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EVOLUTION OF WAVINESS ON THE SURFACE OF A STRAINED ELASTIC SOLID DUE TO STRESS-DRIVEN DIFFUSION

L. B. FREUND
Division of Engineering, Brown University, Providence, RI 02912, U.S.A.

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Abstract—Surface diffusion is one mechanism by which surfaces roughen during high temperature processing of semiconductor materials. Here, the free energy of an elastic crystal is assumed to be the sum of the elastic strain energy and the surface energy, and these two quantities determine the chemical potential for mass transport by surface diffusion. A gradient in chemical potential along the surface provides the driving force for diffusive mass transport which tends to lower the overall free energy of the system. These concepts are applied in considering the transient evolution of waviness of a nearly flat surface in a highly strained elastic solid. In particular, the three-dimensional problem of growth or decay of an initial slight depression in a nominally flat surface is studied by solving the mass transport equation. The process can be described in considerable detail by adhering to an assumption that the amplitude of surface fluctuations is small.

1. INTRODUCTION

A characterizing feature of a homogeneous elastic body is that there is a well defined *reference configuration* to which it returns when all applied loads are removed. While typically viewed as being immutable, there are circumstances under which the shape of the bounding surface of the body in this configuration can change over time as, for example, in condensation/evaporation or diffusion processes. Condensation and evaporation are physical processes central to making high quality semiconductor materials for microelectronic applications. Furthermore, many temperature cycles are often involved in the various steps required for manufacture of complex devices. The focus here is on the particular change-of-shape mechanism of mass transport by surface diffusion. The discussion is limited to cases where any mass rearrangement is coherent, so that there is a well defined reference configuration at any time. The discussion will also be limited to processes with no net gain or loss of mass.

Mass transport by stress-driven diffusion is typically slow, and it can occur to a significant degree only when the process under consideration has the features of relatively high stress, high temperature and small size scale. These features are characteristic of strained-layer semiconductor material systems, of course, for which the magnitude of stress can exceed 1 GPa, the materials are grown or processed at temperatures of 500–600°C, and submicron physical dimensions are typical. Such systems provide the basis for the present discussion.

The materials under consideration are deformed, in general, and are always in mechanical equilibrium. They are not necessarily in thermodynamic equilibrium, however, so they evolve in time in such a way as to decrease the system free energy. The surface field representing the tendency for the system to change the shape of its reference configuration is the chemical potential field (Herring, 1953; Gibbs, 1928). Under circumstances for which this change can arise only through mass transport over the surface of the material, the chemical potential at a point on the surface is defined as the increase in Helmholtz free energy (isothermal potential energy) of the system due to the addition of one atom at that point on the surface at fixed local strain. The basic idea is that, if the chemical potential is lower in some region than in an adjacent region, atoms will diffuse toward the region of lower chemical potential, thereby lowering the free energy of the system. In general, material tends to diffuse against the chemical potential gradient along the surface. It must be recognized that the chemical forces involved are orders of magnitude greater than the mechanical forces. Nonetheless, it appears that stress can play a role in diffusion in cases where the gradients of chemical forces are very small. A development of concepts relevant to crystal growth is provided by Tsao (1993) and various surface diffusion issues have been considered by Rice and Chuang (1981), Mullins and Sekerka (1985), Leo and Sekerka (1989) and Gurtin and Struthers (1990).

The discussion proceeds in several steps. First, the chemical potential is defined as a function of position on the surface in terms of deformation and surface shape, under the assumption that the Helmholtz free energy of the system can change only as a result of a change in net surface area or net elastic strain energy of the material. Chemical potential variations were examined by Mullins (1957) in the absence of stress, and he showed that the flat surface shape is stable under small perturbations in shape as long as the surface energy had a positive value. In the presence of stress, it can be shown that the elastic energy of a body with a flat surface *always diminishes* if the surface becomes wavy (Freund and Jonsdottir, 1993). Thus, this effect counteracts the effect of surface energy, and offers the possibility that the flat surface shape is unstable under small perturbations in shape. The case of periodic perturbations of an originally flat surface in a homogeneously stressed material was considered by Asaro and Tiller (1972), Srolovitz (1989) and Grinfeld (1986, 1993) in order to determine the stability of the flat surface under fluctuations in surface shape. The general finding is that the surface is stable if the wavelength of the perturbations is smaller than some critical value, but unstable if the characteristic length is greater than this value. The critical wavelength which discriminates between stability and instability is proportional to the ratio of the local surface energy to the local elastic strain energy, as must be so on dimensional grounds alone. The stability condition is now well known, and similar applications to strained layers have been developed more recently (Spencer *et al.*, 1991; Freund and Jonsdottir, 1993). As an example of a fully *transient* phenomenon, the time dependent evolution of a surface shape from a localized, nonperiodic defect under plane strain conditions was considered by Freund (1994), and this study is extended here to three-dimensional perturbations.

2. DIFFUSIVE SURFACE TRANSPORT IN A STRAINED SOLID

To consider the phenomenon of stress-driven mass transport by surface diffusion in an elastic crystal, the bulk material and the material immediately adjacent to the surface are viewed as different phases of the same material (Herring, 1953). The bulk material is idealized as an elastic continuum and the "surface" as a pre-stressed elastic membrane attached to the boundary of the bulk material. The thickness of the surface layer does not enter into the formulation. In general, the surface and bulk phases exert tractions on each other, they deform together and they are described by different constitutive relations.

