Energies for Incoherent films: an Analytical Approach

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Energies for incoherent films: an analytical approach

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Abstract

This work discusses the role of interfacial energy for problems involving an epitaxial layer on a rigid substrate. Using the calculus of variations resulting microstructures are determined for a large class of interfacial energies; the qualitative features of these microstructures demonstrate a strong dependence on the smoothness and convexity of the energy. This work is meant to provide insight in deciding appropriate energies for a large class of incoherent interfaces.

1 Introduction

At an interface between crystalline solids two opposing mechanisms compete to determine the resulting structure (cf. e.g. the review article by Matthews [1]). The minimum energy configuration of the bulk material occurs at the stress-free state for each solid. But when the lattice parameters of the two materials differ, complete relaxation to bulk equilibrium would result in a crystalline structure that is discontinuous at the interface. On the other hand, the interface reaches its minimum energy configuration when there is an exact matching of the atoms of the two solids across the interface. This state of perfect coherency is tenable provided the stresses due to the deviation from equilibrium of the bulk material are not too strong. But there is a threshold at which these stresses are too severe to support a coherent interface, and the structure of the interface undergoes dramatic changes: dislocations appear that relax the bulk stresses and an extreme situation may be reached in which all regularity of the atomic bonding at the interface is lost.

A proper choice of interfacial energy is crucial in describing the competition discussed above, but a chief difficulty in deciding on such an energy is the extreme range of behaviors it must embody, as it must characterize: (i) perfect matching of the atoms at the interface; (ii) dislocations distributed in a somewhat regular manner; and (iii) situations in which the abutting lattices are completely mismatched.

Specific interfacial energies have been proposed, some based on microscopic calculations (van der Merwe [2, 3, 4], du Plessis & van der Merwe [5], Fletcher & Adamson [6], Fletcher [7]), others on phenomenological considerations (Leo & Hu [8]), and it

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four classes of energy functions: (i) smooth and convex; (ii) nonsmooth but convex; (iii) nonsmooth and nonconvex; (iv) nonsmooth and concave.

The central effects - namely fine or smooth incoherency and the existence of a threshold for incoherency - depend on whether or not the energy is convex and whether or not the energy is smooth. Nonconvex energies yield finely incoherent interfaces; energies whose convex envelope is nonsmooth exhibit a threshold effect.

Our specific results may be described as follows. Consider first a smooth and convex energy $f(\gamma)$ (Figure 1), for instance quadratic in γ. Then our analysis shows that the interface is always smoothly incoherent, and there is no threshold for incoherency.

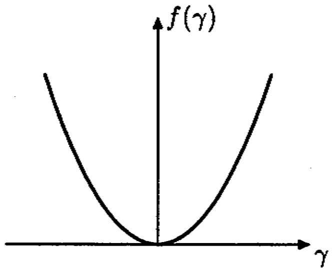

Figure 1. Smooth convex energy f.

For convex energies that are not smooth at $\gamma = 0$ (Figure 2) the interface remains coherent for small thicknesses, but the equilibrium state is one of smooth incoherency when the threshold thickness is exceeded. Such energies might be appropriate to systems with large misfit.

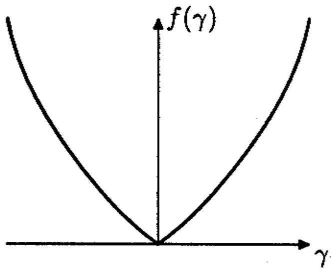

Figure 2. Nonsmooth convex energy f.

A more interesting type of behavior, for an interfacial energy that is not smooth at $\gamma = 0$ (Figure 3), occurs when the energy is concave for small values of γ but ultimately convex for large values. Such an energy was proposed by Leo & Hu [8] and results in an interface that, although coherent for small thicknesses, becomes finely incoherent above a threshold, with the infimum of the energy realized by sequences corresponding to fine mixtures of coherent and incoherent patches. A drawback of this choice of energy is its special form: it is necessary to assign in advance, as a constitutive parameter, the incoherency strain that determines the mixture.

The mathematical techniques we use in this paper are based on classical results of the calculus of variations, and the general approach follows closely ideas developed by Leo & Hu in [8] for the interfacial energy function displayed in Figure 4. We essentially compute the minima of the total energy functional (bulk and interfacial energies), and then analyze corresponding minimizing sequences.

We are currently working to extend the results to non-quadratic bulk energies and curved interfaces.

