Evolution of surface waviness in thin films via volume and surface diffusion

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Abstract

Deformation mechanisms involving mass transport by stress driven diffusion influence a large number of technological problems. We study the formation of undulations on surfaces of stressed films at high temperature by exploring the deformation kinetics governed by volume and surface diffusion. A governing equation is derived that gives the amplitude change of such surfaces as a function of time. A parametric study is then carried out using a range of practically important input values of the film material properties. The results show that at the dominant instability wavelength, under low stress and high temperature conditions, the roughening is only caused by volume diffusion, while smoothing is only caused by surface diffusion. The results from the current model are compared to experimental observations reported in the literature for the roughening of metallic film surfaces under the low stress and high temperature conditions common in thermal barrier systems.

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1 INTRODUCTION

Surface morphological instabilities driven by stresses have attracted considerable attention in the last two decades due to their importance in technology. The stability of a solid surface under stress was first addressed by Tiller and co-workers (Asaro & Tiller, 1972; Vasudev *et al.*, 1975) while analyzing the role of surface diffusion and surface dissolution – condensation through an adjoining liquid in stress corrosion cracking. The chemical potential gradient driving the mass transport processes was assumed to be arising from the stress variation along the surface and the surface curvature. In their analysis, however, volume diffusion by a vacancy mechanism was neglected since it was believed to be slow at typical temperatures encountered for stress-corrosion cracking. Similar stability analysis was done independently by Grinfeld (1993) and Srolovitz (1989). The problem of a stressed solid surface (or surface-vapor interface) becoming unstable at high temperature was later observed during thin film growth and annealing (LeGoues *et al.*, 1990; Jesson *et al.*, 1993; Ozkan *et al.*, 1997; Gao & Nix, 1999). Such instabilities were analyzed based on the surface diffusion mechanism driven by gradients in surface chemical potential (Bruinsma & Zangwill, 1987; Spencer *et al.*, 1991; Gao, 1994; Freund & Jonsdottir, 1993; Freund, 1995; Colin *et al.*, 1998), an approach same as that of Tiller and co-workers (Asaro & Tiller, 1972; Vasudev *et al.*, 1975), and Grinfeld (1993) and Srolovitz (1989).

Although surface diffusion is an important kinetic process, there could be other kinetic processes affecting the evolution of stressed surfaces. One possibility at high temperatures is the diffusion of atoms through the bulk. The chemical potential gradient driving this volume diffusion would arise due to capillarity (Mullins, 1963) and stress variations in the bulk produced by the sinusoidal surface morphology.

Note that for unstressed solid surfaces, capillarity-induced volume fluxes, along with surface diffusion, has been used to predict the decay of surface corrugations by Blakely and coworkers (Blakely & Mykura, 1962; Maiya & Blakely, 1965, 1967; Olson *et al.*, 1972; Keefee *et al.*, 1994) and others (Gjostein & Bonzel, 1968; Liau & Zeiger, 1990). Recently, McCarthy *et al.* (2001) have demonstrated that the smoothing of NiAl surfaces is controlled by the exchange of bulk vacancies with the surface occurring only near the surface atomic step edges. The relative importance of volume fluxes varies with conditions such as operating temperature and stress.

A simple analysis of the evolution of stressed sinusoidal surfaces of small amplitude is presented in this paper by taking into account: (i) surface diffusion driven by gradients in chemical potential along the solid surface, (ii) volume diffusion driven by stress variation along the sinusoidal surface, and (iii) volume diffusion driven by capillarity. The governing equations are obtained, followed by a parametric study to reveal the relative importance of the surface and volume diffusion terms. Although this analysis is general, we will compare the model predictions with the waviness formation observed in metallic films of thermal barrier systems (Panat *et al.*, 2003a).

2 ANALYSIS

Consider a sinusoidal surface of a film over a substrate as shown in Fig. 1. The system is assumed infinitely thick in the 'z' direction, so that a plain strain condition exists throughout. The perturbation on the film surface (referred to from here as the solid surface) is assumed to take the form,

$$h(x,t) \;=\; a(t)\cos(\omega x) \tag{1}$$

where a is the perturbation amplitude, and $\omega = 2\pi/\lambda$ is the frequency with λ being the perturbation wavelength. An arbitrary solid surface profile can be represented by a Fourier series of such sinusoidal perturbations. The perturbation amplitude of the film surface is assumed to be small compared to its thickness, so that the film

can be taken to be infinitely thick while computing the fluxes near the free surface. The slope of the film surface is also assumed to be small, implying $\frac{\partial h(x,t)}{\partial x} << 1$ and $\frac{\partial}{\partial s} \approx \frac{\partial}{\partial x}$, where s is a vector along the film surface. Furthermore, the flux at the interface between the film and substrate is assumed to be negligible.

A remote stress σ_∞ is applied to the film parallel to the x axis. This stress can arise as a result of differential expansion (or contraction) of the film with the substrate due to thermal expansion mismatch, phase transformations, or defects during deposition (Thouless, 1995; Chen *et al.*, 2003; Zhang *et al.*, 2003). We denote σ_∞ positive if compressive. The stress along the solid surface is altered compared to the bulk of the film as a result of the surface perturbation and is given as (Asaro & Tiller, 1972; Vasudev *et al.*, 1975; Gao, 1991a,b),

$$\sigma_x(x, y = 0) = -\sigma_\infty + 2\,\sigma_\infty a\omega \cos(\omega x) \tag{2}$$

The second term on the RHS of Eq. 2 represents the *change* in the stress at the solid surface due to the sinusoidal surface geometry. The chemical potential, χ, along the surface of the wavy solid, is (Asaro & Tiller, 1972; Freund, 1995),

$$\chi = (U - \kappa\gamma)\Omega \tag{3}$$

where κ is the solid surface curvature, Ω is the atomic volume, U is the elastic strain energy per unit volume on the solid surface, and γ is the solid surface energy per unit area, assumed to be isotropic.

The strain energy density at the surface, U, is given by,

$$U(x,t) = \frac{(1-\nu)\sigma_\infty^2}{4G}\left[1 - 4\,a\,\omega\cos\left(\omega x\right)\right] \tag{4}$$

where G is the shear modulus. In writing Eq. 4, the higher order terms of $a\omega$ are neglected as a result of the small slope assumption. If the film in Fig. 1 was not attached to the substrate and free to move, the wavelength, λ, would be a function of time. For a film attached to the substrate, however, it is reasonable to assume that planes remain as planes in the film during surface evolution (Thouless, 1993). In such

a case, $h(x,t) = a(t)\cos(\omega x)$, i.e., the fluctuation amplitude alone varies with time. The chemical potential change along the surface drives atom diffusion, giving rise to a flux along the surface (Fig. 2, also see Asaro & Tiller (1972)),

$$J_s = -\frac{D_s C_s}{kT}\frac{\partial \chi}{\partial x} = \frac{D_s C_s \Omega \sin(\omega x)}{kT}\left[\frac{(1-\nu)\sigma_\infty^2}{G}\, a\omega^2 \; - \; \gamma a \omega^3\right] \tag{5}$$

where D_s is the surface self-diffusivity, C_s is the number of diffusing atoms per unit area, k is the Boltzman's constant, and T is the absolute temperature. If the diffusion is occurring at metal-oxide interface, $C_s\Omega$ is replaced by δ, the effective thickness through which the interfacial diffusion occurs, D_s is replaced by D_i, the interface self diffusivity of the metal atoms, and γ is replaced by γ_i, the sum of interfacial and the oxide surface energies.

