

1 Validation Against the Asaro-Tiller-Grinfeld Instability

1.1 Introduction

The Mullins benchmark considers the smoothing of a sinusoidal free surface by surface energy driven surface diffusion. In that problem, surface energy is the only driving force for surface evolution, and the amplitude of the surface perturbation decreases monotonically with time.

The analytic model developed by Asaro and Tiller [1] and by Grinfeld [2], denoted here as the ATG model, adds a second driving force. The body is subjected to an applied in-plane stress, as shown schematically in Figure 1.1. The applied stress produces a spatially varying elastic strain energy density near an undulating free surface. This strain energy term enters the surface chemical potential and can oppose the smoothing tendency of surface energy. If the elastic driving force is sufficiently large relative to the surface energy term, small perturbations of the surface grow rather than decay.

The ATG problem is therefore a natural extension of the Mullins problem. Mullins smoothing tests surface energy driven surface diffusion. The ATG instability tests whether the implementation can also capture the coupling between solid mechanics, surface stress projection, strain energy density gradients, and surface diffusion.



Figure 1.1: Schematic of a sinusoidally perturbed surface where the underlying substrate is subjected to in-plane stress of σ_0 . The perturbation of the surface is exaggerated for clarity. The evolution of the surface via surface diffusion was analytically solved for by Asaro and Tiller [1] and Grinfeld [2], which provides a useful benchmark for testing the finite element formulation and implementation.

1.2 Objective

The objective of this benchmark is to determine whether the finite element formulation and implementation reproduce the growth rates predicted by the ATG model for a sinusoidally perturbed surface under an applied in-plane stress.

The predicted growth rates from the finite element model are the result of the interactions between surface energy, surface diffusion, and solid mechanics, but these interactions require

additional computations so that all field variables can be accessed in each physics simulation. The analyses use structural continuum elements to compute the stress field in the solid; surface energy elements to generate the capillary normal stress associated with the free surface; cohesive-zone elements as a numerical device for estimating the normal stresses induced by surface energy; projection elements that transfer normal stress from the cohesive-zone representation to adjacent surface nodes; tangential-stress projection elements that estimate the tangential stress along the free surface; and surface-diffusion elements that compute the deposition rate from gradients in chemical potential along the surface. Figure 1.2 provides a schematic showing how some of these interactions are modeled at the surface.

