

1 Micro-Mesas Reference Case

1.1 Introduction

The micro-mesas case is included in the HeavyMetal validation suite as a reference-history validation case for surface-diffusion-driven evolution of a realistic silicon microstructure. Unlike the Mullins and ATG cases, this problem is not validated by comparison to a closed-form analytical solution. Instead, the automated validation workflow checks that selected history files generated by the current version of HeavyMetal reproduce trusted reference histories. In this sense, the formal validation role of the case is regression testing: it verifies that the solution does not change unexpectedly as the code evolves.

The physical formulation used in this calculation is the same surface-energy and surface-diffusion formulation used in the Mullins validation case. Surface curvature produces a chemical-potential gradient along the free surface, and this gradient drives surface transport. The micro-mesas case therefore does not introduce a new governing equation or a new analytical benchmark. Its purpose is instead to apply the same formulation to a more realistic geometry involving large-scale redistribution of material.

1.2 Simulation and Experimental Comparison

Figure 1.1 shows the predicted evolution of two silicon mesas during annealing. The mesas are initially approximately $1\text{ }\mu\text{m}$ wide by $5\text{ }\mu\text{m}$ tall and are annealed at 1100°C in pure hydrogen gas at a pressure of 10 torr. The initially sharp mesa corners round rapidly, the sidewalls relax, and the valleys between the mesas evolve as material is redistributed along the free surface. The sequence demonstrates that the surface-diffusion formulation can produce large-scale shape change in a geometry that is significantly more complex than the idealized sinusoidal perturbations used in the Mullins and ATG validation cases.

The micro-mesas case also provides a useful comparison with experimental observations from Lee and Wu [1]. Figure 1.2 compares experimental cross sections of silicon mesas before and after annealing with corresponding HeavyMetal simulations. The experimental images contain five mesas, while the validation model contains two mesas in order to reduce computational cost and keep the case suitable for routine validation runs. The comparison is therefore not intended as a point-by-point reproduction of the full experimental geometry. Rather, it is intended to test whether the model produces the correct type and approximate rate of morphology evolution.

The key result from the comparison is that the simulated mesas reach a degree of surface evolution comparable to the experiment after approximately 600 s, whereas the experimental anneal time reported by Lee and Wu [1] was 300 s. Thus, the predicted surface-evolution rate differs from the observed rate by roughly a factor of two. Given the uncertainties in the experimental conditions and model inputs, this level of agreement is considered satisfactory.