A gradient in the vacancy concentration arises at right angles to the surface due to surface curvature (Mullins, 1963). The fraction of concentration of vacancies in the solid is then given by (Mullins, 1963),

$$C(x,y) = C_v - \frac{C_v \gamma \Omega}{kT}\,\kappa\, e^{\omega y} \tag{6}$$

where C_v is the fraction of concentration of vacancies in the solid in equilibrium with a flat surface. While writing Eq. 6, it is assumed that the vacancy volume is same as the atomic volume (Mullins, 1963; Blakely & Mykura, 1962). The concentration gradient in the vacancies will result in a vacancy flux at the film surface (Fig. 2),

$$J_{v1} = -\, D_v \frac{\partial [C(x,y)/\Omega]}{\partial y}\bigg|_{y=o} = \frac{D_v C_v \gamma}{kT} a\omega^3 \cos(\omega x) \tag{7}$$

where D_v is the vacancy self-diffusivity. Note that for most metals, the product, $D_v C_v$, is equal to the volume self-diffusivity of the solid, D_1. We replace $D_v C_v$ by D_1 in the current analysis. While writing Eq. 7, the gradient of vacancy concentration normal to the surface is approximated as $\partial[C(x,y)/\Omega]/\partial y$, and computed at $y = 0$ due to the small slope assumption (Mullins, 1963). Equation 7 implies that there is a net flux of the solid atoms from crests to the troughs (Fig. 2) as a result of a net flux of vacancies from troughs to crests. Thus, the vacancy flux given by Eq. 7 tends to "flatten" the surface profile.

A volume diffusive flux can also be driven by a variation of stress along the surface (see Eq. 2). The stress at the crests is relaxed, while it is amplified at the troughs. The atoms on the troughs have a higher chemical potential compared to that on the crests. This process is analogous to diffusional creep of grains in a polycrystalline material (Shewmon, 1989), with grain size being replaced by the fluctuation wavelength. To compute the chemical potential gradient, we need the decay of stress σ_x near the surface. A closed form solution (Asaro & Tiller, 1972; Vasudev *et al.*, 1975) is,

$$\sigma_x(x,y) = -\sigma_\infty \; - \; a\sigma_\infty(-\omega^2\, y - 2\omega)e^{\omega y}\cos(\omega x) \tag{8}$$

The gradient of σ_x along y axis will give rise to the volume fluxes shown in Fig. 2. We compute the diffusive flux from the chemical potential gradient due to variation of $\sigma_x(x,y)$ normal to the surface; a process similar to diffusional creep (Shewmon, 1989), as,

$$J_{v2} = -\,\frac{D_1}{kT\Omega}\frac{\partial[-\sigma_x(x,y)\,\Omega]}{\partial y}\bigg|_{y=o} = \frac{3D_1}{kT}\,a\,\omega^2\,\sigma_\infty\cos(\omega x) \tag{9}$$

Note that the crests will experience a flux of atoms along the positive y axis and vice versa. This flux will tend to roughen the surface for compressive remote stress.

All mass transport processes mentioned above are assumed to take place in the region close to the surface and hence the volume flux *at* the surface can be used to compute the velocity of the surface as shown in Fig. 3. Conservation of mass at a surface element (Fig. 3) gives the normal velocity,

$$V_n = \frac{\partial h(x,t)}{\partial t} = -\Omega\frac{\partial J_s}{\partial x} + \Omega\,(-J_{v1} \; + \; J_{v2}) \tag{10}$$

The rate of change of fluctuation amplitude can then be computed from the definition of $h(x,t)$, along with Eqs. 5, 7 and 9, as

$$\begin{aligned}\frac{1}{a(t)}\frac{\mathrm{d}a(t)}{\mathrm{d}t} \;\; &= \;\; \frac{D_{s\circ}C_{s\circ}\Omega^2}{kT}\;e^{-q_s/kT}\;\left[\frac{(1-\nu)\sigma_\infty^2}{G}\;\omega^3 \; - \; \gamma\,\omega^4\right] \\ &+ \;\; \frac{D_{1\circ}\Omega}{kT}\;e^{-q_1/kT}\,[3\sigma_\infty\omega^2 \; - \; \gamma\,\omega^3]\end{aligned} \tag{11}$$

Here, D_sC_s and D_1 are replaced by $D_{s\circ}C_{s\circ}\exp(-\,q_s/kT)$ and $D_{1\circ}\exp(-\,q_1/kT)$, with q_s and q_1 being the corresponding activation energies. The first term in Eq. 11 tends

to roughen the surface, irrespective of the sign of remote stress, while the third term roughens the surface only for compressive remote stress. The ω^2 (or $1/\lambda^2$) dependence of the third term in Eq. 11 is similar to the $1/(\text{grain size})^2$ dependence of the strain rate (Shewmon, 1989) during creep of a polycrystalline material. The rate of the amplitude increase per unit amplitude ($(1/a)(\mathrm{d}a/\mathrm{d}t)$) in the present problem is thus analogous to the creep strain rate.

The second and the fourth terms in Eq. 11 represent the tendency of the sinusoidal surface to flatten. In absence of remote stress, we go back to the case described by Mullins (1963) where the surface *always* flattens through diffusion at high temperatures. The decay constant during corrugation smoothing (Blakely & Mykura, 1962; Maiya & Blakely, 1965, 1967; Olson *et al.*, 1972; Keefee *et al.*, 1994; Gjostein & Bonzel, 1968; Liau & Zeiger, 1990) is now replaced by a 'decay' or an 'amplification' constant depending upon the surface undulation frequency. The terms in Eq. 11 that have the most influence on the surface evolution at a given ω include $D_1/(D_sC_s)$ and σ_∞. We carry out this analysis in the next section by taking input values for the variables in Eq. 11 from the literature.