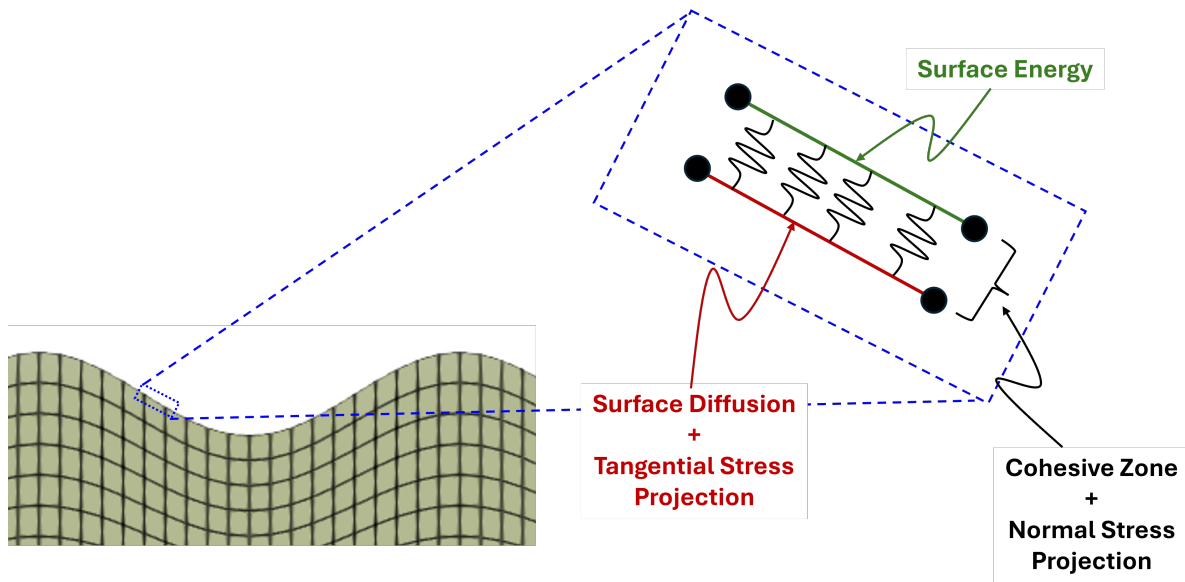


Figure 1.2: Schematic of the elements used to simulate stress- and strain energy-driven diffusion along a free surface: surface energy elements that give rise to a normal stress on the surface; cohesive-zone elements with a linear response that are used to estimate the normal stresses within the cohesive zone and projection elements that transfer the normal stresses to adjacent nodes; and tangential-stress projection elements combined with the surface diffusion elements themselves.

The Mullins benchmark primarily validates the surface energy contribution to the chemical potential. The ATG benchmark adds the strain energy density contribution. Agreement with the ATG solution therefore provides evidence that the tangential-stress projection, the strain energy contribution, and the surface diffusion coupling are functioning correctly.

1.3 The Chemical Potential

Surface diffusion is driven by gradients in chemical potential along a surface. The chemical potential is the change in free energy associated with adding atoms to, or removing atoms from, the surface. If a small normal displacement of the surface is denoted by Δh , the associated

change in volume per unit surface area is approximately

$$\Delta V = \Delta h. \quad (1.1)$$

The number of atoms added per unit surface area is therefore

$$\Delta N = \frac{\Delta V}{\Omega} = \frac{\Delta h}{\Omega}, \quad (1.2)$$

where Ω is the atomic volume. The chemical potential is the change in free energy per atom, so the chemical potential can be written as the atomic volume multiplied by the free energy per unit volume.

For a stressed solid surface, two mechanical contributions are important. First, material added at the surface carries elastic strain energy density ψ . This gives a contribution of

$$\mu_\psi = \Omega\psi. \quad (1.3)$$

Second, if the surface is subjected to a normal stress σ_{nn} , adding material by moving the surface in the normal direction does mechanical work against that normal stress. With the sign convention used here, this contribution is

$$\mu_{\sigma_{nn}} = -\Omega\sigma_{nn}. \quad (1.4)$$

Thus the chemical potential may be written as

$$\mu = \mu_0 + \Omega(\psi - \sigma_{nn}), \quad (1.5)$$

where μ_0 is the chemical potential in the absence of stress, and $\Omega(\psi - \sigma_{nn})$ represents the combination of the strain energy density and mechanical work terms. This is the form used for the comparisons of the HeavyMetal predictions to the ATG analytic solution.

This expression also clarifies the relationship between the Mullins and ATG benchmarks. The Mullins benchmark is not obtained by arbitrarily discarding physics. Rather, it is the limiting case in which the strain energy density contribution is absent or negligible compared with the normal stress contribution. For example, if the local stress state is dominated by the surface normal stress, and if the strain energy density associated with that stress is approximated as

$$\psi \simeq \frac{\sigma_{nn}^2}{2E}, \quad (1.6)$$

then the chemical potential can be written as

$$\mu = \mu_0 + \Omega\sigma_{nn} \left(\frac{\sigma_{nn}}{2E} - 1 \right). \quad (1.7)$$

For metals, $\sigma_{nn}/2E$ is typically much smaller than one, so the strain energy contribution associated with the normal stress is often negligible. In that limit, the chemical potential is well approximated by

$$\mu = \mu_0 - \Omega \sigma_{nn}. \quad (1.8)$$

In the Mullins case, surface energy is the cause of the normal stresses acting on the surface, and no external forces are applied. The chemical potential is therefore controlled primarily by the surface energy-induced normal stress. The ATG instability arises when an applied in-plane stress creates a spatially varying elastic field, and therefore a spatially varying ψ , that is no longer negligible compared with the surface energy contribution.

