

1 Mullins Surface Diffusion Benchmark

1.1 Introduction

The Mullins benchmark considers the smoothing of an initially sinusoidal free surface by surface energy driven surface diffusion. In this problem, the underlying solid is unstressed and the only driving force for surface evolution is the reduction of surface area, and therefore total surface energy. Peaks and valleys in the surface have different curvature, which produces spatial variations in chemical potential along the surface. Surface diffusion then transports material in a direction that reduces these variations in chemical potential and smooths the surface.

Mullins derived an analytic solution for the small-amplitude evolution of a sinusoidally perturbed surface [1]. For small slopes, the governing equation is linear, and the amplitude of the sinusoidal perturbation decays exponentially with time. This provides a direct benchmark for the HeavyMetal surface evolution formulation.

1.2 Objective

The objective of this benchmark is to determine whether the finite element implementation reproduce the Mullins analytic decay rate for a sinusoidal free surface evolving by surface diffusion. Note that the finite element analysis does not impose the Mullins decay rate directly. Instead, the surface energy elements generate the capillary normal stress associated with the free surface. Cohesive-zone elements and normal stress projection elements are used to transfer this normal stress information to the surface nodes. The surface diffusion elements then compute the material deposition/removal rate from gradients in chemical potential along the surface. Figure 1.1 shows the element-level coupling used for this benchmark.

1.3 Analytic Mullins Solution

The general form of the mechanically driven chemical potential used in the surface diffusion formulation is

$$\mu = \mu_0 + \Omega(\psi - \sigma_{nn}). \quad (1.1)$$

For the Mullins benchmark, the underlying substrate is not subjected to applied stresses. The strain energy density term is therefore negligible, and the chemical potential is controlled primarily by the normal stress acting on the surface:

$$\mu \simeq \mu_0 - \Omega\sigma_{nn}. \quad (1.2)$$

For a surface with isotropic surface energy γ , the surface energy produces a capillary normal stress proportional to the curvature. With the sign convention used here, the curvature contribution gives

$$-\sigma_{nn} = \gamma\kappa, \quad (1.3)$$

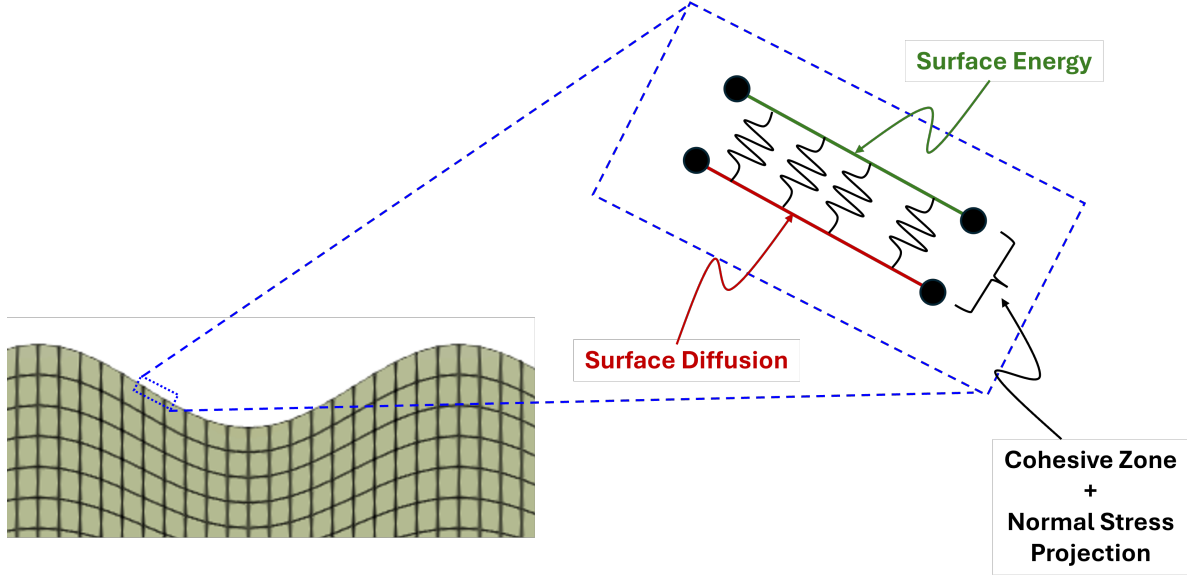


Figure 1.1: Schematic of the elements used for the Mullins surface diffusion benchmark. Surface energy elements generate the capillary normal stress associated with the free surface. Cohesive-zone and normal stress projection elements transfer the normal stress information to adjacent nodes, where it is used by the surface diffusion elements to compute deposition and removal rates.

so that the spatially varying part of the chemical potential becomes

$$\mu = \mu_0 + \Omega\gamma\kappa. \quad (1.4)$$

Only gradients in chemical potential affect the surface flux, so the constant reference value μ_0 does not influence the evolution.