Free energy of the material at constant temperature is assumed to exist in the form of isothermal elastic strain energy, represented by $U(\varepsilon_{kl})$ and measured per unit volume of material in the reference configuration with strain ε_{ij}, and surface free energy, represented by $U_s(\varepsilon_{ij}^{(s)})$ and measured per unit area of surface in the same configuration with surface strain $\varepsilon_{ij}^{(s)}$. Thus, the total free energy is

$$\mathscr{F}(t) = \int_B U(\varepsilon_{ij})\,\mathrm{d}B + \int_S U_s(\varepsilon_{ij}^{(s)})\,\mathrm{d}S \tag{1}$$

where B is the volume occupied by the bulk phase and S is the surface of this volume, as shown in the sketch in Fig. 1. The reference configuration is that configuration for which the bulk phase is totally stress free, which is usually not a realizable state without application of external loading. The constitutive relations for the bulk material and surface material are contained in the definitions of U and U_s, respectively. The time rate of change of free energy due to change in the shape of the free surface described by the local normal velocity v_n is

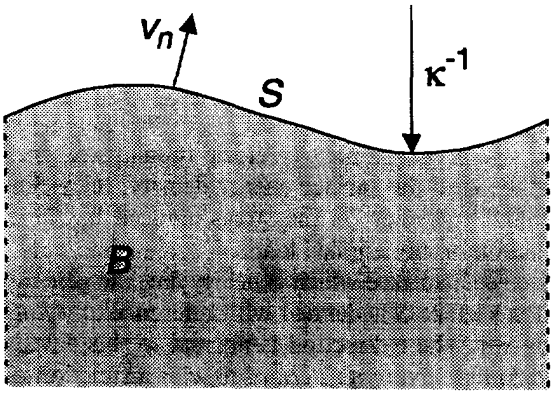

Fig. 1. Schematic of a material with a free surface which changes its shape over the course of time. The local normal velocity is v_n.

$$\dot{\mathscr{F}}(t) = \int_B \frac{\partial U}{\partial t}\,\mathrm{d}B + \int_S U v_n\,\mathrm{d}S + \int_S \frac{\partial U_s}{\partial t}\,\mathrm{d}S - \int_S \kappa U_s v_n\,\mathrm{d}S \tag{2}$$

where $\kappa = \kappa_1 + \kappa_2$ is the sum of the local principal curvatures of the surface, which is twice the mean surface curvature. According to the sign convention adopted, curvature is positive at a point if the center of curvature is in the direction of the outward normal n_i to the surface S. The interpretation of the various terms in this result is relatively straightforward. The first term accounts for changes in the deformation at a bulk material particle as time goes on, the second term accounts for local changes in the instantaneous amount of bulk material involved, the third term accounts for the deformation of the free surface, and the last term accounts for local changes in the amount of free surface. It is assumed in writing (2) that no exchange of energy with the external world takes place. Thus, the instantaneous rate of work being done on the bulk phase must be equal but opposite to the instantaneous rate of work being done on the surface phase. In other words, the sum of the first and third terms in (2) is necessarily zero. Thus, the rate of change of free energy reduces to

$$\dot{\mathscr{F}}(t) = \int_S [U - \kappa U_s] v_n\,\mathrm{d}S. \tag{3}$$

The product $v_n\,\mathrm{d}S$ can be interpreted as the atomic volume of the material, say Ω, times the number of atoms being added per unit time to the area $\mathrm{d}S$. Consequently, the local chemical potential for the surface, viewed as a function of position over the surface, is

$$\chi = [U - \kappa U_s]\Omega. \tag{4}$$

Mass diffuses along the surface in response to a local gradient in chemical potential. The mass flux **j** is given by

$$\mathbf{j} = -\frac{D_s c_s}{kT} \nabla_S \chi \tag{5}$$

where D_s is the surface diffusivity, c_s is the concentration of diffusing species (often taken as the surface density of atom sites or some fixed fraction of this density), k is Boltzman's constant and T is the absolute temperature. The operator ∇_S is the interior gradient operator in the surface S. If $\mathbf{e}_1$ and $\mathbf{e}_2$ are any two vectors tangent to the surface at a point, with $\mathbf{e}_1 \cdot \mathbf{e}_2 = 0$, then $\mathbf{j} \cdot \mathbf{e}_1$ is the number of atoms moving along the surface in the direction of $\mathbf{e}_1$ per unit time per unit distance in the direction of $\mathbf{e}_2$.

Conservation of mass at each point along the surface requires that the normal velocity is proportional to the divergence of the local surface flux. In the present context,

$$v_n = -\Omega \nabla_S \cdot \mathbf{j} = \frac{D_s c_s \Omega^2}{kT} \nabla_s \cdot \nabla_s [U - \kappa U_s]. \tag{6}$$

Thus, given the elastic strain energy density along the surface, the local curvature distribution along the surface, and the surface energy density, (6) yields the normal velocity of the surface. Note that U depends on the stress induced by the action of the surface tension, as well as the action of any applied loads.

If attention is limited to a surface which is nearly flat, the general expressions simplify enormously. Suppose the surface S is defined with reference to a *flat surface* with interior rectangular coordinates x, y. The z direction is normal to this flat surface. Then a nearly flat surface can be specified by giving its z coordinate as a function of position x, y at any time t, say $z = h(x, y, t)$. The surface is "nearly flat" if

$$\sqrt{h_{,x}^2 + h_{,y}^2} \ll 1 \tag{7}$$

for all time. If it is further assumed that the surface energy does not change significantly from its reference value γ for the flat surface, then the surface evolution equation (6) takes the form

$$h_{,t}(x, y, t) = \frac{D_s c_s \Omega^2}{kT} \nabla^2 [U(x, y, t) - \gamma \nabla^2 h(x, y, t)] \tag{8}$$

where $\nabla^2 \varphi = \partial^2 \varphi / \partial x^2 + \partial^2 \varphi / \partial y^2$ is the two-dimensional Laplacian operator in the x, y plane. This is the partial differential equation of primary interest here. The task which must be completed prior to searching for solutions to (8) is to establish the way in which U depends on h. This is done in the next section.