2 Statement of the problem

Our model describes the equilibrium of an epitaxial layer on a rigid substrate. Assuming that the layer has height h, but is infinite in the other directions, we study a model problem for a plane section of the film, within the context of plane elasticity.

We assume that the layer occupies the infinite strip $\mathbb{R} \times [0, h] \subset \mathbb{R}^2$. We let (x, y) denote cartesian coordinates in $\mathbb{R}^2$ with $x \in \mathbb{R}$ and $y \in [0, h]$, and we write $\mathbf{i} = (1, 0)$ and $\mathbf{j} = (0, 1)$. We limit our discussion to plane displacements $\mathbf{u}(x, y)$ of the layer and to situations in which $\mathbf{u}(x, y)$ is periodic in x. With this in mind, we divide the strip into cells of unit length, write $\Omega = [0, 1] \times [0, h]$ for a typical cell, and restrict attention to behavior in Ω. Periodicity then requires that $\mathbf{u}(1, y) - \mathbf{u}(0, y)$ be constant. We assume that the layer cannot separate from the substrate; thus, since $y = 0$ defines the interface between the layer and the substrate,

$$\mathbf{u}(x, 0) \cdot \mathbf{j} = 0 \qquad x \in [0, 1], \tag{1}$$

and the periodicity condition takes the stronger form

$$\mathbf{u}(1, y) = \mathbf{u}(0, y) + (\text{const.})\mathbf{i} \qquad y \in [0, h]. \tag{2}$$

Let

$$u(x, y) := \mathbf{u}(x, y) \cdot \mathbf{i};$$

we define the *incoherency strain* $\gamma(x)$ by

$$\gamma(x) := u_x(x, 0),$$

and refer to the interface as *coherent* if

$$\gamma(x) = 0 \qquad x \in [0, 1],$$

and *incoherent* otherwise.

We work within the theory of small deformations, so that

$$\mathbf{E} = \tfrac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^{\top})$$

represents the strain in the layer. Note that $\gamma = \mathbf{i} \cdot \mathbf{E}(x, 0)\mathbf{i}$. The displacement is measured from a configuration of the layer in which the lattices of the film and the layer are perfectly matched; this configuration, in which $\mathbf{E} = \mathbf{0}$, will not correspond to a minimum energy state of the film, which we assume to occur at a strain $\mathbf{E}_0$. We assume that this *mismatch strain* has the specific form

$$\mathbf{E}_0 = e_0 \mathbf{i} \otimes \mathbf{i},$$

Moreover, for $q > 1$,

$$W^{1+1/q,q}(\Omega,\mathbb{R}^2) \subset C^{0,1-1/q}(\overline{\Omega},\mathbb{R}^2),$$

while for $q = 1$, and since Ω is a rectangle (see [13], Lemma 5.8),[1]

$$W^{2,1}(\Omega,\mathbb{R}^2) \subset C^0(\overline{\Omega},\mathbb{R}^2).$$

By the trace theorem for polygons (see e.g [14], Theorems 1.5.2.1 and 1.5.2.8) and Sobolev's embeddings, we can define the trace $\tau\mathbf{u}$ of any $\mathbf{u} \in W^{1+1/q,q}(\Omega,\mathbb{R}^2)$ as a continuous function on $\partial\Omega$ such that

$$\tau\mathbf{u}\big|_{\Gamma_j} \in W^{1,q}(\Gamma_j,\mathbb{R}^2), \qquad j = 1,\dots,4,$$

where Γ_j are the sides of Ω. In what follows, when the meaning is clear, we will denote $\tau\mathbf{u}$ simply by $\mathbf{u}$.

Letting W denote the space

$$W = \{\mathbf{u} \in W^{1+1/q,q}(\Omega,\mathbb{R}^2) \;:\; \mathbf{u}\,\text{satisfies (1) and (2)}\},$$

we consider the

Minimization problem (M). *Find a displacement field* $\mathbf{u} \in W$ *such that*

$$J(\mathbf{u}) \le J(\hat{\mathbf{u}}) \qquad \text{for all} \qquad \hat{\mathbf{u}} \in W.$$

If $\mathbf{u} \in W$ is a solution of (M), then so is $\mathbf{u} + c\mathbf{i}$, for any scalar constant c. We may therefore assume, without loss of generality, that $u(0,0) = 0$ for all $\mathbf{u} \in W$. Thus, for each fixed $\alpha \in \mathbb{R}$, consider the spaces

$$\begin{aligned} W_\alpha &= \{\mathbf{u} \in W \;:\; u(1,0) = \alpha,\ u(0,0) = 0\},\\ \hat{W}_\alpha &= \{u \in W^{1,q}([0,1]) \;:\; u(1) = \alpha,\ u(0) = 0\}. \end{aligned}$$