For a small-amplitude sinusoidal surface,

$$h(x, t) = A(t) \cos(kx), \quad (1.5)$$

where

$$k = \frac{2\pi}{\lambda}, \quad (1.6)$$

the small-slope approximation is assumed:

$$kA \ll 1. \quad (1.7)$$

Under this approximation, the curvature is

$$\kappa \simeq -\frac{d^2h}{dx^2}. \quad (1.8)$$

For the sinusoidal perturbation,

$$\frac{d^2h}{dx^2} = -k^2 A \cos(kx), \quad (1.9)$$

and therefore

$$\kappa \simeq k^2 A \cos(kx). \quad (1.10)$$

The chemical potential variation along the surface is then

$$\mu = \mu_0 + \Omega \gamma k^2 A \cos(kx). \quad (1.11)$$

The surface flux is taken to be proportional to the surface gradient in chemical potential:

$$J = -M \frac{d\mu}{dx}, \quad (1.12)$$

where M is the surface mobility. In the notation used for the validation calculations,

$$M = \frac{D_s \Gamma}{k_B T}, \quad (1.13)$$

where D_s is the surface diffusivity, Γ is the surface atomic density, k_B is Boltzmann's constant, and T is absolute temperature.

Conservation of mass along the surface gives

$$\frac{dh}{dt} = -\Omega \frac{dJ}{dx}. \quad (1.14)$$

Substituting the flux law gives

$$\frac{dh}{dt} = \Omega M \frac{d^2 \mu}{dx^2}. \quad (1.15)$$

Using Equation (1.11) and

$$\frac{d^2}{dx^2} \cos(kx) = -k^2 \cos(kx), \quad (1.16)$$

gives

$$\frac{dh}{dt} = -M \Omega^2 \gamma k^4 A \cos(kx). \quad (1.17)$$

Since $h(x, t) = A(t) \cos(kx)$, the amplitude satisfies

$$\frac{dA}{dt} = \omega A, \quad (1.18)$$

where

$$\omega = -M \Omega^2 \gamma k^4. \quad (1.19)$$

It is convenient to define

$$B = M \Omega^2 \gamma, \quad (1.20)$$

so that

$$\omega = -B k^4. \quad (1.21)$$

The analytic solution for the amplitude is therefore

$$A(t) = A_0 \exp(-Bk^4t). \quad (1.22)$$

The negative sign indicates that the sinusoidal perturbation decays with time. Shorter wavelengths decay much more rapidly than longer wavelengths because of the fourth-power dependence on wavenumber. This same fourth-power dependence also makes surface diffusion simulations numerically demanding. As the spatial resolution is refined, the smallest surface element length decreases, and the stable or accurate time increment decreases rapidly. As a practical matter, the maximum useful time step scales roughly with the fourth power of the characteristic surface element length.

1.4 Benchmark Setup

The benchmark uses a sinusoidal free surface with wavelength λ and initial amplitude A_0 . The computational domain contains multiple wavelengths, and the underlying substrate is initially unstressed. The surface evolves by surface diffusion driven only by surface energy.

The material properties are taken from the silicon material definition used for the surface evolution validation cases. These properties include the surface energy, surface diffusivity, atomic volume, and elastic constants. Although elastic constants are present in the material definition, the Mullins benchmark does not include an applied stress and therefore does not activate the strain energy density driving term.

The finite element model uses the same surface evolution infrastructure that is used in later, more complex benchmarks. Surface energy elements generate the capillary normal stress. Cohesive-zone and projection elements recover and project the normal stress to the surface nodes. Surface diffusion elements compute the resulting normal deposition/removal rate from the gradient in chemical potential.

The primary benchmark output is the normalized perturbation amplitude,

$$\frac{A(t)}{A_0}. \quad (1.23)$$

The finite element amplitude is computed from selected node-history files at peaks and valleys of the sinusoidal surface. The analytic comparison is

$$\frac{A(t)}{A_0} = \exp(\omega t), \quad (1.24)$$

where $\omega = -Bk^4$.

For the current validation case, the mesh uses 15 elements per wavelength. This case is inexpensive enough to run in the automated validation workflow while still providing a clear comparison with the analytic Mullins decay rate.

Table 1.1: Primary input parameters for the Mullins benchmark case.