3. STRAIN MODIFICATION DUE TO SLIGHTLY WAVY SURFACE

Consider an isotropic elastic body with a flat, traction free surface. A Cartesian coordinate system is introduced with the origin in the surface and the z direction coinciding with the direction of the outward normal vector to the surface. The body is assumed to be strained homogeneously due to remotely applied loads. For the purposes of this discussion, it is assumed that the surface is strained isotropically, so that $\varepsilon_{xx}(x, y, 0) = \varepsilon_{yy}(x, y, 0) = \varepsilon_0$ initially, where ε_0 is a (positive or negative) constant; this implies a remote state of stress for which the only nonzero components of stress are $\sigma_{xx} = \sigma_{yy} = \sigma_0 = 2\mu\varepsilon_0(1+\nu)/(1-\nu)$ where μ is the elastic shear modulus and ν is the Poisson ratio. More general initial uniform strain or nonuniform strain arising from subsurface inhomogeneities such as dislocations, misfitting inclusions or other strain producing features can be taken into account by following the same general approach. However, this additional level of complexity is not needed here.

Suppose that the material is coherently rearranged so that the stress free shape of the surface becomes slightly wavy. The new shape of the surface is given by the function $h(x, y)$, the distance of the new surface measured from the initial plane surface. (The time parameter plays no role in the discussion of this section and it is suppressed.) The strain distribution will be modified from its original uniform value due to the waviness of the surface, and this modification can be easily calculated for any $h(x, y)$ provided that $\sqrt{h_{,x}^2 + h_{,y}^2} \ll 1$. To see more clearly the quantity which must be determined, consider the strain energy along the surface for the case when a uniform initial strain $\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_0$, $\varepsilon_{xy} = 0$ is perturbed by a strain $\Delta\varepsilon_{ij}$ due to surface waviness. The strain energy density along the traction free surface is then

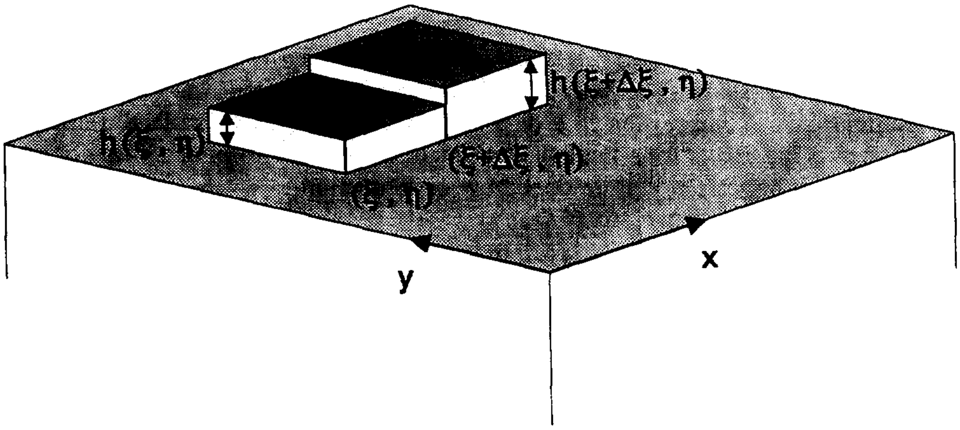

Fig. 2. Schematic showing the method of construction of a wavy surface by addition of blocks to an initially flat surface.

$$U = \frac{\mu}{(1-\nu)}[(\varepsilon_0+\Delta\varepsilon_{xx})^2+(\varepsilon_0+\Delta\varepsilon_{yy})^2+2\nu(\varepsilon_0+\Delta\varepsilon_{xx})(\varepsilon_0+\Delta\varepsilon_{yy})]+2\mu\Delta\varepsilon_{xy}^2$$

$$\approx \frac{2\mu(1+\nu)\varepsilon_0^2}{(1-\nu)}\left[1+\frac{\Delta\varepsilon_{xx}+\Delta\varepsilon_{yy}}{\varepsilon_0}\right] = U_0+\Delta U \tag{9}$$

to first order in variations of the strain. Thus, the quantity to be calculated is ΔU which results from the surface fluctuation $h(x,y)$.

The viewpoint is adopted that the change in shape is effected simply by adding and subtracting thin blocks of mass from the initial flat surface. This is illustrated in the sketch in Fig. 2. The initially flat material is strained an amount ε_0 along its free surface. The blocks are then added (or subtracted) with this same strain. For example, the block located by coordinates $x=\xi$, $y=\eta$ must be added with a force along its sides of $2\mu\varepsilon_0 h(\xi,\eta)(1+\nu)/(1-\nu)$ per unit length in the coordinate directions to maintain this strain, whereas the next block at $x=\xi+\Delta\xi$ $y=\eta$ must be added with a force of $2\mu\varepsilon_0 h(\xi+\Delta\xi,\eta)(1+\nu)/(1-\nu)$ per unit length along its sides. For a smooth surface, $h(\xi+\Delta\xi,\eta)$ must be interpreted as $h(\xi,\eta)+h_{,\xi}(\xi,\eta)\,\Delta\xi$. As long as the externally applied forces are applied to each block, the strain is still uniform everywhere. The removal or cancellation of the external forces, necessary to satisfy the condition of zero surface traction, induces a strain field in the material, however, and this is the *change* in strain associated with waviness of the material surface. Essentially, for the interface shared by the two blocks shown in Fig. 1, this strain field is the field of a concentrated tangential surface force of magnitude

$$P_\xi(\xi,\eta) = 2\mu\varepsilon_0\left(\frac{1+\nu}{1-\nu}\right)\frac{\partial h}{\partial \xi}(\xi,\eta)\Delta\xi \tag{10}$$

acting in the x direction per unit length in the y direction. Generalizing to a two-dimensional array of such blocks for the three-dimensional problem under consideration, the change in strain in the material appearing in (9) is given by

$$\Delta U(x,y) = U_0\frac{1+\nu}{\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{(x-\xi)h_{,\xi}(\xi,\eta)+(y-\eta)h_{,\eta}(\xi,\eta)}{[(x-\xi)^2+(y-\eta)^2]^{3/2}}\,d\xi\,d\eta \tag{11}$$

where the elastic field for a concentrated tangential surface load on an elastic half space has been incorporated. This is commonly known as the Cerruti problem in elasticity. More formal discussions of this general issue have been presented by Gao (1991) and Wu (1994).