1.4 Analytic ATG Solution

For a sinusoidal surface perturbation,

$$h(x, t) = A(t) \cos(kx), \quad (1.9)$$

with

$$k = \frac{2\pi}{\lambda}, \quad (1.10)$$

the small-slope approximation is assumed:

$$kA \ll 1. \quad (1.11)$$

The surface energy contribution can be written in terms of the curvature-induced normal stress. To first order in the surface amplitude, the curvature contribution gives

$$-\sigma_{nn} = \gamma k^2 A \cos(kx). \quad (1.12)$$

Therefore the surface energy contribution to the chemical potential is

$$\mu_{\text{surface}} = \Omega \gamma k^2 A \cos(kx). \quad (1.13)$$

This is the Mullins contribution. By itself, it produces smoothing.

The elastic contribution comes from the strain energy density. For the classical linear ATG solution, the surface tangential stress along a sinusoidally perturbed surface is

$$\sigma_{tt}(x) = \sigma_0 [1 - 2kA \cos(kx)], \quad (1.14)$$

up to a sign convention for whether $\cos(kx) = 1$ corresponds to a peak or a valley. The important point is that the first-order stress perturbation has amplitude

$$\Delta \sigma_{tt} = 2\sigma_0 kA. \quad (1.15)$$

For plane strain, the elastic strain energy density associated with the tangential stress is

$$\psi = \frac{\sigma_{tt}^2}{2E_p}, \quad (1.16)$$

where

$$E_p = \frac{E}{1 - \nu^2}. \quad (1.17)$$

Substituting the first-order stress expression into Equation (1.16) gives

$$\psi = \frac{\sigma_0^2}{2E_p} [1 - 2kA \cos(kx)]^2. \quad (1.18)$$

Keeping only terms through first order in kA ,

$$\psi = \frac{\sigma_0^2}{2E_p} [1 - 4kA \cos(kx)]. \quad (1.19)$$

Thus

$$\psi = \frac{\sigma_0^2}{2E_p} - \left(\frac{2\sigma_0^2}{E_p} \right) kA \cos(kx). \quad (1.20)$$

The first term is spatially uniform and does not contribute to surface diffusion. The second term is spatially varying and is the part that drives the ATG instability. The elastic contribution to the chemical potential is therefore

$$\mu_{\text{elastic}} = -\Omega \left(\frac{2\sigma_0^2}{E_p} \right) kA \cos(kx). \quad (1.21)$$

Combining the surface energy and elastic contributions gives

$$\mu = \mu_{\text{surface}} + \mu_{\text{elastic}}, \quad (1.22)$$

or

$$\mu = \Omega \left[\gamma k^2 - \left(\frac{2\sigma_0^2}{E_p} \right) k \right] A \cos(kx). \quad (1.23)$$

This expression shows the competition between the two effects. The surface energy term is stabilizing. The elastic strain energy term is destabilizing when the applied stress is large enough.

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

$$J = -M \frac{d\mu}{dx}, \quad (1.24)$$

where

$$M = \frac{D_s \Gamma}{k_B T} \quad (1.25)$$

is the surface mobility. Conservation of mass along the surface gives

$$\frac{dh}{dt} = -\Omega \frac{dJ}{dx}. \quad (1.26)$$

Substituting the flux law,

$$\frac{dh}{dt} = \Omega M \frac{d^2 \mu}{dx^2}. \quad (1.27)$$

Using Equation (1.23) and

$$\frac{d^2}{dx^2} \cos(kx) = -k^2 \cos(kx), \quad (1.28)$$

gives

$$\frac{dh}{dt} = -M\Omega^2 k^2 \left[\gamma k^2 - \left(\frac{2\sigma_0^2}{E_p} \right) k \right] A \cos(kx). \quad (1.29)$$

Rearranging,

$$\frac{dh}{dt} = M\Omega^2 \left[\left(\frac{2\sigma_0^2}{E_p} \right) k^3 - \gamma k^4 \right] A \cos(kx). \quad (1.30)$$

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

$$\frac{dA}{dt} = \omega A, \quad (1.31)$$

where

$$\omega = M\Omega^2 \left[\left(\frac{2\sigma_0^2}{E_p} \right) k^3 - \gamma k^4 \right]. \quad (1.32)$$

