SPPARKS Assignment Report

I will start off with an emphasis on a few simulation parameters which appear to be in a state of contrast with respect to their descriptions/depictions in the research paper and the official Sandia website. Furthermore, the values of some critical parameters have not been furnished in the paper. In a state of uncertainty, the Sandia website shall be regarded as the authentic source of descriptions of all the simulation parameters and hence, were adhered to during the simulation setup and the creation of the implicit codes therein.

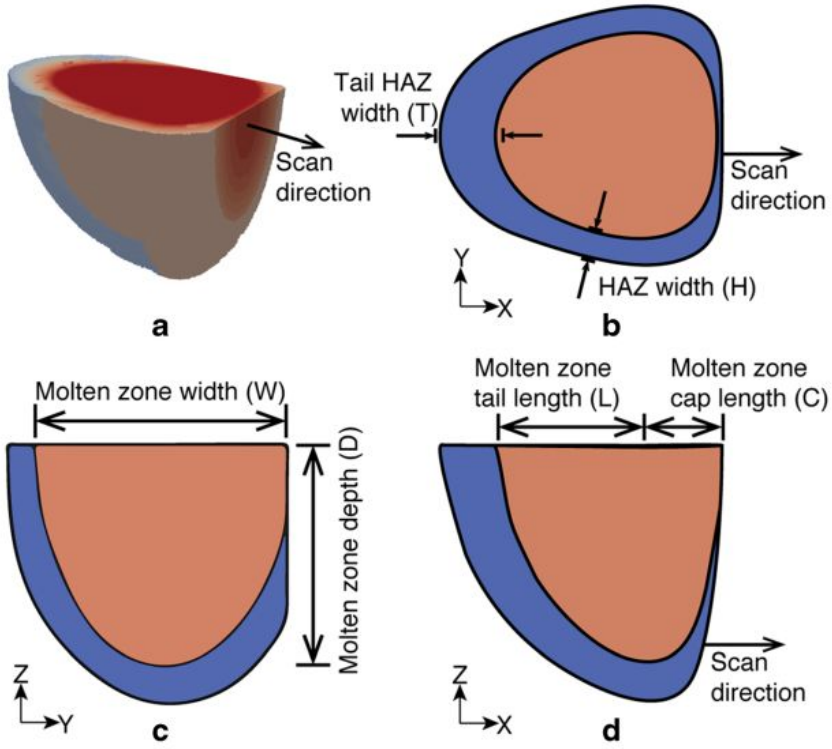

Fig: Melt pool depiction in paper

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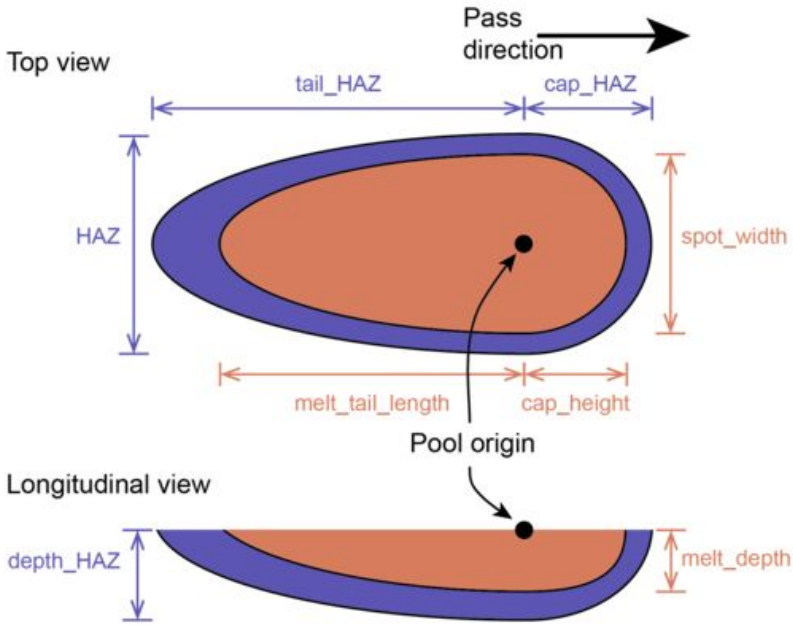

Fig: Melt pool depiction on Sandia website (Link)

Clearly, contrast between the following parameters *which actually mean the same thing* can be seen as per the two depictions above:

1. *HAZ width (H) and HAZ*
   As per the Sandia website, this value *must* be greater than the width (W) of the melt pool
2. *Tail HAZ width (T) and tail_HAZ*
   As per the Sandia website, this value *must* be greater than the melt tail length (L) of the melt pool

In the paper, the values of these parameters do not satisfy the imposed constraints and hence, the respective modifications were made and implemented in the simulations (*). Please refer to the tables below. The red cells represent the parameter values that are not furnished in the paper but were crucial for the simulations.