4. TRANSIENT EVOLUTION OF SURFACE SHAPE

The results of the foregoing sections are now combined to analyse an initial value problem for surface shape. The body is again assumed to be a half space subjected to an isotropic tension or compression in a direction parallel to the free surface. Initially, the surface is nearly flat except for a small fluctuation in shape in the form of a local depression. The shape of this imperfection is described by some function

$$h(x,y,0) = h_I(x,y) \tag{12}$$

where $h_I(x,y) \to 0$ as $\sqrt{x^2+y^2} \to \infty$. Attention here is limited to the case of imperfections with two-fold reflective symmetry, that is, $h_I(x,y) = h_I(x,-y) = h_I(-x,y)$. The surface is assumed to evolve according to the partial differential equation (8), and a solution of this equation is sought for $t > 0$.

The equation is most conveniently addressed when expressed in terms of non-dimensional variables. These are denoted by the same symbols as the corresponding dimensional quantities but with an asterisk subscript. The normalizations used are

$$U_* = \frac{U}{U_0}, \quad t_* = t\left(\frac{U_0}{\gamma}\right)^4 \frac{\gamma D_s c_s \Omega^2}{kT}, \quad x_* = x\frac{U_0}{\gamma}, \quad h_* = h\frac{U_0}{\gamma} \tag{13}$$

and similarly for other parameters with the dimension of length. In terms of the non-dimensional parameters, the surface evolution equation becomes

$$\frac{\partial h_*}{\partial t_*}(x_*,y_*,t_*) = \nabla_*^2[U_*(x_*,y_*,t_*) - \nabla_*^2 h_*(x_*,y_*,t_*)] \tag{14}$$

where ∇_*^2 is the Laplacian operator in terms of non-dimensional coordinates in the flat reference surface. This equation is solved subject to the initial condition

$$h_*(x_*,y_*,0) = h_I{}^*(x_*,y_*) = h_I(x,y)U_0/\gamma \tag{15}$$

and the asymptotic behavior

$$h_*(x_*,y_*,t_*) \to 0 \quad \text{as} \quad \sqrt{x_*^2+y_*^2} \to \infty. \tag{16}$$

This equation is readily solved by means of Fourier transforms. For symmetric surface fluctuations, which is the case being considered here, the real Fourier cosine transform can be used. The solution then has the representation

$$h_*(x_*,y_*,t_*) = \int_0^\infty \int_0^\infty H(\alpha,\beta,t_*)\cos\alpha x_* \cos\beta y_* \, d\alpha \, d\beta \tag{17}$$

where H is the time dependent spectral density function for the surface shape. Substitution into the governing equation (14) and an interchange of order of integration yields the condition for determining $H(\alpha,\beta,t_*)$ in the form

$$\frac{\partial H}{\partial t_*}(\alpha,\beta,t_*) = -\omega(\alpha,\beta)H(\alpha,\beta,t_*), \quad \omega(\alpha,\beta) = (\alpha^2+\beta^2)^{3/2}[(\alpha^2+\beta^2)^{1/2} - 2(1+\nu)]. \tag{18}$$

The solution is

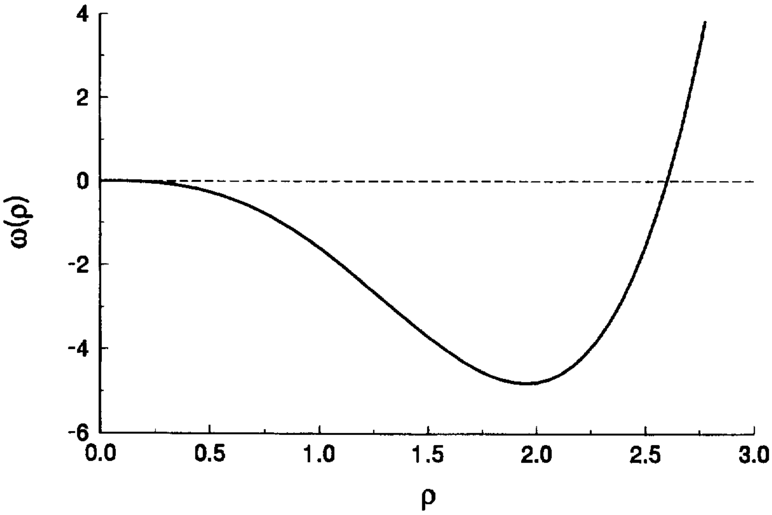

Fig. 3. A plot of the function ω defined in (18) as a function of $\rho = \sqrt{\alpha^2+\beta^2}$ for $\nu = 0.3$. The local minimum occurs at $3(1+\nu)/2$.

$$H(\alpha,\beta,t_*) = H_\text{I}(\alpha,\beta)\,\mathrm{e}^{-\omega(\alpha,\beta)t_*} \tag{19}$$

where $H_\text{I}(\alpha,\beta)$ is the double cosine transform of $h_{\text{I}*}(x_*,y_*)$. Thus, the solution of the partial differential equation (14) subject to the initial condition and constraint on remote behavior is

$$h_*(x_*,y_*,t_*) = \int_0^\infty\int_0^\infty H_\text{I}(\alpha,\beta)\,\mathrm{e}^{-\omega(\alpha,\beta)t_*}\cos\alpha x_*\cos\beta y_*\,\mathrm{d}\alpha\,\mathrm{d}\beta. \tag{20}$$

The result that the surface can be unstable is immediately evident in this result. The function $\omega(\alpha,\beta)$ is positive for sufficiently large values of $\alpha^2+\beta^2$, but there is always a circle of radius $2(1+\nu)$ in the plane of the transform parameters α, β inside of which $\omega(\alpha,\beta) < 0$. This function is plotted in Fig. 3 versus $\rho = \sqrt{\alpha^2+\beta^2}$. Consequently, any portions of the spectral density $H_\text{I}(\alpha,\beta)$ of the initial data inside this circle will grow in magnitude as time increases. The precise way in which this growth occurs depends on the detailed shape of the initial imperfection, so a specific case is considered next.