Then W_α and $\hat{W}_\alpha$ are convex, and each $\mathbf{u} \in W_\alpha$ satisfies

$$\begin{aligned} &\mathbf{u}(1,y) = \mathbf{u}(0,y) + \alpha\mathbf{i}, \qquad && y \in [0,h],\\ &\mathbf{u}(x,0)\cdot\mathbf{j} = 0, && x \in [0,1]. \end{aligned} \tag{6}$$

Thus, since each cell has unit length, the subscript α *represents the average value of the incoherency strain* $\gamma = u_x$ *corresponding to any* $\mathbf{u} \in W_\alpha$.

Our first step in attacking problem (M) is to determine the infimum of the functional J. We accomplish this by first computing

$$\inf_{\mathbf{u}\in W_\alpha} J(\mathbf{u})$$

and then minimizing over all $\alpha \in \mathbb{R}$. To facilitate this, we introduce the *convex envelope* f^{**} of f defined by

$$f^{**} = \sup\{\, g \le f \;:\; g \quad \text{convex}\}.$$

[1]For arbitrary Lipschitz domain we only have the weaker inclusion $W^{2,1}(\Omega,\mathbb{R}^2) \subset C^0(\Omega,\mathbb{R}^2) \cap L^\infty(\Omega,\mathbb{R}^2)$.

Granted incoherency, if $f^{**}(\alpha_{min}) = f(\alpha_{min})$, then the problem (M) has a solution $\mathbf{u}$ and there is a well-defined incoherency strain γ defined over the interface; in this case we will refer to the interface as being *smoothly incoherent.* On the other hand, for $h > h_c$ and $f^{**}(\alpha_{min}) < f(\alpha_{min})$ (so that α_{min} is not a point of interfacial stability), (M) has no solution; that is, there is no function $\mathbf{u} \in W$ that minimizes J. In this case we will refer to the interface as *finely incoherent.* For such situations, even though (M) has no solution, one can derive physically meaningful results by studying the properties of *minimizing sequences*; that is, sequences $\{\mathbf{u}_n\}$ with the property that $\mathbf{u}_n \in W$ and

$$J(\mathbf{u}_n) \to \inf_{\mathbf{u}\in W} J(\mathbf{u}),$$

or equivalently

$$J(\mathbf{u}_n) \to g(\alpha_{min}).$$

For any such sequence, let $\gamma_n(x) = \frac{\partial u_n(x,0)}{\partial x}$, so that

$$\alpha_n = \int_0^1 \gamma_n(x)\, dx$$

is the average incoherency strain associated with $\mathbf{u}_n$.

We may prove the following

Theorem on Minimizing Sequences. *Let $\{\mathbf{u}_n\}$ be a minimizing sequence for the problem (M) with α_n the average incoherency strain associated with $\mathbf{u}_n$. Then*

$$\begin{aligned} &\alpha_n \to \alpha_{min}, \\ &\mathbf{u}_n \to \tilde{\mathbf{u}}_{min} \qquad in \quad W^{1,2}(\Omega, \mathbb{R}^2), \end{aligned} \tag{13}$$

as $n \to \infty$, where

$$\tilde{\mathbf{u}}_{min}(x,y) := \alpha_{\min}\, x\mathbf{i} + \frac{\nu(e_0 - \alpha_{\min})}{(1-\nu)}\, y\mathbf{j}. \tag{14}$$

Thus the minimizing sequences always converge in bulk to a smooth deformation.

At the interface, although minimizing sequences may not have a classical limit when (M) has no solution, the "generalized limit", however it be visualized, corresponds to a well defined average incoherency strain, namely α_{min}, the incoherency strain associated with the infimum of J.