3 RESULTS AND DISCUSSION

We start by analyzing Eq. 11 for constant temperature as applied in various experimental studies of surface evolution of stressed (Ozkan *et al.*, 1997; Panat *et al.*, 2003a) and unstressed surfaces (Blakely & Mykura, 1962; Maiya & Blakely, 1965, 1967; Olson *et al.*, 1972; Keefee *et al.*, 1994). First, a brief literature survey of the typical values of the relevant parameters in Eq. 11 is presented, especially those pertaining to the thermal barrier systems. The remote stress (σ_∞) in the films can vary widely. In films of thermal barrier systems, this stress is in tens of MPa at high temperatures (Panat *et al.*, 2003b; Karlsson & Evans, 2001; Pan *et al.*, 2003). In thin film roughening experiments, this stress is typically in the GPa range (Gao, 1991a; Freund, 1995; Gao & Nix, 1999).

Few q_1 values for Ni-based bond coat alloys used in thermal barrier systems and related materials have been reported in literature. For NiAl, the activation energy for interdiffusion, q_1 of 2.71-3.25 eV (Pan *et al.*, 2003) has been reported. The q_1 for Ni is about 2.89 eV (Porter & Easterling, 1981). For surface diffusion, the reported q_s values for Ni vary considerably, from 0.82 eV (Gjostein & Bonzel, 1968), to 1.54-1.85 eV (Maiya & Blakely, 1967). This variation is due to surface conditions and surface orientation. To the authors' knowledge, q_s for metal film surfaces in thermal barrier systems has not been experimentally determined. The ratio of $D_1/(D_sC_s)$ can vary over a few orders of magnitude depending upon conditions such as crystal orientation, temperature, and surface cleanliness. For Ni, this ratio has been reported to vary from about 1.5×10^{-25} m^2 at 1273 K and 1.8×10^{-24} m^2 at 1473 K (Gjostein & Bonzel, 1968; Porter & Easterling, 1981). $D_1/(D_sC_s)$ is also reported to vary for Ni, from 2.5×10^{-25} m^2 to 10^{-24} m^2 at 1273 K, and 1.3×10^{-24} m^2 to 3.7×10^{-24} m^2 at 1473 K (Maiya & Blakely, 1967; Porter & Easterling, 1981). For Cu, $D_1/(D_sC_s)$ has been reported to be 7×10^{-27} m^2 at 1273 K (Choi & Shewmon, 1962; Porter & Easterling, 1981); while for α-Fe, this ratio is about 10^{-24} m^2 at all temperatures (Blakely & Mykura, 1963).

The surface energy, γ, of the film is typically of the order of 1 J/m^2. The isothermal (annealing) temperature for roughening experiments in thermal barrier systems is between 1373 K and 1473 K (Deb *et al.*, 1987; Tolpygo & Clarke, 2000; Panat & Hsia, 2003; Panat *et al.*, 2003a). Note that the effect of the isothermal temperature on results is incorporated through the ratio $D_1/(D_sC_s)$.

To gain an insight on the film surface roughening through combined surface and volume diffusion, we find the amplitude change of surface perturbations with time as a function of wavelength from Eq. 11 for a set of input parameters given below. For $G = 100$ GPa, $\nu = 1/3$, $\sigma_\infty = 25$ MPa, $D_1/(D_sC_s) = 10^{-25}$ m^2, $\gamma = 1$ J/m^2, and $\Omega = 4.28 \times 10^{-29}$ m^3 (from Blakely & Mykura, 1961, for Ni), Eq. 11 gives,

$$\ln\left(\frac{\mathrm{a}(t)}{\mathrm{a}_\circ}\right)\Bigg|_{\hat{\lambda}} = \frac{8\pi^3 D_s C_s \Omega^2 \sigma_\infty^6\, t}{kT\gamma^3 G^3}\, \hat{\lambda}^{-3}\left[P - Q\,\hat{\lambda}^{-1} + R\,\hat{\lambda} - S\right] \qquad (12)$$

where P, Q, R, and S are parameters equal to 4.2×10^3 N/m^2, 3.9×10^4 N/m^2, 5.5×10^6 N/m^2, and 2.9×10^3 N/m^2, respectively for the chosen set of material parameters, $\hat{\lambda} = 2\pi\sigma_\infty^2/(\omega\gamma G)$ is the dimensionless wavelength, a(t) is the fluctuation amplitude at time t, while a$_\circ$ is the initial amplitude.

The normalized amplitude change of the film a(t)/a$_\circ$ as a function of wavelength λ from Eq. 12 is plotted in Fig. 4a. The plot reveals different rates of amplitude change for perturbations of different wavelengths. For surface undulations with wavelengths less than a critical value, λ_{cr} (Fig. 4a), the amplitude decreases with time. This value is about 15 μm in the present case. It can be seen that in this region ($\lambda < \lambda_{cr}$), the logarithm of amplitude ratio is negative, i.e., amplitude decreases rapidly as the wavelength of waviness decreases. On the other hand, undulations with wavelength greater than λ_{cr} increase in amplitude at varying relative rates with time. The result also shows that the maximum amplitude change occurs at a wavelength, λ_{max} (Fig. 4a), of about 21 μm in the present case. The components with wavelengths close to this peak point grow faster than components of other wavelengths. The evolution of the film described by Fig. 4a is qualitatively similar to that if we consider surface diffusion alone as shown in Fig. 4b (also see Asaro & Tiller (1972); Freund (1995)) or volume diffusion alone as shown in Fig. 4c. However, the critical and the maximum wavelengths is significantly larger when considering surface diffusion alone (about 1510 μm and 2010 μm respectively), or considerably smaller when considering volume diffusion alone (about 0.08 μm and 0.13 μm respectively). Thus, for the set of parameters used to plot Fig. 4, neither of the two diffusion paths alone can explain the waviness formation seen in thermal barrier systems (Panat *et al.*, 2003a) where the wavelength of waviness is seen to be tens of micrometers.

Figure 4 suggests that given enough time to evolve, the film surface wavelengths should be relatively independent of the initial surface features and be dominated by wavelengths close to λ_{max}. For the material parameters used to obtain Fig. 4, the contribution to roughening by the first term of Eq. 11 is negligible compared to the third term at λ_{max}. Also, at λ_{max}, the contribution to smoothing of perturbations

by the fourth term of Eq. 11 is negligible compared to the second term. Thus, at the dominant instability wavelength for the material parameters considered, the only destabilizing mechanism for the surface perturbations is volume diffusion, while the only stabilizing mechanism is surface diffusion. Under these conditions,

$$\lambda_{max} \;=\; \sqrt{2}\;\lambda_{cr} \;=\; 2\pi\;\left(\frac{2\Omega\gamma}{3\sigma_\infty}\frac{D_sC_s}{D_1}\right)^{1/2} \tag{13}$$