Before proceeding, it is worthwhile to note the general uncertainty about the actual values of the physical parameters which appear in this calculation, particularly concerning the estimates of time scale. The physical length scale over which these effects can be expected in the processing of semiconductor materials is roughly in the range of wavelengths between about 10 nm and 10 μm. Some guidance on the time scale is available from the discussion of the kinetics of adsorbate atoms given by Zangwill (1988). He argues that the diffusivity should depend on the absolute temperature T and it should have the Arrhenius form

$$D_s = D_{s0}\,\mathrm{e}^{-E_m/kT}. \tag{21}$$

The activation barrier for surface diffusion E_m is thought to be about 5 to 20% of the chemical binding energy, or about 0.5 eV. The simplest form for the pre-exponential factor D_{s0} is $\lambda a^2/4$ where λ is the natural frequency of vibration of the diffusing atom in its local energy well, and a is the spacing between local well minima; this estimate is based on a random walk model. For silicon, $a \approx 0.54\times10^{-9}$ m and $\gamma \approx 1$ J/m^2. Let $\lambda = 10^{14}$/s. The chemical binding energy is estimated as $E_b = 2\gamma a^2$, and the diffusion barrier height is chosen as $E_m = E_b/10$. For a modulus of 10^{11} N/m^2 and a biaxial strain of 0.01, the strain energy density U_0 is about 10^6 J/m^3. The atomic volume for the diamond cubic structure is about $\Omega \approx 5/a^3$. If the concentration of diffusing atoms is chosen to be 1% of the surface atoms sites, that is, as $c_s = 0.01/a^2$, then these values of the parameters in (13) imply that a unit of normalized time $t_* = 1$ corresponds to a physical time of about 10 s at a temperature of 800 K.

5. AN EXAMPLE

As a specific example, suppose that the imperfection has the shape

$$h_I(x,y) = -A\,\mathrm{e}^{-x^2/a^2-y^2/b^2} \tag{22}$$

where A, a and b are parameters characterizing the shape of the imperfection, each with dimension of length. When $A > 0$ this represents a smooth ellipsoidal depression in the surface. For this case,

$$H_I(\alpha,\beta) = -A_*\frac{a_*b_*}{\pi}\,\mathrm{e}^{-\frac{1}{4}(a_*^2\alpha^2+b_*^2\beta^2)} \tag{23}$$

where the length parameters have been normalized according to (13). Thus, the integral to be evaluated is

$$h_*(x_*,y_*,t_*) = -A_*\frac{a_*b_*}{\pi}\int_0^\infty\int_0^\infty \mathrm{e}^{-\frac{1}{4}(a_*^2\alpha^2+b_*^2\beta^2)}\,\mathrm{e}^{-\omega(\alpha,\beta)t_*}\cos\alpha x_*\cos\beta y_*\,\mathrm{d}\alpha\,\mathrm{d}\beta. \tag{24}$$

The integrand is smooth and rapidly decaying at remote portions of the integration domain, so this double inverse transform integral can be readily evaluated numerically. However, by converting to polar coordinates, one of the integrations can be done in closed form so this coordinate transformation is incorporated.

The variables r_*, θ are used to represent the polar coordinates in the physical plane, so that

$$x_* = r_*\cos\theta, \quad y_* = r_*\sin\theta. \tag{25}$$

In the transform parameter plane, the polar coordinates are denoted by ρ, φ so that

$$\alpha = \rho\cos\varphi, \quad \beta = \rho\sin\varphi. \tag{26}$$

The cosine factors in the integrand are then recast in the form (Abramowitz and Stegun, 1965)

$$\begin{aligned}\cos\alpha x_*\cos\beta y_* &= \tfrac{1}{2}\cos\left[r_*\rho\cos(\theta+\varphi)\right]+\tfrac{1}{2}\cos\left[r_*\rho\cos(\theta+\varphi)\right]\\ &= J_0(r_*\rho)+2\sum_{k=1}^{\infty}(-1)^k J_{2k}(r_*\rho)\cos 2k\theta\cos 2k\varphi\end{aligned} \tag{27}$$

where J_m is the ordinary Bessel function of the first kind of order m. The exponential part of the integrand representing H_I takes the form

$$\mathrm{e}^{-\frac{1}{4}(a_*^2\alpha^2+b_*^2\beta^2)} = \mathrm{e}^{-\frac{1}{8}\rho^2(a_*^2+b_*^2)}\,\mathrm{e}^{-\frac{1}{8}\rho^2(a_*^2-b_*^2)\cos 2\varphi}. \tag{28}$$

When recast in this way, the integrand is no longer symmetric in a_* and b_* so, without loss of generality, it is assumed once and for all that

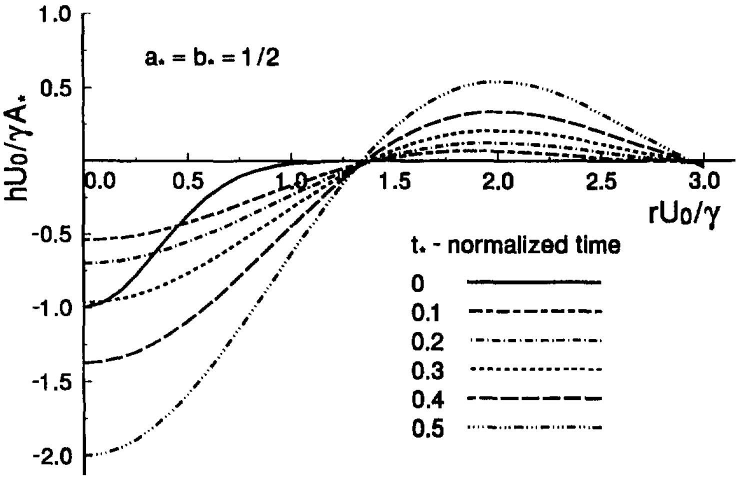

Fig. 4. Profile of surface shape for $a_* = 1/2$ versus normalized radial distance for axially symmetric surface imperfection for six values of normalized time t_*.

