MULTIPHYSICS SIMULATION OF THE THERMAL RESPONSE OF A NANOFIBROUS TARGET IN A HIGH-INTENSITY BEAM

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Abstract

Nanofibrous structures are of high interest to the fields of engineering and materials science, and investigation of their properties as well as discovery of novel applications for them both constitute lively areas of research. A very promising application of nanofiber mats lies in the field of accelerator technology: beam targets made from nanofiber mats offer a solution to the problem of advancing the "intensity frontier"-the limit on the beam intensities that can be realized in fixed target experiments and neutrino production facilities. However, testing has shown that the survivability of these nanofiber targets depends strongly on their manufacturing parameters, such as the packing density of fibers. In this work, we will use multiphysics simulations to perform a thermal study on how nanofiber targets react to high intensity beams, so that the dependency of the targets' lifetime on their construction parameters can be better understood.

INTRODUCTION

Most neutrino beams are produced by exposing a fixed target to a high-energy proton beam. The intensity of this "primary" beam in turn determines the intensity of the neutrino beam, and so far they have operated at max intensities on the order of one megawatt—the NuMI beamline at Fermilab recently set a record beam power of 893 kW. However, future installations are expected to reach higher intensities: the Long Baseline Neutrino Facility, for example, calls for a primary beam power of 1.2 MW [1], with an accelerator upgrade planned in the horizon of 2030 to raise the power to 2.4 MW, bringing us to the multi-megawatt regime.

Attaining these intensities is not just a matter of accelerator technology—the fixed target must *survive* many beam cycles for these facilities to be practical. The upper bound on the intensities reachable with current technology is known as the *intensity barrier*, and its advancement is therefore necessary to meet the demands of future neutrino experiments.

In facilities such as NuMI, the convention is to use solid graphite targets with water cooling. Although such targets have operated successfully to date, there is question as to whether they will retain suitable lifetimes at the multimegawatt scale. The primary weakness of these solid targets is that their uniform lattice allows thermal stress waves induced by the pulsed beam to easily propagate, leading to fatigue failure. This issue will only be exacerbated by *larger* amplitude stress waves from higher beam power in the future. The High Power Targetry Research and Development (HPT R&D) Group at Fermilab has been studying [2,3] a potential solution—a nanofibrous target material, consisting of an electrospun array of Yttria-Stabilized Zirconia nanofibers. These nanofiber "mats" are porous, and so the open space between fibers dissipates any thermal stress waves caused by the beam, avoiding the central weakness of existing targets. Their porosity *also* allows us to cool the targets internally by forcing helium gas through them. They also demonstrate resistance to radiation damage without additional treatment [2]. These advantages suggest that these nanofiber targets pose a novel solution to breaking the intensity barrier.

Such nanofiber targets are an emergent topic, and thus are under rigorous testing. One such test at HiRADMat [2]-a facility at CERN which provides a single pulse beam for thermal shock tests of target materials-revealed that the construction parameters of the nanofiber mats, namely their Solid Volume Fraction (SVF), strongly affect their survival. The SVF, notated f, is defined as the percentage volume of the mat occupied by *solid* material. The target with a higher SVF developed a hole at its center, whereas the one with a lower SVF remained undamaged. The exact mode of failure of the denser target is as of yet unknown; there was no evidence of melting, but one suggested explanation is that pockets of gas in the denser mat may cause such damages by limiting diffusion. While this test demonstrates that lowering the SVF increases target lifetime, it comes at the price of a lower neutrino yield, and so the choice of SVF is delicate.

MODELS AND THEORY

In order to optimize the performance of these targets, it is essential to characterize their thermal properties, which thus allows us to *predict* how they will respond to beam heating for a set of prescribed construction parameters. The nanoscale structure of these targets, however, makes theoretical descriptions and simulations of their behavior difficult. It is impossible to model all of the constituent fibers of a nanofiber target explicitly—however, the fact remains that the behavior at the individual-fiber level cannot be ignored. There are significant nanoscale effects present which add up to change the qualities of the whole.

This task becomes tractable, however, by using Porous Media Models (PMMs), which translate the behavior at the nansocale to the macroscale by computing *effective material parameters* of a new, *homogenous* material. In this way, the explicit nanoscale geometry is "forgotten", but the effects are retained by adjusting the properties of a replacement

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bulk material. It then becomes tenable for us to perform simulations by applying these effective material parameters to a greatly simplified domain.