4 Proofs

Proof of the Theorem on the Infimum of J. Fix $\mathbf{u} \in W$ and let $\alpha := u(1,0)$. Then

$$J(\mathbf{u}) = F(\mathbf{u}) + I(u(x,0)) \geq \inf_{\mathbf{v}\in W_\alpha} F(\mathbf{v}) + \inf_{v\in \hat{W}_\alpha} I(v).$$

Consider the auxiliary problem:

(M_α): minimize $F(\mathbf{u})$ on W_α.

and in turn

$$\inf_{\mathbf{u}\in\mathcal{}} J(\mathbf{u}) \geq g(\alpha_{min}).$$

Next, we prove the reverse inequality. By Corollary 2.2.9 of Dacorogna [16],

$$f^{**}(\alpha_{min}) = \inf\{\lambda f(\gamma_a) + (1-\lambda) f(\gamma_b) : \lambda \in [0,1],\ \gamma_a,\ \gamma_b \in \mathbb{R} \\ \lambda\,\gamma_a + (1-\lambda)\gamma_b = \alpha_{min}\}; \tag{18}$$

thus, for any fixed $k \in \mathbb{N}$, we can find $\lambda_k \in [0,1]$ and $\gamma_{a,k},\ \gamma_{b,k} \in \mathbb{R}$, with

$$\alpha_{min} = \lambda_k\,\gamma_{a,k} + (1-\lambda_k)\gamma_{b,k}, \tag{19}$$

such that

$$f^{**}(\alpha_{min}) \leq \lambda_k f(\gamma_{a,k}) + (1-\lambda_k) f(\gamma_{b,k}) \leq f^{**}(\alpha_{min}) + \frac{1}{k}. \tag{20}$$

Let $I_{a,k} \subset [0,1]$ be any measurable set with $|I_{a,k}| = \lambda_k$ and define $I_{b,k} := [0,1]\backslash I_{a,k}$. Then $|I_{b,k}| = (1-\lambda_k)$. Let

$$g_k(x) = \begin{cases} \gamma_{a,k} & x \in I_{a,k}, \\ \gamma_{b,k} & x \in I_{b,k}, \end{cases}$$

and let

$$u_k(x) = \int_0^x g_k(t)\,dt - \alpha_{min}\,x \qquad x \in [0,1].$$

Since $u_k(1) = u_k(0) = 0$, we can extend u_k by periodicity to all of $\mathbb{R}$. For $n \in \mathbb{N}$, let

$$u_{n,k}(x) = \alpha_{min} x + \frac{1}{n}\,u_k(nx).$$

Then, for a.e. $x \in [0,1]$,

$$u'_{n,k}(x) = \begin{cases} \gamma_{a,k} & n\,x \in I_{a,k}, \\ \gamma_{b,k} & n\,x \in I_{b,k}, \end{cases}$$

and, as $n \to \infty$, we may use Theorem 2.1.5 of Dacorogna [16] to conclude that

$$u_{n,k} \overset{*}{\rightharpoonup} \alpha_{min} x \qquad \text{in } W^{1,\infty}([0,1];\mathbb{R}) \tag{21}$$

Fix $\varepsilon > 0$ and let $\psi_\varepsilon \in C_0^\infty([0,h];\mathbb{R})$ be a cut–off function, with $0 \leq \psi_\varepsilon(y) \leq 1$, such that $\psi_\varepsilon(y) \equiv 1$ on $[2\varepsilon, h]$, $\psi_\varepsilon(y) \equiv 0$ on $[0,\varepsilon]$, and

$$|\psi'_\varepsilon(y)| \leq C/\varepsilon \qquad \text{for all } y \in [0,h].$$

Let

$$\mathbf{u}_{n,\varepsilon,k}(x,y) := \Big(\psi_\varepsilon(y)\,\alpha_{min} x + (1-\psi_\varepsilon(y))u_{n,k}(x)\Big)\mathbf{i} - \frac{\nu(\alpha_{min} - e_0)}{(1-\nu)}\,y\mathbf{j}. \tag{22}$$

Then

$$|\mathbf{u}_{n,\varepsilon,k}(x,y) - \tilde{\mathbf{u}}(x,y)| = (1-\psi_\varepsilon(y))|u_{n,k}(x) - \alpha_{min} x| \leq ||u_{n,k} - \alpha_{min} x||_{L^\infty([0,1];\mathbb{R})}$$

$\{y=0\}$ of Ω is by construction $u(x,0)=\alpha_{min}x$, which must, in turn, minimize the interfacial energy functional $I(u)$. Thus

$$f^{**}(\alpha_{min}) = I(u) = \int_0^1 f(\alpha_{min})\,dx = f(\alpha_{min}).$$

Conversely, if this relation holds, the minimum exists and is given by $\tilde{\mathbf{u}}$.

□

Proof of the Theorem on Minimizing Sequences. Notice first that, by (7) and (8),

$$g_{blk}(\alpha_n) \le F(\mathbf{u}_n) \quad \text{and} \quad g_{int}(\alpha_n) \le I(u_n).$$

Thus, $g(\alpha_n) \le J(\mathbf{u}_n)$. But $J(\mathbf{u}_n) \to g(\alpha_{min}) \le g(\alpha_n)$ and g is strictly convex. Thus $\alpha_n \to \alpha_{min}$ and we have $(13)_1$.