The value of λ_{max} changes with $D_1/(D_sC_s)$ and stress σ_∞ as shown in Fig. 5. Other parameters used to plot Fig. 5 are the same as those used for Fig. 4a. The dominant surface wavelength in Fig. 5 increases with decreasing volume diffusion relative to surface diffusion (i.e. decreasing $D_1/(D_sC_s)$). Fig. 5 also shows that the values of λ_{max} decrease with increasing stress at a given relative diffusional rate, $D_1/(D_sC_s)$. This is due to the fact that the λ_{max} predicted by surface diffusion alone in Eq. 11 decreases faster with stress (proportional to σ_∞^2) compared to that predicted by volume diffusion alone (proportional to σ_∞). Results similar to those in Fig. 5 are plotted in Fig. 6 for low (Fig. 6a) and high (Fig. 6b) stress values. In Fig. 6a, the inclusion of volume diffusion terms has considerable effect on the value of λ_{max} ('y' axis has a logarithmic scale) when the film remote stress is low. At high stress levels in GPa range, though (Fig. 6b), the effect of volume diffusion would be insignificant. The neglect of volume diffusion terms in Eq. 12 while analyzing the epitaxial thin film roughening problems (Freund & Jonsdottir, 1993; Freund, 1995) is thus justified for practical ranges of material properties. Further, the range of dominant film wavelengths seen in Fig. 6b is in agreement with the values reported in thin film roughening experiments (Ozkan *et al.*, 1997; Gao & Nix, 1999), in line with previous analysis (Bruinsma & Zangwill, 1987; Spencer *et al.*, 1991; Gao, 1991b; Freund & Jonsdottir, 1993; Freund, 1995). Note that the effect of temperature on λ_{max} can be qualitatively assessed from Fig. 5. As the annealing temperature decreases, the ratio $D_1/(D_sC_s)$ decreases since q_s is smaller than q_1. Hence, decreasing temperature is equivalent to a decreasing $D_1/(D_sC_s)$ in Fig. 5. The actual rate of this decrease will depend on $(q_1 - q_s)$.

The film roughening behavior described in the current analysis (Eq. 11) is sensitive to the sign of the remote stress, unlike that predicted by considering surface diffusion alone (Asaro & Tiller, 1972; Bruinsma & Zangwill, 1987; Srolovitz, 1989; Spencer *et al.*, 1991; Freund & Jonsdottir, 1993; Grinfeld, 1993; Freund, 1995; Colin *et al.*, 1998). For compressive remote stress (Figs. 4, 5, and 6), the volume diffusion driven by the remote stress tends to roughen the film surface, while that due to surface tension (i.e. γ) tends to smooth out the perturbations. For tensile remote stress, however, both of the volume diffusion mechanisms flatten the surface perturbations (see Eq. 11). At a low tensile stress, volume diffusion and hence this effect is dominant. As the tensile stress is increased, roughening due to surface diffusion increasingly dominates over flattening due to volume diffusion. Fig. 7 illustrates such a behavior at low (Fig. 7a) and high (Fig. 7b) film tensile stress levels. Note that all the other parameters used to plot Figs. 7 are similar to those used while plotting Fig. 4. Thus, the current model suggests that films under low tensile stress will have no tendency to roughen, while films under high tensile or compressive stress would tend to show surface roughening.

4 COMPARISON WITH EXPERIMENTS

Recently Panat *et al.* (2003a) conducted annealing experiments on nickel aluminide films on a Ni-based superalloy (René N5) substrate. These coatings are used as thermal barriers in jet engines and gas turbines (Goward, 1998). Panat *et al.* (2003a) observed that nominally flat surfaces of these coatings "rumple", or roughen, to form surface undulations. Figure 8 shows such a surface after an anneal of about 25 hours at 1200 °C in vacuum. The wavelength of the surface undulations of these films was of the order of 50 μm. A Rutherford Backscattering Spectroscopy (RBS) analysis of the surfaces of these films indicated that no segregation of either Ni or Al occurred. Further, calculations indicate that the contribution to the roughening process via evaporation of the metal elements at high temperature is negligible. Thus

mass transport via surface and volume diffusion driven by the stress in the film is likely to be the mass transport mechanism in roughening of these films (Fig. 8). Note that the chemical compositions of these films evolved during the anneal. Initially, the film surface consisted of Ni, Al, Co and Cr, while after the anneal, the RBS analysis showed that the surface consisted of W (< 2 at %), in addition of the Ni, Al, Co and Cr. We believe that the additional W results from interdiffusion between the film and substrate.

The nickel aluminide films used by Panat *et al.* (2003a) are deposited on the René N5 substrate at about 1080 °C. The thermal expansion coefficients of the materials in such systems dictate that they be under tensile stress below (and under compressive stress above) the processing temperature (Watanabe *et al.*, 2002; Karlsson & Evans, 2001; Chen *et al.*, 2003; Panat *et al.*, 2003b). The yield behavior of these films (Pan *et al.*, 2003) suggests that the film remote stress at high temperatures be about 20-30 MPa compressive. From the above discussion and the roughening predictions of the current model (Figs. 5 and 6), it can be seen that the experimental observations (Fig. 8) agree with the model reasonably well. It is worthwhile to note that the surface and volume diffusivities of the nickel aluminide films is not known. At the same time, the microstructural changes occuring in the films during the high temperature anneal (Panat *et al.*, 2003a) can potentially change the properties of the surface and the bulk. Lastly, the current analysis describes one-dimension roughening, while in practice, the roughening occurs in two dimensions (Fig. 8).

Some estimates can be made for the amplitude change predicted by the current model. For conditions used to plot Fig. 5, when the remote stress is 25 MPa, λ_{max} is 21 μm (i.e. $D_1/(D_sC_s) = 10^{-25}$ m^2), and $D_{s\circ}\exp(\text{-}q_s/(kT))$ is 10^{-9} m^2/s, we get $\ln(\text{a}/\text{a}_\circ) = 5.68 \times 10^{-6}\, t$ (t in seconds). This implies that the wave amplitude (for the maximum wavelength) increases by about 67 % after 25 hour isothermal heating. For an order of magnitude higher $D_{s\circ}\exp(\text{-}q_s/(kT))$, with the same $D_1/(D_sC_s)$, this increase is over two orders of magnitude.

Note that the film surfaces form high diffusivity paths for diffusion when com-

pared to the bulk (Shewmon, 1989). At the same time, the grain boundaries in polycrystalline films can also become high diffusivity paths compared to the bulk under certain conditions. Such effects have been observed in Cu thin films (Weiss *et al.*, 2001) and in films of thermal barrier systems (Panat *et al.*, 2003a). However, the effect of grain boundary diffusion on surface evolution decreases as the temperature is increased since the activation energy for grain boundary diffusion is less than that for bulk diffusion. The decreasing importance of grain boundary diffusion with increasing temperature has been observed by Panat *et al.* (2003a) in polycrystalline nickel aluminide films of thermal barrier systems.