In the case of our nanofiber targets, the major physical processes at play are the fluid flow of the helium through the nanofiber mat, the deposition of energy from the beam generating heat, and the conduction of heat along nanofibers. Thermal radiation is also an important mode of heat transport because of the high temperatures expected, and we did find a PMM to handle radiation, due to Lee [4,5]. However, the simulation software we used for this work, ANSYS Fluent, can only handle radiation in porous media at very high porosities [6], $\epsilon \sim 1$, where the porosity, ϵ , is defined as the percentage of the material's volume which is void space or fluid and relates to the SVF by $\epsilon = 1 - f$. The average porosity of our samples is $\epsilon \approx 0.637$, and so we were forced to neglect this effect for now.

The energy deposition per volume, E_D , caused by the beam was estimated using MARS [7-9], a popular collection of programs for predicting the effects of high energy particles upon materials. We considered a pencil beam $(\sigma \approx 0.50 \text{ mm})$ of 120-GeV protons incident on a uniform cylinder of radius 1 cm with density 0.28 g/cm^3 . We treated this as a pulsed beam, with $N = 10^{13}$ protons per 10-µs pulse, and a 1.8 s cooldown: values inspired by the NuMI beamline. From this, we obtained the heating caused by the beam as a function of distance from the target center, which we used as a source term in the energy equation to represent the contribution from the primary beam.

To handle the fluid flow of the helium through the nanofibrous target, we used a well-known approach called Darcy's Law [10], which models flow through a porous medium by introducing a momentum source term to the fluid governing equations of the form:

$$\vec{S} = -\frac{\mu}{\alpha}\vec{u}$$

where μ is the dynamic viscosity, \vec{u} is the velocity field, and α is the permeability (to fluid flow) of the porous medium. To estimate α for our nanofiber mat, we used the Λ -methods described in [11, 12]. The permeability is where the nanoscale structure enters the problem, and in general depends on the direction of the fluid flow (e.g., cross- or thru-flow).

Finally, in order to characterize the heat transfer due to conduction, we used a model for the effective thermal conductivity of a fibrous structure with a gaseous interstitial medium developed by Bhattacharyya [13]. It is a nonlinear combination of the thermal conductivity of both the gas phase, k_g , and that of a single fiber, k_0 , taking the form:

$$k_{\rm eff}(T) = k_0 + \frac{k_g - k_0}{1 + \frac{f}{1 - f} \left[1 + \frac{5}{6} \frac{k_g - k_0}{k_g + k_0}\right]} \,,$$

with the average SVF of our samples being $f \approx 0.363$. The contribution to the thermal conductivity from the helium gas, k_g , was predicted using a model developed by Daryabeigi [14].

ANSYS SIMULATIONS

With the PMMs in hand, we sought to perform a multiphysics simulation of a nanofiber mat being exposed to a high intensity, pulsed particle beam. This work was the first such attempt to simulate the thermal response of one of our nanofiber mats. We decided to use ANSYS Fluent for the task, due to its ability to handle many physical effects, porous media, and its comparatively intuitive interface.

In these simulations, we modeled a 10 mm \times 10 mm nanofiber target in a 20 mm × 20 mm surrounding helium medium, with the beam normal and centered to the target surface. We used a structured mesh of identical square elements of side length 0.2 mm. A velocity inlet (5 m/s) and outflow were used for boundary conditions in the vertical directions to represent a cross-flow cooling apparatus. The target can be regarded as stacked 2D planes in which the nanofibers are oriented randomly, and since the mats are only 1 mm thick, the energy deposition by the beam is identical on all layers. This led us to use a thin-target approximation, reducing the problem to 2D. The other boundaries were treated as insulating, and have a Neumann condition. This setup is depicted in Fig. 1.

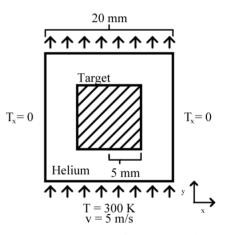


Figure 1: Illustration of the 2D problem.

Darcy's Law is implemented easily in ANSYS Fluent by selecting porous media conditions in the zone setup. In the case of cross flow, the permeability was predicted to be $\alpha \approx 2.524 \cdot 10^{-15} \text{ m}^2$, describing a "semi-pervious" material. Using a custom material library, we incorporated Bhattacharyya's effective thermal conductivity model by performing a fifth-order polynomial fit to capture the temperature dependence of k_{eff} . For other temperature dependent material properties-for which we had a closed-form expression, such as helium's density, viscosity, and thermal conductivity-we wrote User Defined Functions (UDFs).