Let $\tilde{\mathbf{E}}$ be the strain associated to $\tilde{\mathbf{u}}_{min}$; then, by (17), we have

$$F(\mathbf{u}_n) - F(\tilde{\mathbf{u}}_{min}) = \int_\Omega w(\mathbf{E}_n - \tilde{\mathbf{E}})\,dx\,dy + \int_\Omega \tilde{\mathbf{T}}\cdot(\mathbf{E}_n - \tilde{\mathbf{E}})\,dx\,dy,$$

and applying the divergence theorem and the periodicity boundary conditions, the last integral may be written as

$$\int_0^h \{\mathbf{i}\cdot\tilde{\mathbf{T}}(1,y)\mathbf{i}\}(\alpha_n - \alpha_{min})\,dy,$$

which vanishes as $n\to\infty$ by $(13)_1$. Thus, by the positive-definiteness of the quadratic form $w(\mathbf{E})$, it follows that $\mathbf{E}_n \to \tilde{\mathbf{E}}$ in $L^2(\Omega, \mathbb{R}^{(2\times 2)})$, and Korn's inequality (cf. the appendix) yields the desired result.

□

5 On the structure of minimizing sequences

5.1 Oscillating sequences

The minimizing sequence (22) constructed in the proof of the Theorem on the Infimum of J becomes particularly simple if we assume that there exist $\lambda \in [0,1]$, and $\gamma_a, \gamma_b \in \mathbb{R}$ such that

$$f^{**}(\alpha_{min}) = \lambda f(\gamma_a) + (1-\lambda) f(\gamma_b), \qquad \alpha_{min} = \lambda\gamma_a + (1-\lambda)\gamma_b. \tag{23}$$

Indeed, we may then replace g_k, u_k and $\mathbf{u}_{n,\varepsilon,k}$ respectively by

$$g(x) = \begin{cases} \gamma_a & x \in I_a, \\ \gamma_b & x \in I_b, \end{cases} \qquad \text{with } |I_a| = \lambda \text{ and } |I_b| = (1-\lambda),$$

$$u(x) = \int_0^x g(t)\,dt - \alpha_{min}\,x, \qquad u_n(x) = \alpha_{min}x + \frac{1}{n}u(nx), \tag{24}$$

Let $\{\mathbf{u}_n\}$ be a minimizing sequence for the problem (M) with α_n the average incoherency strain associated with $\mathbf{u}_n$. We have already proved that

$$\begin{aligned} &\alpha_n \to \alpha_{min}, \qquad \int_0^1 f(\gamma_n)\,dx \to f^{**}(\alpha_{min}), \\ &\mathbf{u}_n \to \tilde{\mathbf{u}}_{min} \qquad \text{in} \quad W^{1,2}(\Omega, \mathbb{R}^2), \end{aligned} \tag{27}$$

where $\tilde{\mathbf{u}}_{min}$ is defined in (14). By the growth condition (26) and $(27)_2$, we have, in particular, that

$$\int_0^1 |\gamma_n| dx \le M$$

for all $n \in \mathbb{N}$. In turn

$$|u_n(x)| \le \int_0^1 |\gamma_n| dx \le M.$$

Hence, again by (26), $(27)_2$, and Dunford–Pettis criterion, there exists a subsequence u_{n_k} which converges weakly to some function v in the space $W^{1,1}([0,1],\mathbb{R})$. On the other hand, since by the continuity of the trace operator u_n converges to $\alpha_{min} x$ in $L^2([0,1],\mathbb{R})$, then, necessarily, $v(x) = \alpha_{min} x$ and thus the *entire* sequence u_n converges weakly to $\alpha_{min} x$ in $W^{1,1}([0,1],\mathbb{R})$. There are now two cases.