5 CONCLUSIONS

In this paper we present a simple analysis describing the evolution of sinusoidal surfaces of stressed films by considering the diffusion of atoms through the film volume and along the film surface. The volume diffusion is shown to be influential at relatively low stress levels (tens of MPa) typically encountered in films in thermal barrier systems, while is not important at high stress levels (in GPa range) typically encountered in thin film technology. Other factors influencing the relative importance of volume diffusion are the ratio of the volume self diffusivity to the product of the surface self diffusivity with the surface defect concentration. The inclusion of volume diffusion terms in the stability analysis implies a different behavior of the film surfaces under a tensile and a compressive stress. This effect is however shown to affect the stability only at low stress levels. The current study shows that at the dominant instability wavelength and under low stress and high temperature conditions, the only important destabilizing mechanism is volume diffusion, while the only important stabilizing mechanism is surface diffusion. The current model explains the surface instabilities reported for films of thermal barrier systems reasonably well.

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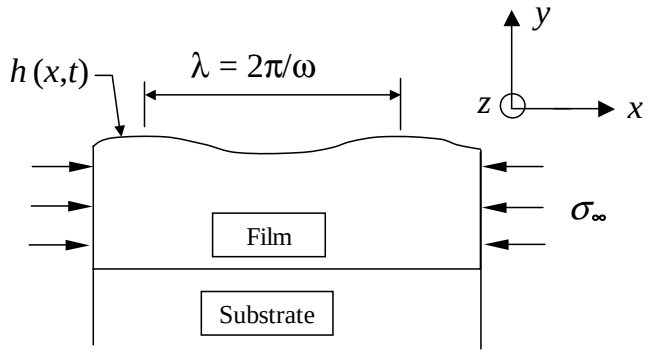

Figure 1: Sinusoidal perturbations of free surface of the stressed solid.

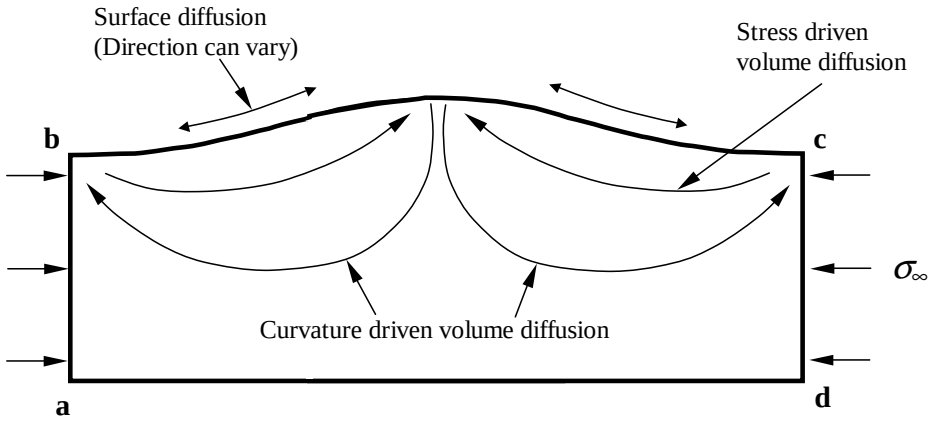

Figure 2: A portion on the film surface between two troughs showing various diffusion processes.

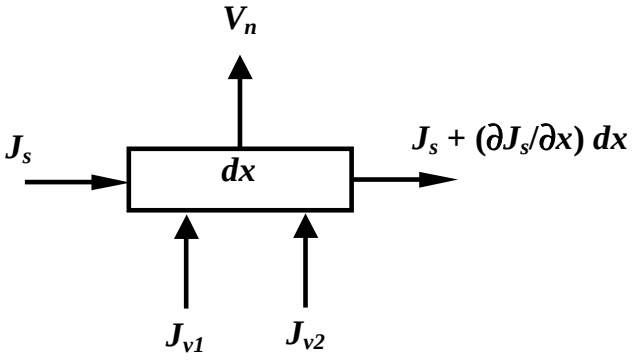

Figure 3: Diffusion along surface element of the surface.