The solution is

$$A(t) = A_0 \exp(\omega t). \quad (1.33)$$

The perturbation grows when $\omega > 0$, or

$$\left(\frac{2\sigma_0^2}{E_p} \right) k^3 > \gamma k^4. \quad (1.34)$$

The neutral condition is

$$k_{\text{crit}} = \frac{2\sigma_0^2}{E_p \gamma}, \quad (1.35)$$

and the fastest-growing mode is

$$k_{\text{max}} = 0.75 k_{\text{crit}}. \quad (1.36)$$

The corresponding wavelength is

$$\lambda_{\text{max}} = \frac{2\pi}{k_{\text{max}}}. \quad (1.37)$$

This fastest-growing wavelength was used to define the ATG benchmark geometry.

1.5 Benchmark Setup

The benchmark uses a sinusoidal surface with wavelength equal to the fastest- growing ATG wavelength predicted from the selected silicon material properties and the applied stress. The computational domain contains three wavelengths. The right-side displacement is chosen to produce the desired nominal stress:

$$U_{\text{rhs}} = \frac{3\lambda_{\text{max}}\sigma_0}{E_p}. \quad (1.38)$$

The benchmark cases use $\sigma_0 = 500$ MPa, $\epsilon/\lambda = 0.01$, and $T = 1100^\circ\text{C}$. The material parameters are taken from the silicon material definition used for the surface-evolution validation cases. The strain energy-density contribution to surface diffusion is active for this benchmark. This distinguishes the ATG calculation from the Mullins calculation, where surface evolution is driven only by surface energy.

Table 1.1: Primary input and derived parameters for the ATG benchmark cases.

Parameter	Symbol	Value	Units
Applied nominal stress	σ_0	500	MPa
Wavelength	λ	$3.99027407 \times 10^{-3}$	mm
Initial amplitude	ϵ	$3.99027407 \times 10^{-5}$	mm
Amplitude/wavelength	ϵ/λ	0.01	—
Number of periods	n_{periods}	3	—
Temperature	T	1100	$^\circ\text{C}$
Plane-strain modulus	E_p	1.587679606×10^5	MPa
Right-side displacement	U_{rhs}	$3.76991118 \times 10^{-5}$	mm
Analytic growth rate	ω_{analytic}	$1.76041055 \times 10^{-5}$	1/s

Two mesh densities are emphasized in the results below: 20 and 30 elements per wavelength. The 20-element-per-wavelength case is suitable for the automated validation suite because it is computationally less expensive. The 30-element-per-wavelength case provides a higher-resolution comparison to the analytic solution and is retained to support the validation documentation.

1.6 Results

Figure 1.3 shows the spatial variation of the σ_{11} component of stress near the sinusoidally perturbed surface. For this geometry, σ_{11} is a close proxy for the surface tangential stress σ_{tt} . As expected, the tangential stress is higher in the valleys and lower near the peaks. This produces a spatial variation in elastic strain energy density along the surface.

The strain energy contribution tends to drive material transport in a direction that increases the perturbation amplitude. This is opposite to the effect of surface energy, which tends to smooth

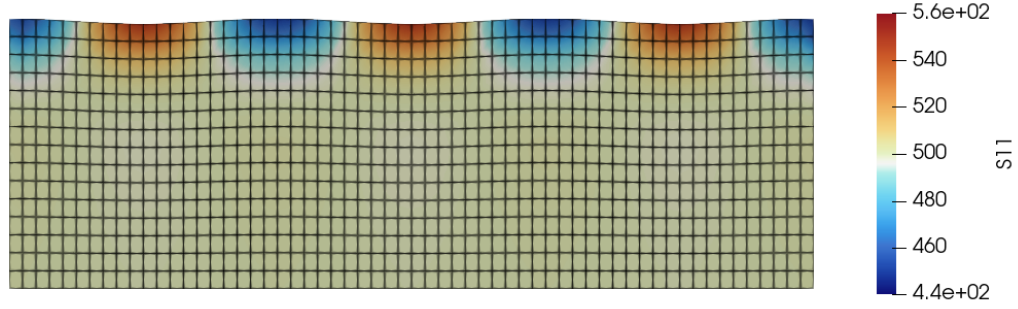


Figure 1.3: Spatial variation of σ_{11} near the sinusoidally perturbed surface.

the surface. The ATG instability occurs when the destabilizing elastic contribution exceeds the stabilizing surface energy contribution.