If $f^{**}(\alpha_{min}) = f(\alpha_{min})$ then $\tilde{\mathbf{u}}_{min}$ is a classical solution of the problem (M). Thus we may focus on the complementary situation

$$f^{**}(\alpha_{min}) < f(\alpha_{min}). \tag{28}$$

Let

$$A_{min} := \{\gamma \in \mathbb{R} : f^{**}(\gamma) = f^{**}(\alpha_{min}) + (f^{**})'_+(\alpha_{min})(\gamma - \alpha_{min})\}.$$

The set A_{min} is clearly closed, convex and non empty, since $\alpha_{min} \in A_{min}$. Moreover it is also bounded, since by (26)

$$\lim_{\gamma \to \infty} \frac{f^{**}(\gamma)}{\gamma} = \infty.$$

Thus $A_{min} = [\gamma_a, \gamma_b]$, where $0 \le \gamma_a \le \alpha_{min} \le \gamma_b$. If $\gamma_a < \gamma_b$, then

$$f(\gamma_a) = f^{**}(\gamma_a) \qquad \text{and} \qquad f(\gamma_b) = f^{**}(\gamma_b). \tag{29}$$

Indeed, suppose, for example, that $f(\gamma_b) > f^{**}(\gamma_b)$. By continuity we can find $\rho > 0$ and $0 < \varepsilon_0 < \gamma_b - \gamma_a$ such that

$$f(\gamma) > f^{**}(\gamma) + \rho \qquad \text{for all } \gamma \in [\gamma_b - \varepsilon_0, \gamma_b + \varepsilon_0].$$

Consider the function

$$f_1(\gamma) = f^{**}(\gamma_b - \varepsilon) + \frac{f^{**}(\gamma_b + \varepsilon) - f^{**}(\gamma_b - \varepsilon)}{2\varepsilon}(\gamma - (\gamma_b - \varepsilon)),$$

where we have chosen $0 < \varepsilon \le \varepsilon_0$ so small that

$$f^{**}(\gamma) < f_1(\gamma) \le f(\gamma) - \frac{1}{2}\rho \qquad \text{for all } \gamma \in (\gamma_b - \varepsilon, \gamma_b + \varepsilon).$$

In conclusion we have shown that for n sufficiently large

$$|\{x \in [0,1] : \quad \mathrm{dist}(\gamma_n, \{\gamma_a\} \cup \{\gamma_b\}) \geq \varepsilon\}| \leq \varepsilon,$$

that is (31).

Since γ_n converges weakly to α_{min} in $L^1([0,1],\mathbb{R})$, we can apply the Fundamental Theorem on Young measure (see e.g. [20]) to obtain the existence of a weak* measurable map $\nu : [0,1] \to \mathcal{M}(\mathbb{R})$ such that the following hold

(i) $\nu_x \geq 0$, $||\nu_x||_{\mathcal{M}(\mathbb{R})} = \int_{\mathbb{R}} d\nu_x = 1$ for a.e. $x \in [0,1]$;

(ii) supp $\nu_x \subset \{\gamma_a\} \cup \{\gamma_b\}$ for a.e. $x \in [0,1]$.

Thus for a.e. $x \in [0,1]$

$$\nu_x = \lambda(x)\delta_{\gamma_a} + (1-\lambda(x))\delta_{\gamma_b}, \qquad \text{where} \quad 0 \leq \lambda(x) \leq 1.$$

On the other hand, since

$$\alpha_{min} \equiv \langle \nu_x, \mathrm{id} \rangle = \int_{\mathbb{R}} y \, d\nu_x(y) = \lambda(x)\gamma_a + (1-\lambda(x))\gamma_b,$$

it follows that $\lambda(x) \equiv \lambda$. Hence

$$\nu_x = \lambda\delta_{\gamma_a} + (1-\lambda)\delta_{\gamma_b}$$

and the proof is complete.

5.3 Concentrating sequences

Condition (23) may not be satisfied in the important case in which f is strictly concave. We have

$$f^{**}(\gamma) = m\gamma, \qquad \text{with } m = \lim_{\gamma \to +\infty} \frac{f(\gamma)}{\gamma}.$$

This may be proved using the inequalities $f^{**}(\lambda\gamma) \leq \lambda f^{**}(\gamma) \leq \lambda f(\gamma) \leq f(\lambda\gamma)$: taking $\lambda = \overline{\gamma}/\gamma < 1$ we obtain that

$$\frac{f^{**}(\overline{\gamma})}{\overline{\gamma}} \leq \frac{f(\gamma)}{\gamma} \leq \frac{f(\overline{\gamma})}{\overline{\gamma}},$$

and taking the limit as $\gamma \to +\infty$ we have the above representation for the convex envelope of f.