$$a_* \geqslant b_*. \tag{29}$$

Then, with the aid of the integral identity (Abramowitz and Stegun, 1965)

$$\int_0^{\pi/2} \mathrm{e}^{-c\cos 2\varphi} \cos 2k\varphi \, \mathrm{d}\varphi = \frac{\pi}{2}(-1)^k I_k(c) \tag{30}$$

for any *non-negative* constant c, where I_k is the modified Bessel function of the first kind of order k, the solution takes the form

$$h_*(r_*, \theta, t_*) = -A_* \frac{a_* b_*}{2} \int_0^\infty \mathrm{e}^{-\frac{1}{8}\rho^2(a_*^2+b_*^2)-\omega(\rho)t_*} \left\{ J_0(r_*\rho) I_0(\tfrac{1}{8}\rho^2(a_*^2-b_*^2)) \right.$$
$$\left. + 2\sum_{k=1}^{\infty} J_{2k}(r_*\rho) I_k(\tfrac{1}{8}\rho^2(a_*^2-b_*^2)) \cos 2k\theta \right\} \rho \, \mathrm{d}\rho. \tag{31}$$

This form is fully equivalent to (24) but is somewhat easier to evaluate numerically.

The case of an axisymmetric imperfection, that is, the case of $a = b$ which remains axisymmetric as it evolves, is considered first. In the solution integral (31), each term in the sum enclosed within the curly brackets is zero and $I_0(0) = 1$, greatly simplifying the computations. Numerical results representing the shape of the surface as a function of normalized radial position rU_0/γ and normalized time t_* are shown for $a_* = b_* = 1/2$, 2 and 3 in Figs 4, 5 and 6, respectively. It is clear that the initial exponential shape, given by (22), quickly gives way to a shape which is oscillatory with distance from the center of symmetry. Furthermore, a comparison of the three figures reveals that the characteristic wavelength of the oscillatory shape appears to be about the same, namely, about three in non-dimensional length units.

Still dealing only with the case of axisymmetry, the *rate* at which the oscillations develop and the imperfection grows does appear to depend on the value of a. This is evident from Fig. 7 which shows the depth of the surface fluctuation at the center point $r = 0$ as a function of time for $a_* = b_* = 1/2$, 2 and 3. For $a_* = 1/2$, the amplitude at the center point first *decreases* quite dramatically before gradually beginning to increase as time goes on. For $a_* = 2$ or 3, on the other hand, the amplitude at the center of the imperfection begins to increase immediately at time $t_* = 0$ and it increases thereafter. The *rate of increase* appears to be strikingly different according to the results in Fig. 7. This is indeed the case for the relatively short time behavior. However, the corresponding long time results are

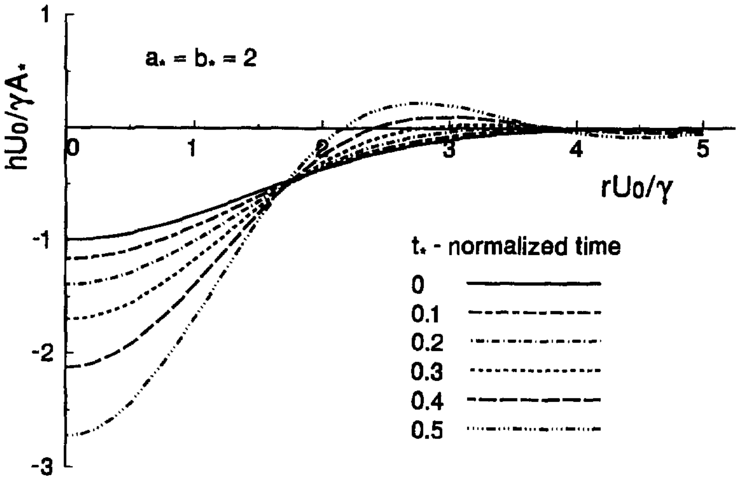

Fig. 5. Same as Fig. 4 for $a_* = 2$.

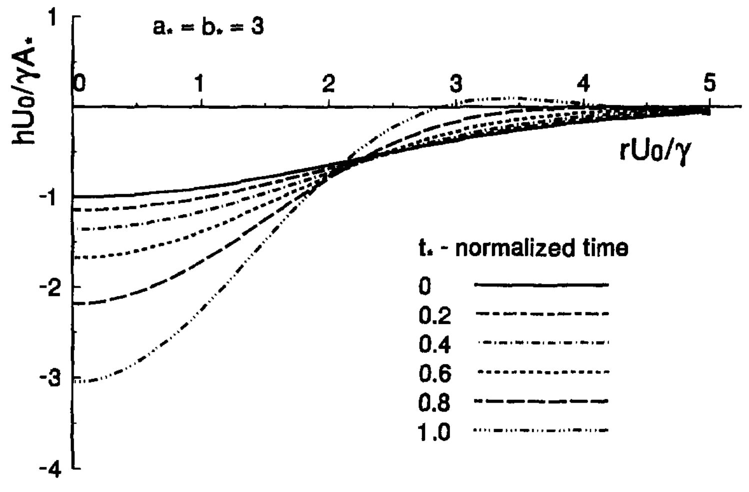

Fig. 6. Same as Fig. 4 for $a_* = 3$.

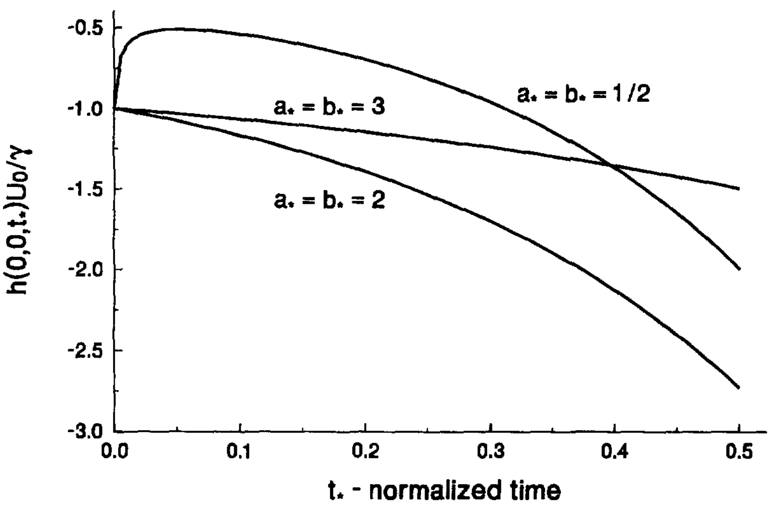

Fig. 7. Amplitude of the imperfection along the axis of symmetry at $r = 0$ versus normalized time for three values of initial imperfection size, as represented by a_*, showing short time behavior.