Figure 1.4 compares the finite-element estimate of the surface normal stress with the capillary prediction $\sigma_{nn} = \gamma\kappa$. The agreement provides a direct check that the surface-energy contribution, the cohesive-zone normal-stress recovery, and the normal-stress projection are producing the expected capillary driving term along the surface.

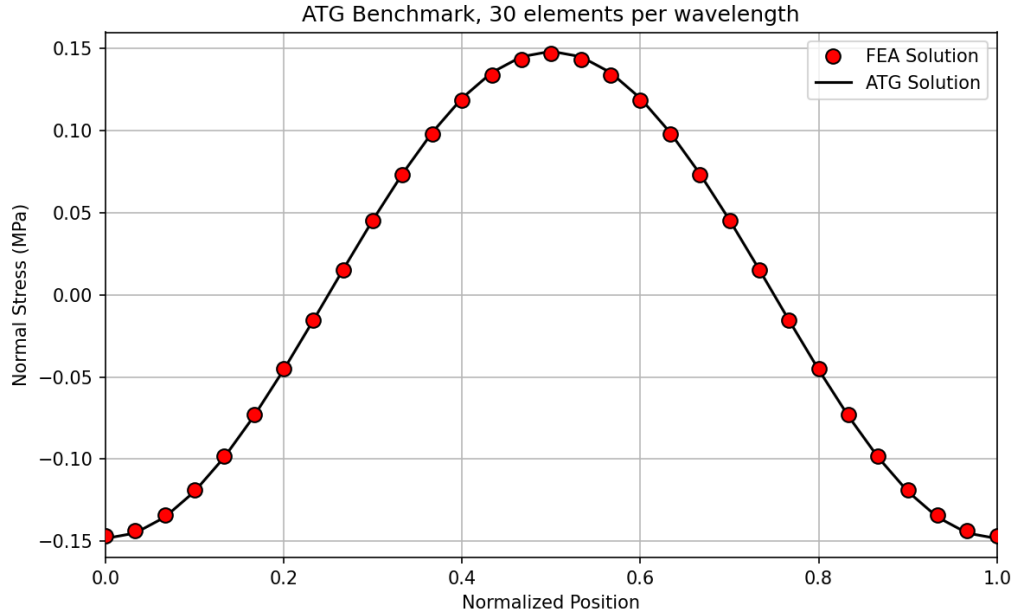


Figure 1.4: Comparison of the finite-element normal stress estimate with the capillary prediction $\sigma_{nn} = \gamma\kappa$.

Figure 1.5 compares the finite-element estimate of the tangential surface stress with the prediction from the linear ATG solution. For the linear ATG solution, the first-order amplitude of the tangential stress perturbation is

$$\Delta\sigma_{tt} = 2\sigma_0 k\epsilon = 4\pi\sigma_0 \left(\frac{\epsilon}{\lambda} \right). \quad (1.39)$$

For the present case, this gives $\Delta\sigma_{tt} = 62.8$ MPa. The finite- element model captures the expected spatial variation in tangential stress, with stress concentration in the valleys and stress reduction near the peaks. The analytic solution predicts slightly larger stress peaks and troughs than the finite-element calculation. This indicates that the finite-element model produces a slightly smaller tangential-stress gradient, and therefore a slightly smaller strain energy density gradient, than the ideal linear ATG solution.