In this case α_{min} can be computed explicitly. Indeed

$$\alpha_{min} = \max\left\{0, e_0 - \frac{m(1-\nu^2)}{Eh}\right\},$$

so that (23) fails when

$$h > \frac{m(1-\nu^2)}{E\, e_0},$$

because $\alpha_{min} > 0$.

where χ_k is the characteristic functions of the set $[0, \frac{1}{k}]$, and

$$x_{h,k} \in \left[\frac{h}{n_k}, \frac{h}{n_k} + \frac{1}{kn_k}\right] \subset \left[\frac{h}{n_k}, \frac{h+1}{n_k}\right].$$

The claim is thus proved.

It is clear that one can also take $\varphi(x, \gamma) = \theta(x)\phi(\gamma)$, where $\theta \in C_0([0, 1]; \mathbb{R})$ and ϕ is positively homogeneous of degree one. Thus we can use the varifold to express the infimum of the interfacial energy in a suggestive form. Let $\theta \in C_0([0, 1]; \mathbb{R})$: then

$$\int_0^1 \theta(x) f(\gamma_k)\, dx = \int_0^1 \theta(x)(f(\gamma_k) - m\gamma_k)\, dx + \int_0^1 \theta(x) m\gamma_k\, dx.$$

The first integral on the right hand side goes to zero as $k \to \infty$, since

$$\left|\int_0^1 \theta(x)(f(\gamma_k) - m\gamma_k)\, dx\right| \leq \alpha_{min} \left(\frac{f(\alpha_{min}k)}{\alpha_{min}k} - m\right) \|\theta\|_\infty.$$

Now, choosing $\varphi(x, \gamma) = \theta(x)\, m\gamma$ we obtain

$$\int_0^1 \theta(x) f(\gamma_k)\, dx \to m\alpha_{min} \int_0^1 \theta\, dx = \int_{[0,1]\times S} \theta f^{**}\, d\Lambda.$$

6 Results for specific forms of the interfacial energy

We now turn to the analysis of various forms of the interfacial energy density f. We will focus on the problem of the dependence of α_{min} on h, where, we recall, α_{min} is the average incoherency strain corresponding to the infimum of J, which is defined in (9). As we have shown in the Existence Theorem, the non-smoothness of f^{**} at zero implies the existence of a critical value for h below which the interface is coherent. Analogously, non-smoothness at other points implies that there are intervals of h within which the interface remains smoothly incoherent with a fixed incoherency strain. Finally, when f^{**} is smooth at α_{min}, the interface is either finely or smoothly incoherent according to the convexity at α_{min}.

6.1 f convex and smooth (Figure 1)

Since in this case $f(\gamma) = f^{**}(\gamma)$, the solution exists in W and is given by $\tilde{\mathbf{u}}_{min}$ in (14). The trace of $\tilde{\mathbf{u}}_{min}$ on the lower boundary of Ω is $u(x) = \alpha_{min}x$, with α_{min} the solution of (9).

Thus the interface is always smoothly incoherent, since the film is uniformly strained with respect to the substrate, and no fine structure appears.

The average strain at the interface α_{min}, which measures incoherency, is related to the variation of the thickness of the layer by the relation

$$h = \frac{1 - \nu^2}{E} \frac{f'(\alpha_{min})}{e_0 - \alpha_{min}} \tag{34}$$

which shows that when $h \to 0$, then $\alpha_{min} \to 0$, and when $h \to +\infty$, then $\alpha_{min} \to e_0$. Note that, by (12), the critical thickness h_c vanishes, and the interface can never be coherent.

In other words, when the mismatch strain is large, the interface loses coherency at the first critical thickness by nucleating finer and finer incoherent patches, but when the second critical thickness is reached, then this fine structure is lost and the layer becomes uniformly strained with respect to the substrate.

6.4 f nonconvex and nonsmooth (Figure 4)

Here there are values $0 < \gamma_1 < \gamma_2 < \ldots$ of the incoherency strain such that $f^{**}(\gamma) = f(\gamma)$ at and only at $\gamma = \pm\gamma_i$. $f^{**}(\gamma)$ is therefore piecewise linear with slope changes when $\gamma = \pm\gamma_i$:

$$f^{**}(\gamma) = \begin{cases} m_1|\gamma| & |\gamma| \leq \gamma_1, \\ m_2|\gamma| + \text{const.} & \gamma_1 \leq |\gamma| \leq \gamma_2, \\ \ldots \end{cases}$$

with $m_1 < m_2$. To fix ideas, assume that the mismatch strain is such that $e_0 \in (\gamma_1, \gamma_2)$: then (12) shows that when the thickness is below the first critical value given by

$$h < h_c := \frac{1-\nu^2}{E}\frac{m_1}{e_0},$$

the interface remains coherent.