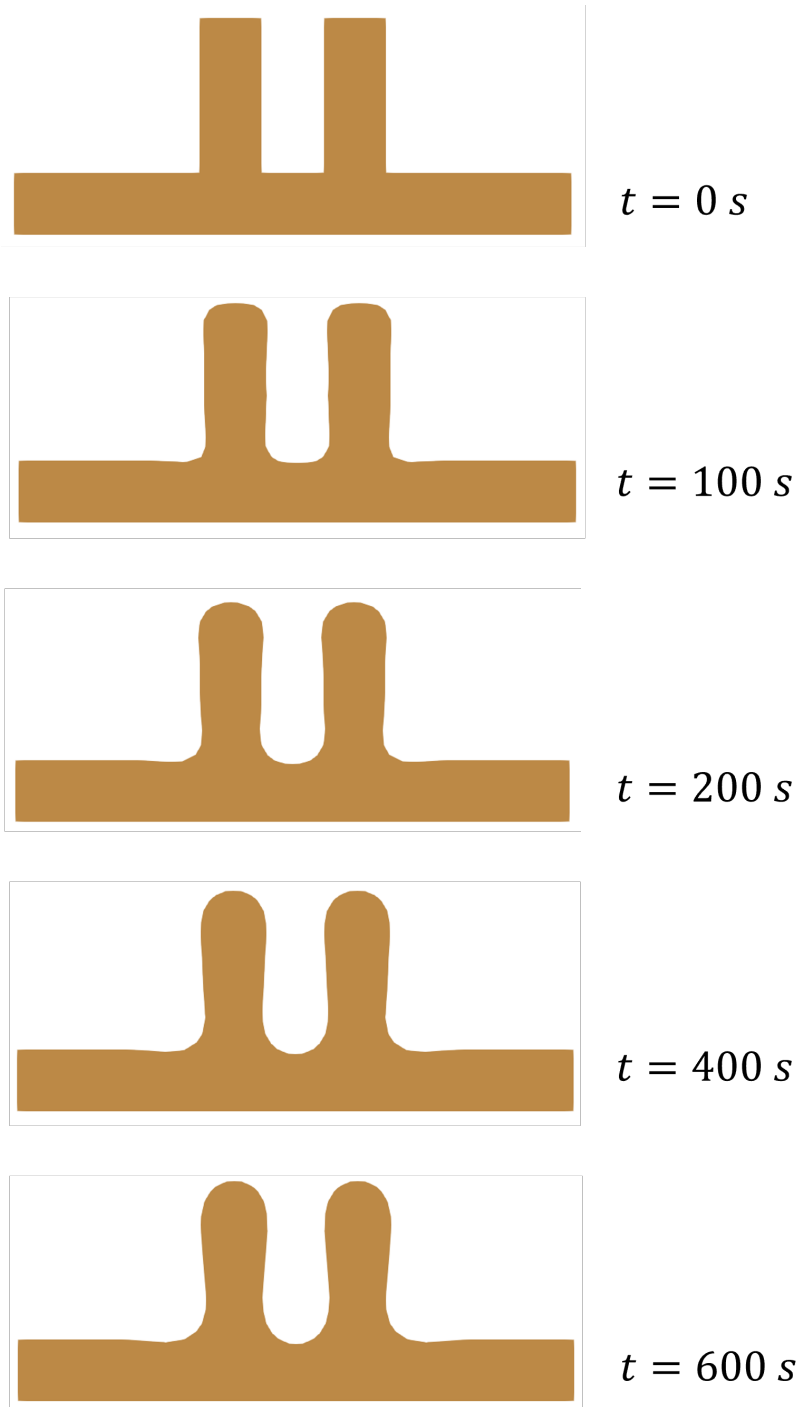


Figure 1.1: Simulation of the evolution of $1 \mu\text{m} \times 5 \mu\text{m}$ micro-etched silicon mesas being annealed at 1100°C in an atmosphere of pure hydrogen gas at a pressure of 10 torr, corresponding to the experimental annealing conditions reported by Lee and Wu [1].

