Goal:

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

Simulation:

Initialize 3D cylindrical grid with cubic cells of zeroes. Iterate through grid, probabilistically (see defect generating probability functions below) changing the state of the current cell to 1, which represents the generation of a defect. Defects are permanent, only can go from 0 to 1, not 1 to 0.

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 OR for probability functions. If sum, then if there are 3 neighboring defect sites, sum(neighbors)=3. If OR, then OR(neighbors)=1.

Two-sided

Other Parameters:

1. Diameter. Default=210.

One-sided

Two-sided

Legend:

bulk

interface

Scale: 1nm=3 monolayers of MgO

Diameter, default = 210

Path = 1

When Diagonals == 1

Path = 1

When Diagonals == 0

Z=4