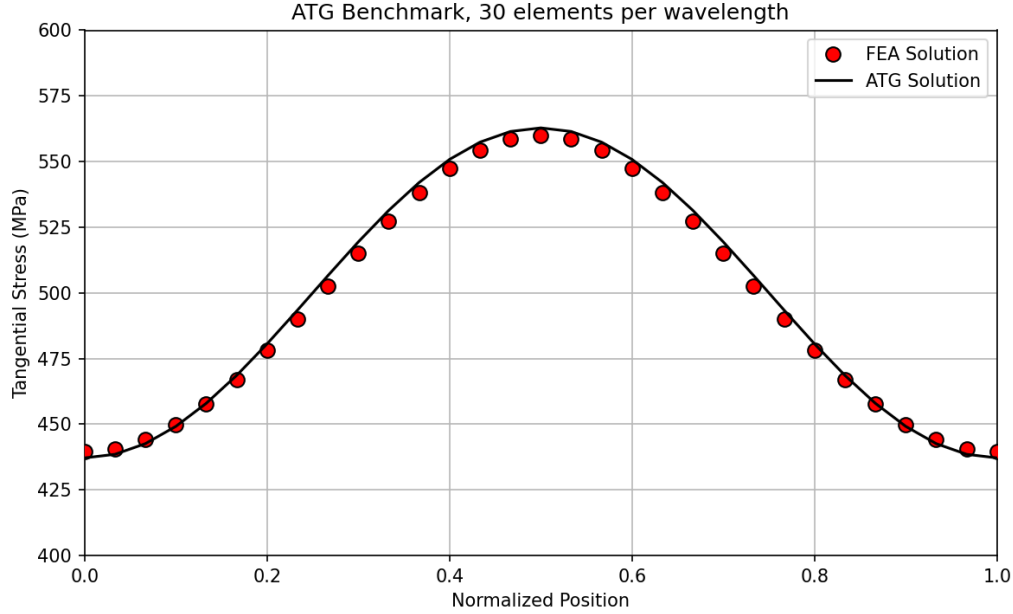


Figure 1.5: Comparison of the finite-element tangential stress estimate with the linear ATG prediction.

This difference is important because the ATG growth rate is controlled by the difference between two competing terms. The destabilizing elastic term and the stabilizing surface energy term are of comparable magnitude. Consequently, a modest underprediction of the tangential-stress gradient can produce a more noticeable reduction in the net growth rate.

Figure 1.6 shows the normalized amplitude as a function of time for the cases with 20 and 30 elements per wavelength. The finite- element results are compared with the analytic ATG growth law $A(t)/A_0 = \exp(\omega t)$.

Table 1.2: Fitted and analytic ATG growth rates for the two mesh densities shown in Figure 1.6.

Elements per wavelength	ω_{FEM} (1/s)	ω_{analytic} (1/s)	Relative error
20	$1.55619467 \times 10^{-5}$	$1.76041055 \times 10^{-5}$	11.6%
30	$1.69629397 \times 10^{-5}$	$1.76041055 \times 10^{-5}$	3.64%

For the 20-element-per-wavelength case, the relative error in the fitted growth rate is approximately 11.6 percent. For the 30-element-per-wavelength case, the relative error decreases to

