 8.96 \text{ g cm}^{-3}. \quad (\text{A8})$$

4. Density of liquid material

The model used to describe the density of liquid phase copper as a function of temperature in FLASH comes from Cahill and Kirshenbaum [38] and is given by

$$\rho_{\text{liquid,Cu}}(T) = \rho_0 + mT, \quad (\text{A9})$$

where $\rho_0 = 9.077 \text{ g cm}^{-3}$, $m = -8.006 \times 10^{-4} \text{ g cm}^{-3} \text{ K}^{-1}$, and T is the temperature measured in Kelvin.

The model used for aluminum is from Leitner *et al.* [37] and is also a linear model

$$\rho_{\text{liquid,Al}}(T) = \rho_0 + mT, \quad (\text{A10})$$

where $\rho_0 = 2.67 \text{ g cm}^{-3}$ and $m = -2.99 \times 10^{-4} \text{ g cm}^{-3} \text{ K}^{-1}$.

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