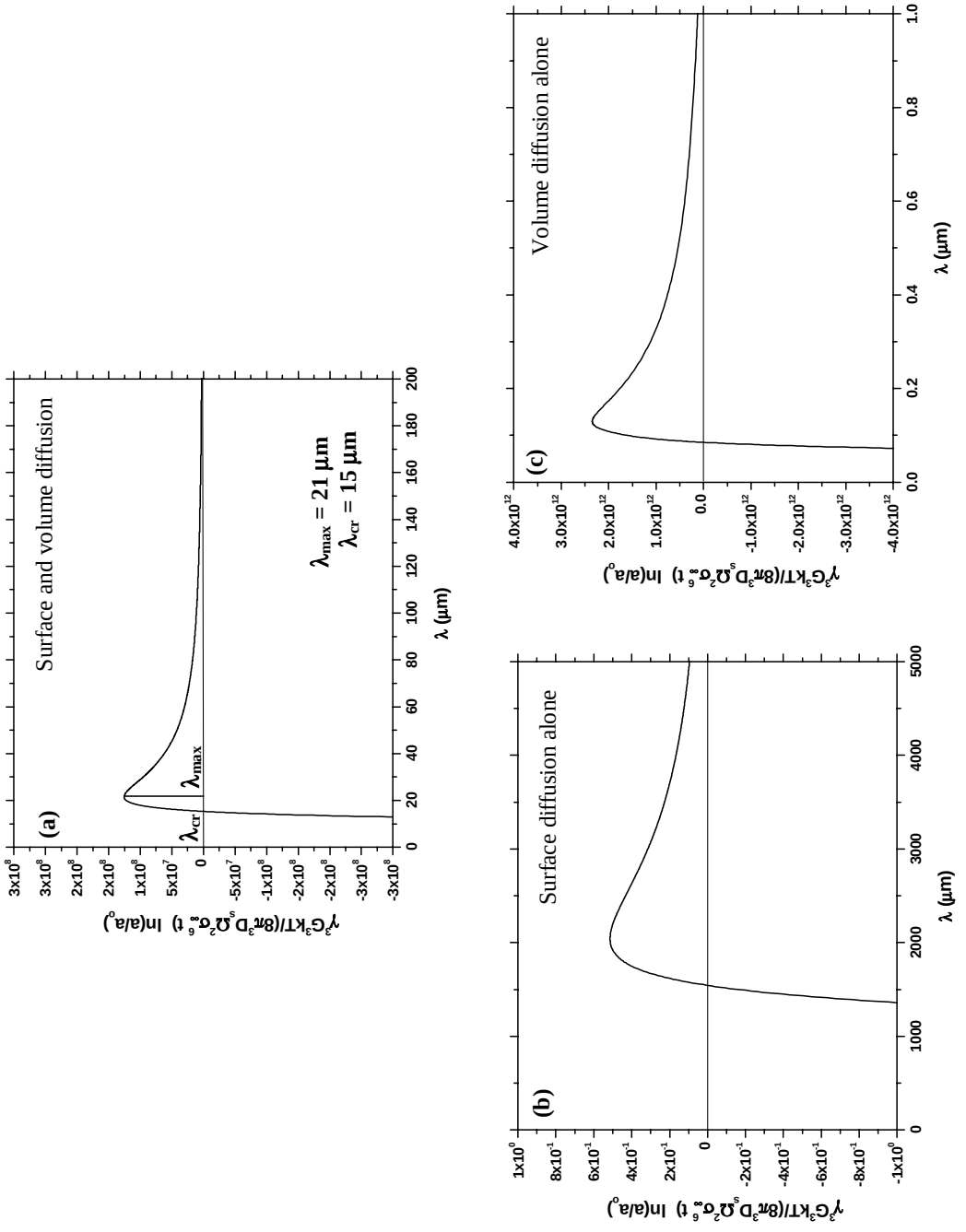

Figure 4: Ratio of amplitude change of a film as a function of wavelength for isothermal temperature history. (a) Considering both surface and volume diffusion, (b) considering surface diffusion alone (first two terms on RHS of Eq. 11) and (c) considering volume diffusion alone (last two terms on RHS of Eq. 11).

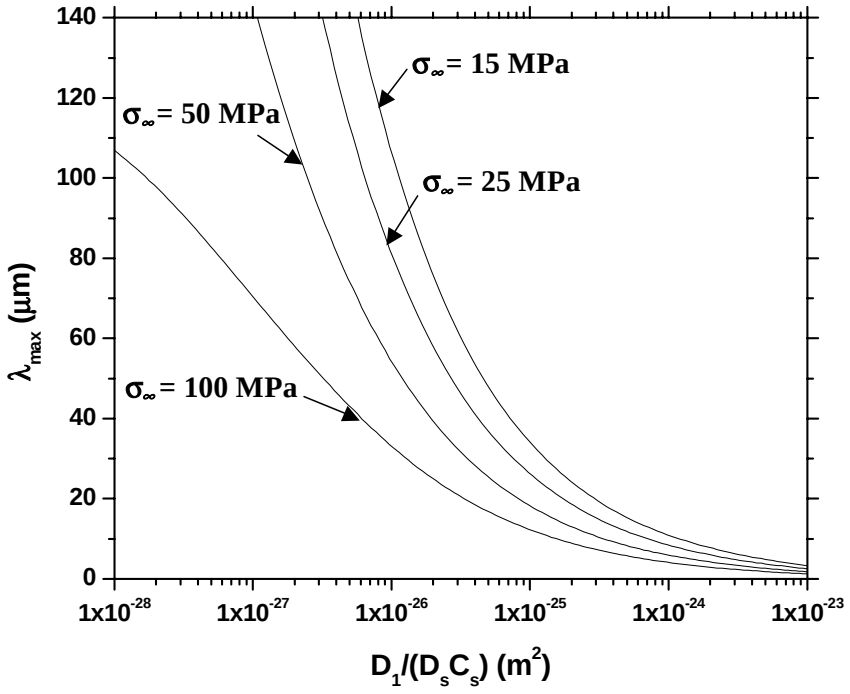

Figure 5: The λ_{max} of a film as a function of $D_1/(D_sC_s)$ [$= D_vC_v/(D_sC_s)$].

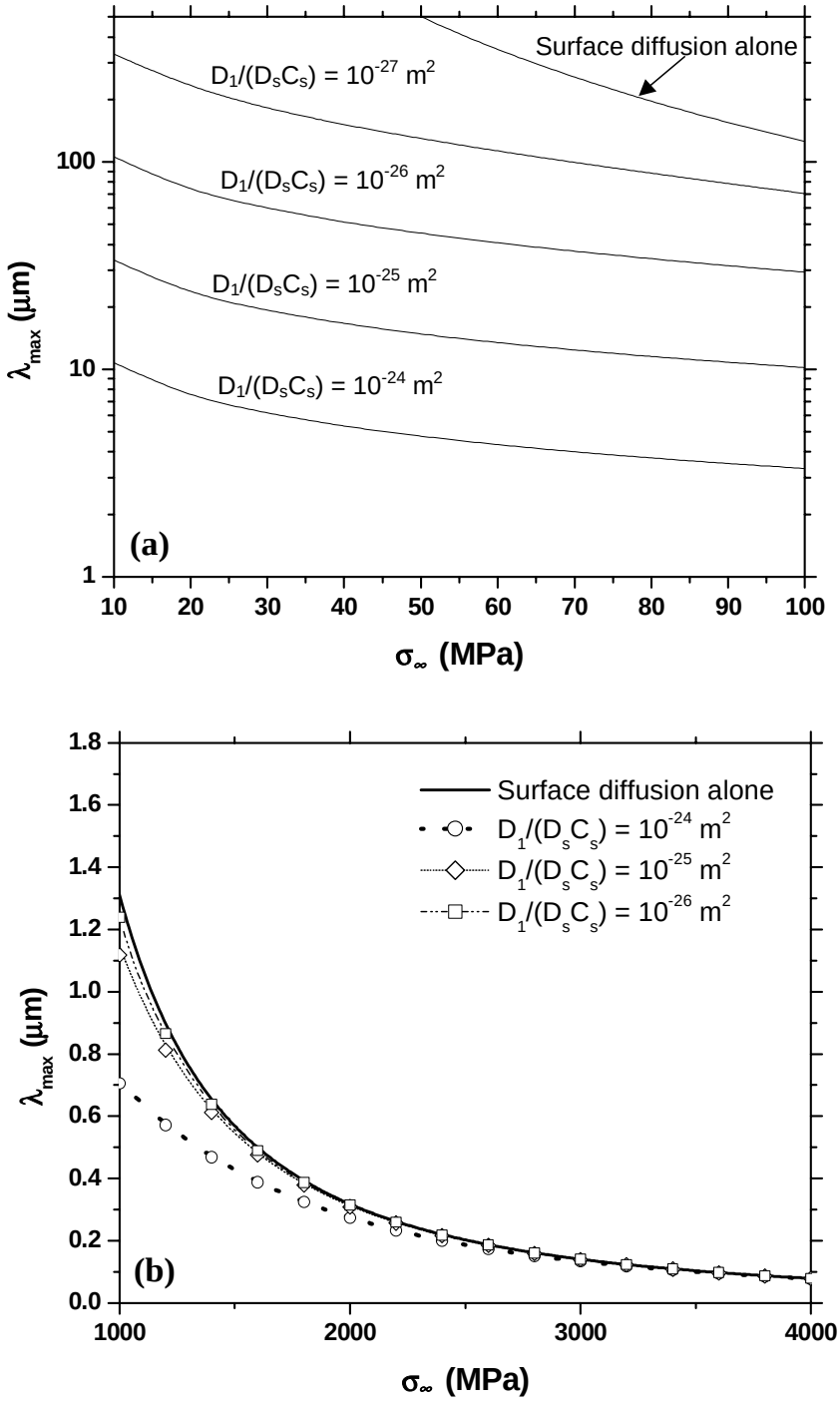

Figure 6: The λ_{max} of a film as a function of the remote stress at (a) low and (b) high stress levels for different $D_1/(D_sC_s)$ values.