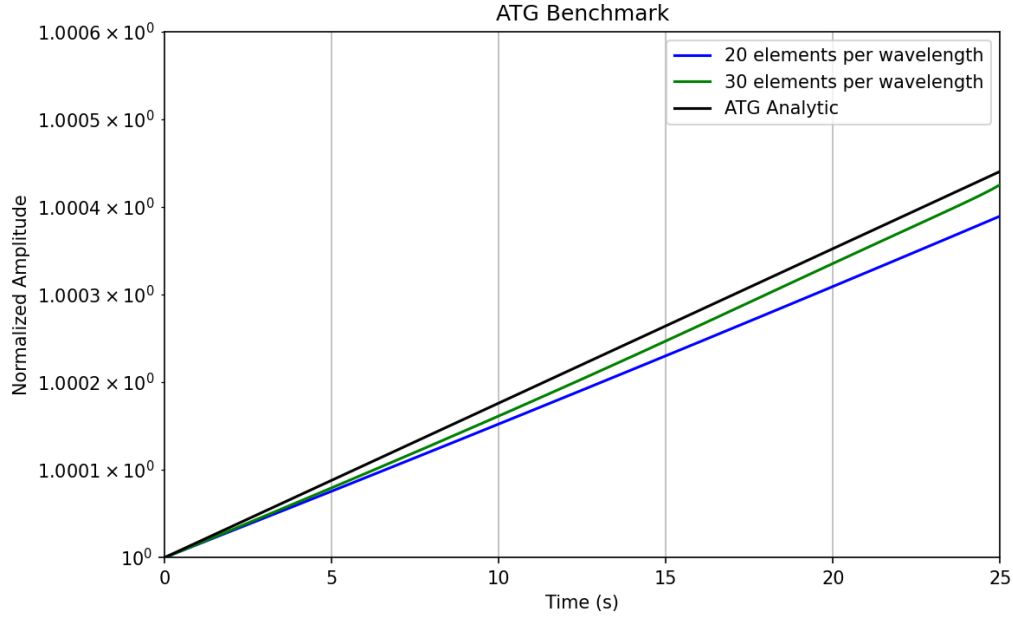


Figure 1.6: Normalized amplitude growth for the 20- and 30-elements-per- wavelength ATG benchmark cases.

approximately 3.64 percent. The 30-element-per-wavelength case grows slightly more slowly than the analytic solution. This is consistent with the tangential-stress comparison in Figure 1.5. The finite-element model predicts slightly lower stress gradients along the surface than the analytic ATG solution, and these lower stress gradients imply lower strain energy-density gradients. Since the strain energy density gradient is the destabilizing term in the ATG instability, a slightly lower gradient should lead to a slightly lower growth rate. That is exactly what is observed.

This consistency provides additional confidence in the calculation. The small discrepancy in amplitude growth is not an unrelated numerical artifact. It follows from the same finite-element approximation of the surface stress field that controls the strain energy driving term in the surface diffusion calculation.

1.7 Discussion

The agreement between the finite-element solution and the analytic ATG solution is notable. The analytic solution is a small-amplitude, linearized, elastic half-space solution. Nevertheless, it provides an excellent prediction for a finite-depth, discretized, multiphysics finite-element calculation.

The finite-element result is also notable because the numerical model does not directly impose the ATG dispersion relation. Instead, the growth rate emerges from the coupled solution of the solid mechanics problem, the estimation and projection of surface stresses, the calculation of chemical-potential gradients, and the resulting surface diffusion deposition rates. The separate

comparisons of normal and tangential surface stress provide intermediate checks on the two stress quantities that enter the surface-diffusion driving force.

In other words, the ATG benchmark is not a check of a single isolated formula. It is an end-to-end test of a relatively long implementation chain:

solid mechanics → tangential stress projection → strain energy-density contribution to chemical potential → surface energy-induced normal stress → cohesive-zone normal stress recovery → normal-stress projection → surface diffusion → normal deposition rate → evolution of surface amplitude.

Given this chain of calculations, the level of agreement with the analytic ATG solution is strong evidence that the formulation and implementation are internally consistent.

The remaining discrepancy in the 30-element-per-wavelength case is also physically consistent. The finite-element model predicts slightly smaller tangential-stress variations than the analytic solution. Since the strain energy-density gradient is the destabilizing term in the ATG instability, this should produce a slightly smaller growth rate. The finite-element amplitude-growth result shows exactly that behavior.

The ATG benchmark is therefore an important complement to the Mullins benchmark. Mullins validates surface energy-driven smoothing. ATG validates the additional coupling to tangential stress, strain energy density gradients, and stress-driven surface instability. Together, the two benchmarks provide strong evidence that the surface diffusion infrastructure is behaving correctly for both stabilizing and destabilizing surface-evolution problems.

For the automated validation workflow, a moderately refined case is used to keep the validation suite computationally efficient. Higher-resolution cases are retained in the validation directory to support documentation and demonstrate convergence toward the analytic solution.

1.8 References

- [1] R. J. Asaro and W. A. Tiller. Interface morphology development during stress corrosion cracking: Part I. Via surface diffusion. *Metallurgical Transactions*, 3:1789–1796, 1972.
- [2] M. A. Grinfeld. Instability of the separation boundary between a non-hydrostatically stressed elastic body and a melt. *Soviet Physics Doklady*, 31:831, 1986.