Parameter	Symbol	Value	Units
Wavelength	λ	0.01	mm
Initial amplitude	A_0	0.0001	mm
Amplitude/wavelength	A_0/λ	0.01	—
Elements per wavelength	n_{ex}	15	—
Solid elements through height	$n_{\text{ey,solid}}$	8	—
Number of periods	n_{periods}	3	—
Temperature	T	1100	$^{\circ}\text{C}$
Time increment	Δt	nan	s
Step time	t_{end}	nan	s
Material file	—	silicon.mtl	—

1.5 Results

Figure 1.2 compares the normalized amplitude from the finite element calculation with the Mullins analytic solution for the 15-elements-per-wavelength silicon case. The amplitude decreases monotonically with time, as expected for surface energy driven smoothing. The finite element solution closely follows the analytic exponential decay curve over the time interval shown.

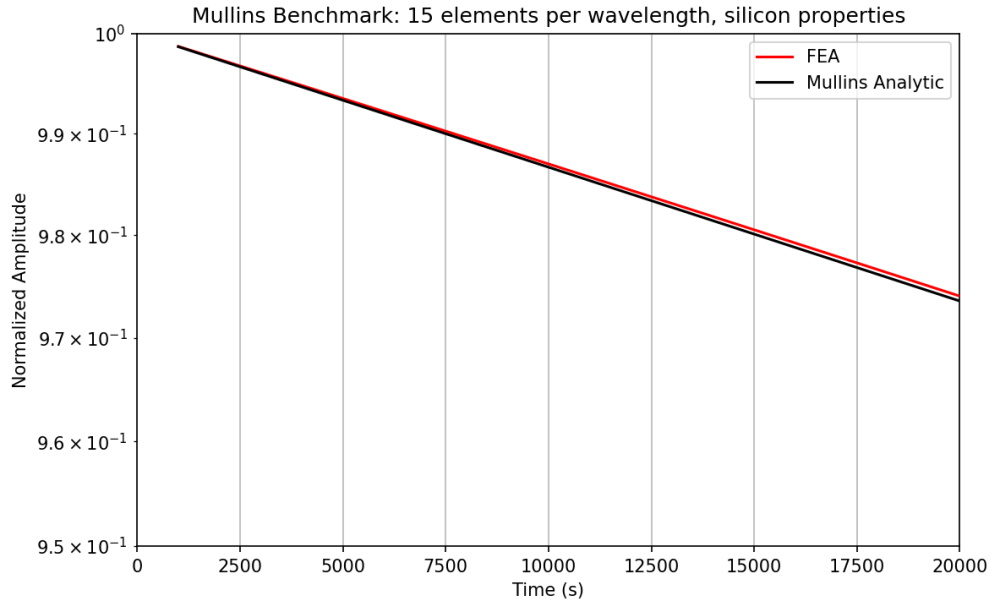


Figure 1.2: Normalized amplitude decay for the 15-elements-per-wavelength Mullins benchmark case. The finite element result closely follows the Mullins analytic solution.

Table 1.2: Fitted and analytic decay rates for the Mullins benchmark case.

Quantity	Symbol	Value	Units
Fitted decay rate	ω_{FEM}	$-1.31505174e - 06$	1/s
Analytic decay rate	ω_{analytic}	$-1.33889378e - 06$	1/s
Relative error	–	1.78%	–

The fitted finite element decay rate is

$$\omega_{\text{FEM}} = -1.31505174e - 06 \text{ s}^{-1}. \quad (1.25)$$

The analytic decay rate is

$$\omega_{\text{analytic}} = -1.33889378e - 06 \text{ s}^{-1}. \quad (1.26)$$

The relative error is therefore approximately

$$\frac{|\omega_{\text{FEM}} - \omega_{\text{analytic}}|}{|\omega_{\text{analytic}}|} = 1.78\%. \quad (1.27)$$

The comparison is especially useful because the finite element solution is not prescribed to follow the Mullins decay law. The decay rate emerges from the coupled calculation of surface energy induced normal stresses, normal stress projection, chemical potential gradients, surface diffusion fluxes, and surface deposition/removal rates.

1.6 Discussion

The Mullins benchmark provides a test of the curvature-driven part of the surface evolution formulation. The surface evolution is driven by the normal stress generated by surface energy, which makes the benchmark a clean test of the surface energy, normal stress projection, and surface diffusion coupling.

The agreement with the analytic solution is significant because the implementation chain is not trivial. The surface energy elements generate normal stresses at the free surface. These stresses are recovered and projected to the adjacent nodes, where they enter the surface diffusion calculation through the chemical potential. Gradients in chemical potential then drive surface fluxes, and the divergence of those fluxes determines the normal deposition/removal rate. Thus, even though the analytic solution is simple, the finite element benchmark is an end-to-end test of the capillarity-driven surface evolution machinery.

The Mullins benchmark validates the stabilizing, curvature-driven portion of the surface evolution formulation. The ATG benchmark in the following section extends this test by adding an applied in-plane stress and the corresponding strain energy density contribution to the chemical potential.

1.7 References

- [1] W. W. Mullins. Theory of thermal grooving. *Journal of Applied Physics*, 28:333–339, 1957.
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