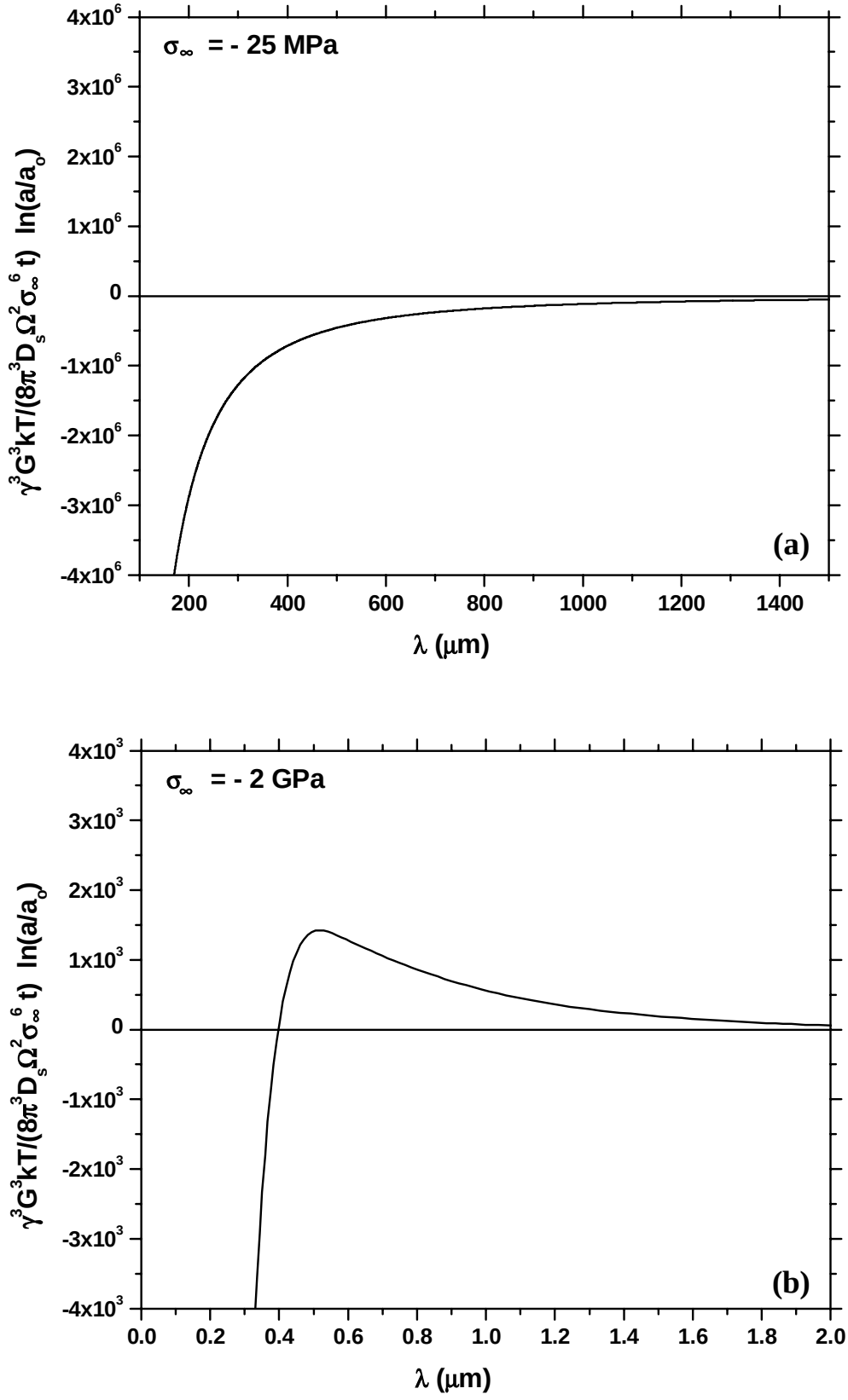

Figure 7: Ratio of amplitude change of a film as a function of wavelength for a tensile film stress of (a) 50 MPa and (b) 2 GPa.

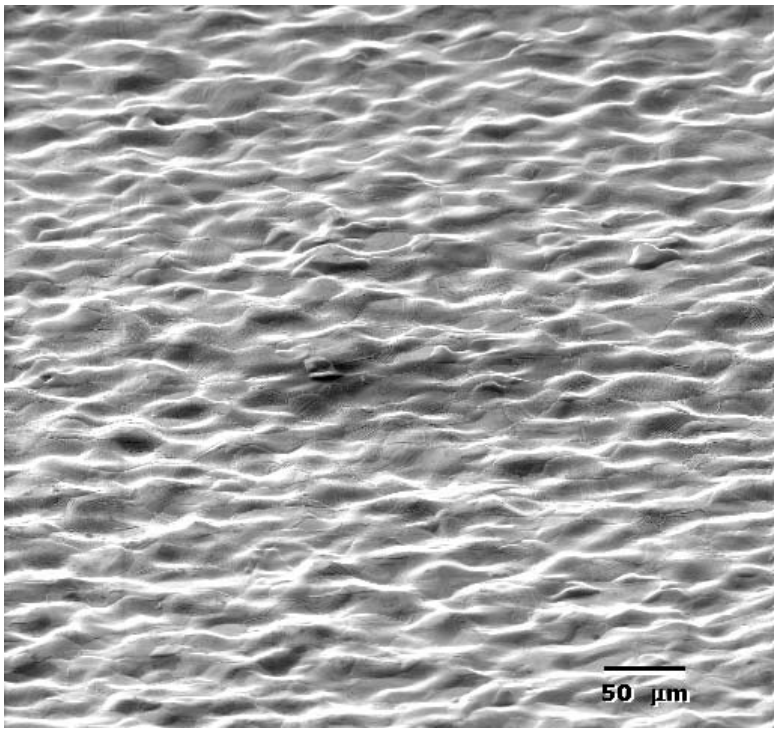

Figure 8: Surface of a nickel aluminide coating (about 50 μm thick) on a superalloy substrate that has developed clear wavy patterns on the surface at 1200 °C in vacuum after 25 hours (from Panat *et al.* (2003a)).