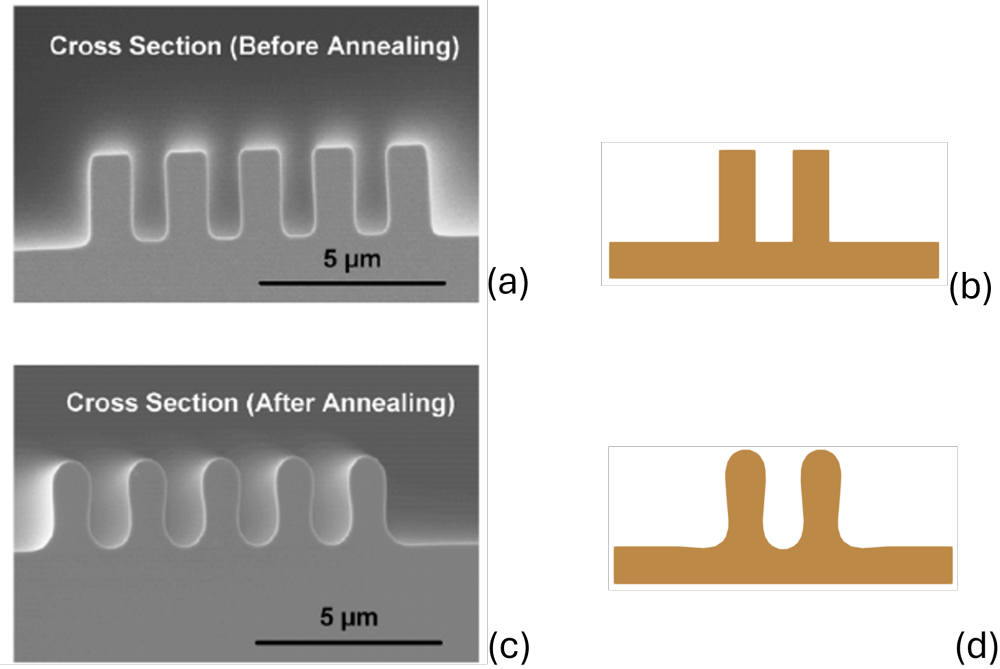


Figure 1.2: Comparison of experimental and simulated silicon mesa evolution: (a) image of five silicon mesas prior to annealing from Lee and Wu [1]; (b) model of two mesas prior to annealing, where only two mesas were considered in the model to reduce validation run times; (c) image of five silicon mesas after being annealed at 1100°C in an atmosphere of pure hydrogen gas at a pressure of 10 torr for 300 s from Lee and Wu [1]; and (d) predicted shapes of silicon mesas after a simulated anneal time of 600 s.

Important uncertainties include the initial mesa dimensions, the thermal ramp history, the actual specimen temperature during annealing, and the surface-transport coefficients used in the simulations.

This case complements the idealized Mullins, ATG, and square-relaxation benchmarks. The Mullins and ATG cases provide direct checks against analytical solutions for simple geometries. The square-relaxation and micro-mesas cases demonstrate that the same surface-transport machinery can produce large-scale morphological evolution in geometries that are farther from small-amplitude sinusoidal perturbations. The micro-mesas case is especially useful because it connects the reference solution used in the automated validation workflow to an experimentally observed silicon surface-evolution problem.

1.3 Reference-History Validation

For the automated validation workflow, selected node histories are tracked at characteristic locations on the mesas. The mesh generator creates named node sets at the bottom-left, bottom-right, top-left, and top-right locations of each modeled mesa. Because the current HeavyMetal history-output workflow supports one tracked node per node set, each tracked

location is written as a separate single-node set.

For an input file named `test.inp`, the corresponding history files are `test.bl1`, `test.br1`, `test.tl1`, `test.tr1`, `test.bl2`, `test.br2`, `test.tl2`, and `test.tr2`. Here, in the file extension b and t refer to the bottom or top of the mesa, l and r refer to the left or right sides of the mesa, and 1 and 2 refer to the individual mesa, going from left to right. The validation workflow compares each generated history file against the corresponding trusted reference-history file. Passing this case means that the tracked histories for the current run remain consistent with the trusted reference solution. The automated check therefore guards against unintended changes in the geometry generation, node-set history output, surface-energy elements, surface-diffusion elements, and reference-history comparison workflow.

1.4 Discussion

Overall, the micro-mesas case serves two related purposes. In the validation workflow, it is a reference-history regression test that guards against unintended changes in surface-evolution behavior. In the broader documentation, it also demonstrates that the same surface-energy and surface-diffusion formulation validated in simpler benchmark problems can reproduce experimentally observed silicon microstructure evolution at a semi-quantitative level.

The agreement with experiment should not be interpreted as a precise parameter-free prediction of the annealing experiment. The model uses a reduced two-mesa geometry, and both the experimental conditions and the material coefficients contain significant uncertainty. Nevertheless, the calculated morphology and characteristic evolution time are comparable to the experimental observations. This makes the micro-mesas case a useful bridge between analytic surface-evolution benchmarks and practical silicon surface-transport simulations.

1.5 References

[1] M.-C. M. Lee and M. C. Wu, "Thermal annealing in hydrogen for 3-D profile transformation on silicon-on-insulator and sidewall roughness reduction," *Journal of Microelectromechanical Systems*, vol. 15, no. 2, pp. 338–343, Apr. 2006. doi: 10.1109/JMEMS.2005.859092.