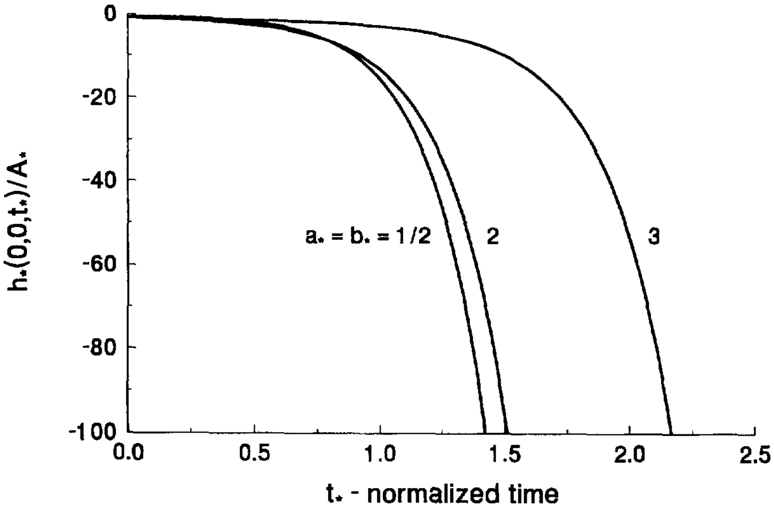

Fig. 8. Same as Fig. 7, except that long time behavior is shown.

shown in Fig. 8 where it is evident that the rate of increase is indeed the same for all values of a_*, a result that is readily established by examining the long time behavior of the solution integral (31). The rate of growth of the fluctuation is approximately $\exp[27(1+\nu)^4 t_*/32]$ as $t_* \to \infty$.

The reason for the behavior shown in Fig. 7 can be seen by considering $H_I(\rho)$, which is the Fourier spectrum of the initial surface shape $h_{I*}(r_*)$. The spectrum includes positive wave numbers roughly in the range $0 < \rho < 2\sqrt{2a_*}$. If a_* is relatively small (large), then the initial surface shape is narrow (broad), and the spectrum $H_I(\rho)$ is broad (narrow). If the spectrum is broad, then as time increases from zero the large wave number or short wave length contributions to the surface shape are suppressed by the term $\exp[-\rho^4 t_*]$ in the integrand of the solution (31). This depression accounts for the early time *decrease* in amplitude seen for $a_* = 1/2$ in Fig. 7 and, to a lesser extent, for $a_* = 2$. On the other hand, if the spectrum is narrow then this time dependent exponential factor has no effect, as seen in the early time behavior for $a_* = 3$ in Fig. 7. As time becomes large, all shapes diverge for long time at a rate determined by the behavior of the integrand near the critical wave number $\rho = 2(1+\nu)$ (Fig. 8).

Cases for which the imperfection shape is eccentric can also be considered in the same way. An example is shown in Fig. 9 for $a_* = 3$ and $b_* = 1.5$, for an initial aspect ratio of 2. The dashed curves show the profile along the major axis (the x axis) and minor axis (the

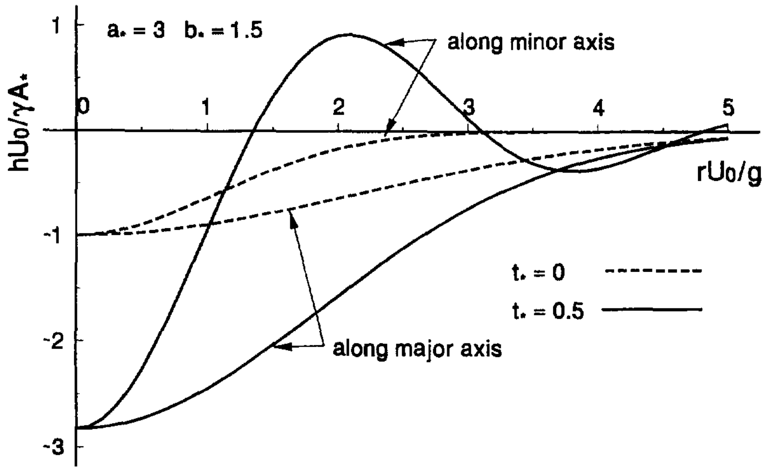

Fig. 9. Profile of an eccentric imperfection with doubly symmetric shape along the major and minor axes for the case of $a_* = 3$, $b_* = 1.5$ for the initial time of $t_* = 0$ and for $t_* = 0.5$.