To proceed further, define two more critical values for h by

$$h_c' := \frac{1-\nu^2}{E}\frac{m_1}{e_0-\gamma_1}, \qquad h_c'' := \frac{1-\nu^2}{E}\frac{m_2}{e_0-\gamma_1},$$

which have the following properties; for h such that

$$h_c < h < h_c',$$

the interface is finely incoherent: (23) holds, and the energy is minimized by sequences as in (24), oscillating between $\gamma_a = 0$ and $\gamma_b = \gamma_1$ (with total volume fraction α_{min}/γ_1), and which represent mixtures of coherent and incoherent patches. The fine structure of the interface is summarized by a Young measure, as in the preceding section.

When the thickness reaches the second critical value, i.e., for

$$h_c' < h < h_c'',$$

the interface structure changes drastically and it becomes smoothly incoherent. Indeed, for all values of the thickness satisfying the above inequality, the relative incoherency strain remains constant and fixed at the value $\gamma \equiv \gamma_1$.

The layer remains 'glued' to the substrate with fixed incoherency strain until the third critical threshold is reached. Beyond this, i.e., for a thickness such that

$$h > h_c'',$$

oscillations appear again, and the interface becomes finely incoherent. In particular, since (23) holds, the minimizing sequences correspond to fine mixtures of different incoherent patches, corresponding to incoherency strains $\gamma_a = \gamma_1$ and $\gamma_b = \gamma_2$, and the fine structure of the interface is again determined by a Young measure.

The interface is always finely incoherent, since the critical thickness vanishes, and relaxes completely to the bulk equilibrium strain, so that the average incoherency strain coincides with the mismatch strain.

If f is concave, the infimum of the energy is not attained, and the structure of the minimizing sequences is as above, with incoherency strain concentrating on sets of measure zero. The fine properties of the interface are described again by a varifold as in Section 6.5.

To construct the minimizing sequences (22) in the proof of the Theorem on the Infimum of J, let $t_k \nearrow \infty$ be such that

$$\lim_{k\to\infty} \frac{f(t_k)}{t_k} = 0.$$

Then we may choose, for example,

$$g_k(x) = \begin{cases} e_0 t_k & x \in \left[0, \frac{1}{t_k}\right] \\ 0 & x \in \left[\frac{1}{t_k}, 1\right] \end{cases}$$

so that

$$u_k'(x) = u_{n_k,k}'(x) = \begin{cases} e_0 t_k & n_k x \in \left[0, \frac{1}{t_k}\right], \\ 0 & n_k x \in \left[\frac{1}{t_k}, 1\right]. \end{cases}$$

Appendix. Korn's inequality

We state and prove here a modified version of Korn's inequality. The proof follows Dautray & Lions [23]. Recall that functions in W are such that $\mathbf{u}(0,0) = 0$.

Theorem 1. *If Ω is a bounded set with regular boundary, then there exists a positive constant C such that*

$$\|\mathbf{E}\|^2_{L^2(\Omega,\mathbb{R}^{(2\times 2)})} \geq C\|\mathbf{u}\|^2_{W^{1,2}(\Omega,\mathbb{R}^2)}$$

for any $\mathbf{u} \in W$, and with $\mathbf{E}$ the strain associated to $\mathbf{u}$.

Proof. The first step is to prove that $\|\mathbf{E}\|^2_{L^2(\Omega,\mathbb{R}^{(2\times 2)})} := \int_\Omega \mathbf{E}\cdot\mathbf{E}\, dx\, dy$ defines a norm on W, i.e., $\|\mathbf{E}\|_{L^2(\Omega,\mathbb{R}^{(2\times 2)})} = 0 \Longrightarrow \mathbf{u} = 0$. To see this, note first that if $\|\mathbf{E}\|_{L^2(\Omega,\mathbb{R}^{(2\times 2)})} = 0$ then $\mathbf{E} = 0$ a.e., and this in turn implies that $\mathbf{u}(x,y) = \mathbf{a} + b(y\mathbf{i} - x\mathbf{j})$, with $\mathbf{a}$ and b constant. But since $\mathbf{u} \in W$, (1) holds and $b = 0$, while $\mathbf{a} = 0$ is a consequence of $\mathbf{u}(0,0) = 0$.

The second step, which shows that the norm $\|\mathbf{E}\|_{L^2(\Omega,\mathbb{R}^{(2\times 2)})}$ is equivalent to the $W^{1,2}(\Omega,\mathbb{R}^2)$ norm on W, is as in Dautray & Lions [23].

□

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