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No.	Authors	Title	Date
959	Kuznetsov, I. R., and D. S. Stewart	Modeling the thermal expansion boundary layer during the combustion of energetic materials—*Combustion and Flame*, in press (2001)	Oct. 2000
960	Zhang, S., K. J. Hsia, and A. J. Pearlstein	Potential flow model of cavitation-induced interfacial fracture in a confined ductile layer—*Journal of the Mechanics and Physics of Solids*, **50**, 549–569 (2002)	Nov. 2000
961	Sharp, K. V., R. J. Adrian, J. G. Santiago, and J. I. Molho	Liquid flows in microchannels—Chapter 6 of *CRC Handbook of MEMS* (M. Gad-el-Hak, ed.) (2001)	Nov. 2000
962	Harris, J. G.	Rayleigh wave propagation in curved waveguides—*Wave Motion* **36**, 425–441 (2002)	Jan. 2001
963	Dong, F., A. T. Hsui, and D. N. Riahi	A stability analysis and some numerical computations for thermal convection with a variable buoyancy factor—*Journal of Theoretical and Applied Mechanics* **2**, 19–46 (2002)	Jan. 2001
964	Phillips, W. R. C.	Langmuir circulations beneath growing or decaying surface waves—*Journal of Fluid Mechanics* (submitted)	Jan. 2001
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966	Bagchi, P., and S. Balachandar	Linearly varying ambient flow past a sphere at finite Reynolds number: Part 2—Equation of motion—*Journal of Fluid Mechanics* **481**, 105–148 (2003) (with change in title)	Feb. 2001
967	Cermelli, P., and E. Fried	The evolution equation for a disclination in a nematic fluid—*Proceedings of the Royal Society A* **458**, 1–20 (2002)	Apr. 2001
968	Riahi, D. N.	Effects of rotation on convection in a porous layer during alloy solidification—Chapter 12 in *Transport Phenomena in Porous Media* (D. B. Ingham and I. Pop, eds.), 316–340 (2002)	Apr. 2001
969	Damljanovic, V., and R. L. Weaver	Elastic waves in cylindrical waveguides of arbitrary cross section—*Journal of Sound and Vibration* (submitted)	May 2001
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971	Subramanian, S. J., and P. Sofronis	Calculation of a constitutive potential for isostatic powder compaction—*International Journal of Mechanical Sciences* (submitted)	June 2001
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981	Adrian, R. J.	Information and the study of turbulence and complex flow—*Japanese Society of Mechanical Engineers Journal B*, in press (2002)	Oct. 2001
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991	Christensen, K. T., and R. J. Adrian	Measurement of instantaneous Eulerian acceleration fields by particle-image accelerometry: Method and accuracy—*Experimental Fluids* (submitted)	Dec. 2001
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1004	Fried, E., and R. E. Todres	Normal-stress differences and the detection of disclinations in nematic elastomers—*Journal of Polymer Science B: Polymer Physics* **40**, 2098–2106 (2002)	June 2002
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1006	Tomkins, C. D., and R. J. Adrian	Spanwise structure and scale growth in turbulent boundary layers—*Journal of Fluid Mechanics* (submitted)	Aug. 2002
1007	Riahi, D. N.	On nonlinear convection in mushy layers: Part 2. Mixed oscillatory and stationary modes of convection—*Journal of Fluid Mechanics* (submitted)	Sept. 2002
1008	Aref, H., P. K. Newton, M. A. Stremler, T. Tokieda, and D. L. Vainchtein	Vortex crystals—*Advances in Applied Mathematics* **39**, in press (2002)	Oct. 2002
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1011	Carlson, D. E., E. Fried, and D. A. Tortorelli	On internal constraints in continuum mechanics—*Journal of Elasticity* **70**, 101–109 (2003)	Oct. 2002
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1014	Brown, E. N., M. R. Kessler, N. R. Sottos, and S. R. White	*In situ* poly(urea-formaldehyde) microencapsulation of dicyclopentadiene—*Journal of Microencapsulation* (submitted)	Feb. 2003
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1021	Fried, E.	The configurational and standard force balances are not always statements of a single law—*Proceedings of the Royal Society* (submitted)	Apr. 2003
1022	Panat, R. P., and K. J. Hsia	Experimental investigation of the bond coat rumpling instability under isothermal and cyclic thermal histories in thermal barrier systems—*Proceedings of the Royal Society of London A*, in press (2003)	May 2003
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1026	Liu, M., K. J. Hsia, and M. Sardela Jr.	In situ X-ray diffraction study of electric field induced domain switching and phase transition in PZT-5H—*Journal of the American Ceramics Society* (submitted)	May 2003
1027	Riahi, D. N.	On flow of binary alloys during crystal growth—*Recent Research Development in Crystal Growth*, in press (2003)	May 2003
1028	Riahi, D. N.	On fluid dynamics during crystallization—*Recent Research Development in Fluid Dynamics*, in press (2003)	July 2003
1029	Fried, E., V. Korchagin, and R. E. Todres	Biaxial disclinated states in nematic elastomers—*Journal of Chemical Physics* **119**, 13170–13179 (2003)	July 2003
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1031	Yoon, H. S., D. F. Hill, S. Balachandar, R. J. Adrian, and M. Y. Ha	Reynolds number scaling of flow in a Rushton turbine stirred tank: Part I—Mean flow, circular jet and tip vortex scaling—*Chemical Engineering Science* (submitted)	Aug. 2003
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1033	Hill, K. M., G. Gioia, and V. V. Tota	Structure and kinematics in dense free-surface granular flow—*Physical Review Letters*, in press (2003)	Aug. 2003
1034	Fried, E., and S. Sellers	Free-energy density functions for nematic elastomers—*Journal of the Mechanics and Physics of Solids*, in press (2003)	Sept. 2003
1035	Kasimov, A. R., and D. S. Stewart	On the dynamics of self-sustained one-dimensional detonations: A numerical study in the shock-attached frame—*Physics of Fluids* (submitted)	Nov. 2003
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1038	Panat, R., K. J. Hsia, and J. W. Oldham	Rumpling instability in thermal barrier systems under isothermal conditions in vacuum—*Philosophical Magazine* (submitted)	Dec. 2003
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1041	Dienberg, C. E., S. E. Ott-Monsivais, J. L. Ranchero, A. A. Rzeszutko, and C. L. Winter	Proceedings of the Fifth Annual Research Conference in Mechanics (April 2003), TAM Department, UIUC (E. N. Brown, ed.)	Feb. 2004
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1044	Panat, R., K. J. Hsia, and D. G. Cahill	Evolution of surface waviness in thin films via volume and surface diffusion—*Journal of Applied Physics* (submitted)	Mar. 2004