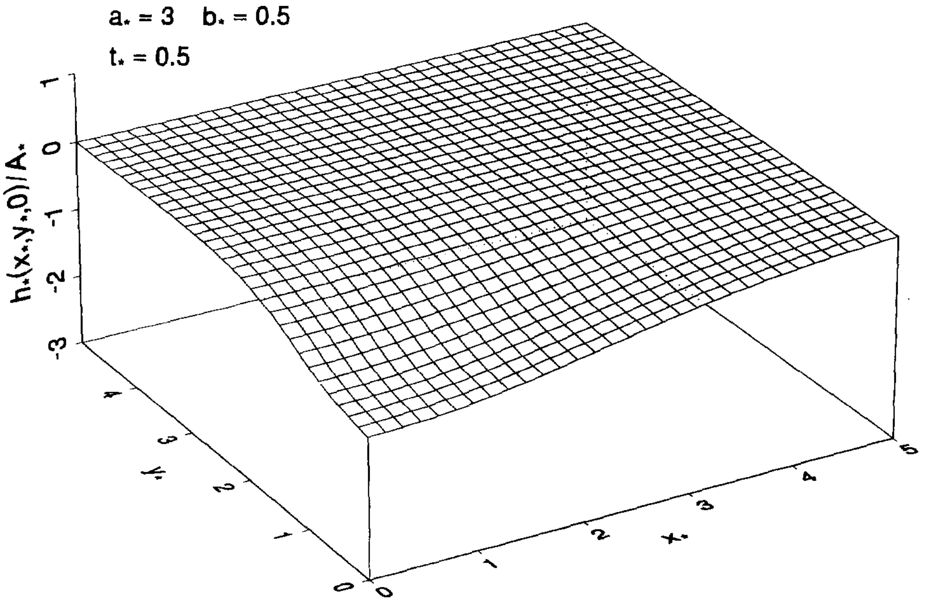

Fig. 10. One quadrant of the full surface shape for the case illustrated in Fig. 9 for $t_* = 0$, showing the initial imperfection in the nearly flat surface.

y axis) at $t_* = 0$, and the solid curves show the surface profile along the same axes for $t_* = 0.5$. The two sets of profiles are shown on the same scale. The general forms of the profiles exhibit the same features already noted for the case of axisymmetry. In addition, it appears that the aspect ratio of the profile is also increasing as time increases. The full surface shapes for this case are shown in Figs 10 and 11. Because of symmetry, only the quadrant $x, y \geqslant 0$ is shown, for both $t_* = 0$ and $t_* = 0.5$. The apparent sharpness at the root of the imperfection in Fig. 11 is due to the coarseness of the mesh of points at which surface height has been calculated. The region $0 \leqslant x, y < 1$ near the root of the imperfection is shown expanded and with a much higher density of mesh points in Fig. 12; it is evident that the root is still flat but the shape has become generally sharper in profile than the original shape.

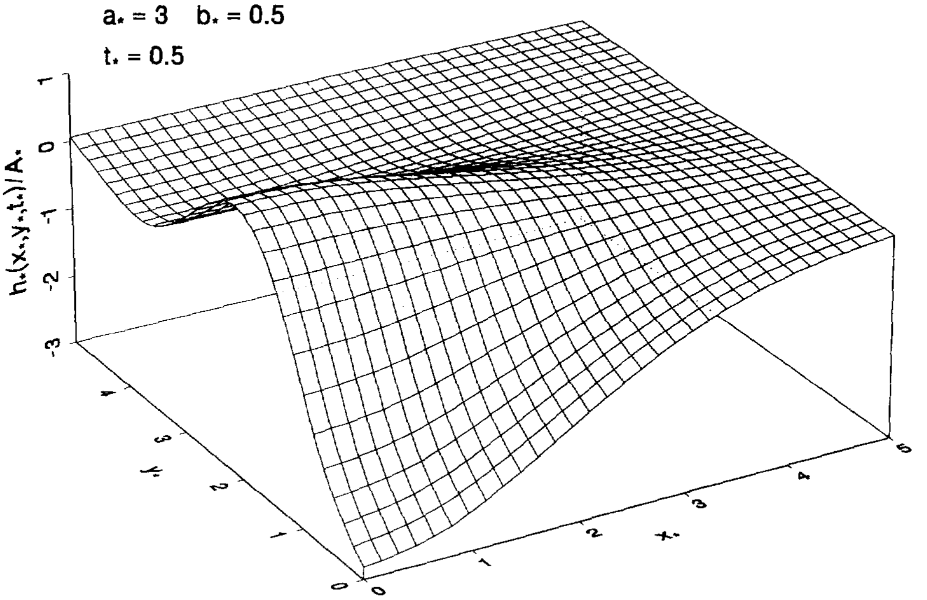

Fig. 11. One quadrant of the full surface shape for the case illustrated in Fig. 9 for $t_* = 0.5$.

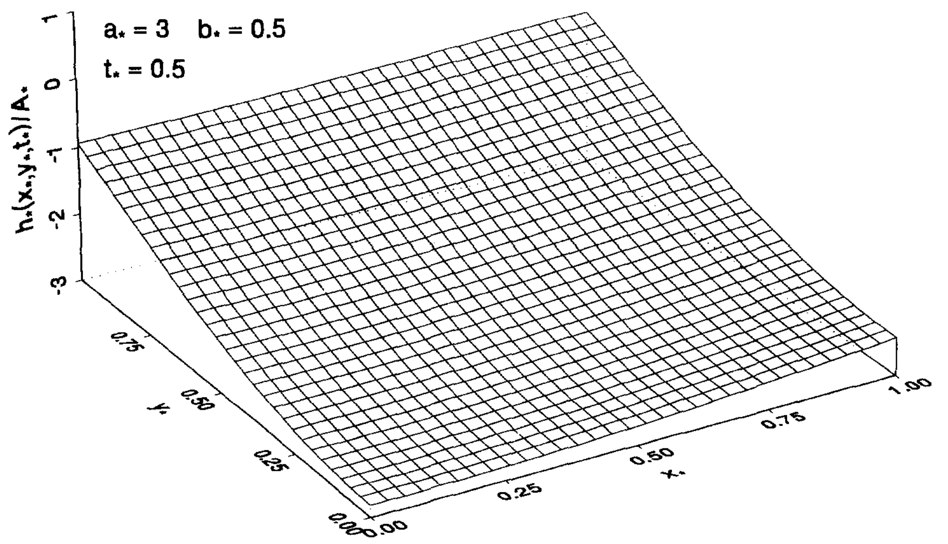

Fig. 12. One quadrant of the root of the imperfection shown in Fig. 11 for $t_* = 0.5$, illustrating that the surface is still locally flat at $x = 0$, $y = 0$ although the overall shape appears to correspond to a sharp root.

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