Goal:

To quantify the effect double-sided vs. single-sided interface defect generation has on time-to-failure statistics.

Simulation:

Initialize 3D cylindrical grid of zeroes. Iterate through grid, generating defects in cylindrical grid along the way. Terminate simulation when there is a path of defects from one interface (X,Y,Z==0) to other interface (X`,Y`,Z==3). Record how many iterations (aka time-to-failure) it took to terminate.

Repeat simulation until a sizable statistic of time-to-failure is collected.

Path is any chain of connections that connects interface to interface. Path can zig-zag or go backwards.

Defect generating probability functions:

OR (see optional Boolean arguments below)

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Tunable parameters to be estimated:

Optional boolean arguments:

1. Whether one-sided or two-sided interface defect formation. If one-sided, then define Z==3 layer as bulk.
2. Whether to define diagonal adjacency as neighbors in the defect generating probability functions and path finding.
3. Whether to use sum or NOR for probability functions. If sum, then if there are 3 neighboring defect sites, sum(neighbors)=3. If NOR, then NOR(neighbors)=1.

One-sided

Scale: 1nm=3 monolayers of MgO

Diameter, default = 270

Two-sided

Legend:

bulk

interface

Path = 1

When Diagonals == 0

Path = 1

When Diagonals == 1

Z=4