Simulation #2				
Parameter	*Denoted by*	*Constraint*	*Value in paper*	*Modified value (as per constraint)*
n_spins	n_spins		NA	1000
spot_width	W		80	80
melt_tail_length	L		60	60
melt_depth	D		50	50
cap_height	C		NA	30 (L / 2)
HAZ	HAZ	> W	5	90 [W + (2 * 5)]
tail_HAZ	T	> L	20	80 (L + 20)
depth_HAZ	depth_HAZ	> D	NA	55 (D + 5)
cap_HAZ	cap_HAZ	> C	NA	35 (C + 5)
exp_factor	exp_factor		NA	0.1
velocity	V		15	15

Simulation #4				
Parameter	*Denoted by*	*Constraint*	*Value in paper*	*Modified value (as per constraint)*
n_spins	n_spins		NA	1000
spot_width	W		90	90
melt_tail_length	L		70	70
melt_depth	D		62.5	62.5
cap_height	C		NA	35 (L / 2)
HAZ	HAZ	> W	35	160 [W + (2 * 35)]
tail_HAZ	T	> L	35	105 (L + 35)
depth_HAZ	depth_HAZ	> D	NA	97.5 (D + 35)
cap_HAZ	cap_HAZ	> C	NA	70 (C + 35)
exp_factor	exp_factor		NA	0.1
velocity	V		7.5	7.5

Note on n_spins

During the creation of the simulation domain in SPPARKS, the domain is fragmented into sites (or voxels) depending on the domain size and the lattice constant. Each site is assigned a spin state and neighboring sites interact with each other for spin flipping. This spin flipping works on an algorithm based on Glauber's dynamics and is dependent on temperature as well as the number of spins specified in the code. Furthermore, the colors observed during the simulation indicate the spin values of the sites. More the number of spins or more the specified temperature, more will be the randomness of the sites' spin states and hence, a homogenous color will be visible throughout the domain. For instance, at *n_spins=10,000*, the domain was entirely reddish and the melt pool movement could not be distinguished. But, at *n_spins=1000*, the domain showed a mix of different colors and the melt pool movement was clearly visible along with a grain's shape, size, and orientation. *However, it's important to note that the colors as such do not have any relation to the physical characteristic/quantification of the microstructure, but they just present a clear view of a grain's shape, size and orientation*.

Note on domain size

It appears that the domain size used for the simulation is not explicitly mentioned in the paper. However, there have been mentions of domain size of *300 x 300 x 200 elements* at a few places in the paper and hence, the same size was used for the assignment simulations. As a matter of fact, the simulation results in the paper and those done by me match for this domain size.

Note on "thresh" command in the codes

The *thresh* command in the code specifies the plane that is used as a reference to view the simulation results. All those sites that satisfy the thresh value(s) will be present in the dumped images. Since the same data was not furnished in the paper, few logical iterations in the codes were carried out to eventually obtain images that resembled the paper's simulations.

Note on simulation times

Using 4 processors, following were the approximate simulation times:

	simulation time
Simulation #2	9 hrs.
Simulation #4	21 hrs.

Note on fine grain sizes in Simulation #2 vs coarser grain sizes in Simulation #4

As is obvious from the simulations results, the grains differ from each other in the two simulations prominently in terms of their sizes. The reason behind this (which has also been mentioned in the paper) is the small melt pool size in simulation #2 where the melt pools don't overlap to as great an extent as they do in simulation #4 between subsequent passes. The extent of overlap determines the size of the grains, hence the observed difference. A rough calculation I did showed that the melt pools overlap ~25 % in simulation #2 whereas they overlap ~85 % in simulation #4 (~3.4 times), given the same hatch spacing to carve out 4 x 4 layers.

(*): Despite the fact that the melt pool depictions in the paper and that on the Sandia website differ a bit, they actually mean the same thing. *There's nothing wrong in the paper, it has just represented them in a different manner*. Indeed, my simulation results matched those of the paper only when the modified parameter values were used in the code. Using the un-modified values, no change in the microstructures were observed during the entire simulation duration, hence justifying the fact that the modifications were indeed necessary.

SIMULATION #2

SIMULATION #4