Finally, to simulate the heating due to the beam, we wrote the data from our MARS simulation in the format of a "profile" file, which integrates source terms particularly well into Fluent. This could then be read to add a spatially-dependent energy source term in the region of the nanofiber mat. In order to account for the fact that the beam is pulsed and not

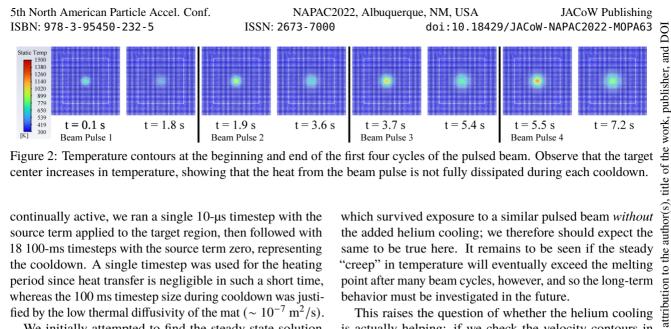


Figure 2: Temperature contours at the beginning and end of the first four cycles of the pulsed beam. Observe that the target center increases in temperature, showing that the heat from the beam pulse is not fully dissipated during each cooldown.

continually active, we ran a single 10-µs timestep with the source term applied to the target region, then followed with 18 100-ms timesteps with the source term zero, representing the cooldown. A single timestep was used for the heating period since heat transfer is negligible in such a short time, whereas the 100 ms timestep size during cooldown was justified by the low thermal diffusivity of the mat (~ 10^{-7} m²/s).

We initially attempted to find the steady-state solution using a pseudo-transient method, but evaluations failed to converge and the max temperature of 5000 K in ANSYS Fluent was exceeded in the entire target region. We reason that this is because the beam heating is an impulse and so the source term cannot be left "on", even when time-averaged. We instead studied the transient solution over a span of four cycles (\approx 7 s), using a second-order SIMPLE solution algorithm. Temperature contours at the beginning and end of each cycle are shown in Fig. 2, with velocity in Fig. 3.

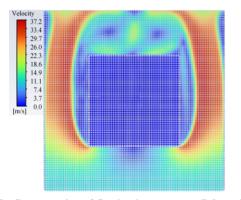


Figure 3: Contour plot of fluid velocity at t = 7.2 s; observe that the velocity drops to zero inside the target.

RESULTS

The transient solution demonstrated quick convergence, and provided both intuitive and illuminating results. Referencing Fig. 2, we see the "pulsed" temperature rise that we would naturally expect from a pulsed heat source. Note, however, that the target center's temperature is increasing with every cycle-and so we infer that the heat from the beam is not being diffused completely during the cooldown.

Nonetheless, the colorbar indicates that the temperature remains below 1500 K, and thus the YSZ fibers are in no danger of reaching their melting point at 2973 K this early. The target's dimensions were selected to mirror those of the low density sample from the HiRADMat experiment [2], which survived exposure to a similar pulsed beam without the added helium cooling; we therefore should expect the same to be true here. It remains to be seen if the steady "creep" in temperature will eventually exceed the melting point after many beam cycles, however, and so the long-term behavior must be investigated in the future.

This raises the question of whether the helium cooling is actually helping: if we check the velocity contours in Fig. 3, we notice that the flow velocity vanishes in the target interior, and that the flow outside resembles that of a bluff body. So, the helium is not actually extracting heat from the target center as intended, only the boundary, implying the permeability $\alpha \sim 10^{-15} \text{ m}^2$ is too low. Increasing the permeability can be accomplished by increasing the nanofiber radius, or reducing the SVF-though this latter choice has consequences as aforementioned.

CONCLUSION

In this work, we used porous media models to determine effective material parameters of a nanofiber target material, and used ANSYS Fluent to simulate the target's thermal response to heating by a high-intensity, pulsed proton beam. The results mostly matched expectations, but a steady increase in overall temperature across beam cycles will require long-term study. It was also observed that the helium flow did not permeate the nanofiber target, suggesting that higher permeability may eliminate the temperature "creep" and greatly improve target survivability and performance, bringing us closer to the goal of advancing the intensity frontier.

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