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H-measures for splitting particles

by

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Abstract

The elastic energy of a sequence of splitting particles is computed in the limit of infinite splitting. The calculation combines the mathematical tool of H-measures with the calculation of Khachaturyan et al. [1] for the elastic energy of cuboidal particles, doublets and octets. In the infinite splitting limit, the elastic energy of particles that split in one spatial dimension (a sequence of plates) decreases monotonically with particle separation, while the elastic energy of particles that split in all three dimensions (a sequence of cubes) exhibits a minimum at a particular interparticle separation.

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1 Introduction

It is well known that minimization of elastic energy can act to refine microstructure in multiphase crystalline solids. An example of such refinement is the laminated martensite twin structures observed in shape memory alloys, see for example [2]. Another interesting case of refinement is the particle splitting observed in diffusional transformations of Ni-based superalloys, see e.g. [3, 4]. Such splitting has been used as evidence for the possibility of elastically driven microstructures consisting of small, roughly equally sized precipitates embedded in a surrounding matrix.

The formation of fine phase microstructures has been studied extensively in the mathematics community by modeling a phase transformation with a nonconvex free energy that depends on a compatible deformation gradient field. The wells in the energy correspond to the different phases observed in the system, while the compatibility constraint on the deformation leads to solutions with coherent interfaces (continuous displacements). Because the solutions to this problem are not smooth, techniques beyond the Euler-Lagrange equations must be used to describe the energy minimizing microstructures. In particular, microstructures are associated with a minimizing sequence such that the energy decreases as the sequence (or microstructure) refines. However, the limit of the sequence, computed in a weak or average sense, is not itself a minimizer of the energy. Therefore, a set of mathematical tools has been developed to characterize the macroscopic properties of a microstructure described by an infinitely fine sequence of functions. One such tool is the H-measure, which was developed independently by Tartar [5] and Gérard [6] (under the name ‘microlocal defect measure’) as a way to calculate certain macroscopic properties associated with the minimizing sequence.

In this paper, we apply H-measures to the problem of splitting particles. The elastic energies of systems of splitting particles was first considered by Khachaturyan et al. [1]. They used Fourier methods to show that the elastic energy of a cuboidal particle in an elastic matrix decreases as it splits first into two plates and then into eight self-similar cubes. Khachaturyan et al. postulated that under further splitting, the elastic energy

decrease would continue were it not for the stabilizing influence of surface energy. However, they did not attempt to compute the limiting elastic energy associated with infinitely split particles.

Using H-measures, we calculate the elastic energy of a particle-matrix system in the limit of infinite particle splitting. Following [1], we consider two cases in the limit of infinite splitting: plate-shaped precipitates and identical cube-shaped precipitates. We find that the energy associated with a cluster of infinitely fine cube-shaped precipitates has a nonzero minimum for a particular cluster size and recovers to the single particle energy as the cluster size tends to infinity. This is consistent with elasticity scaling. In contrast, the energy of splitting into plates tends to zero as the cluster size tends to infinity, consistent with the result that the elastic energy of a thin plate with a $(1, 0, 0)$ habit plane vanishes [1].

In section 2, we present, following [1], the set-up and solution for the elastic energies of a system of rectangular parallelepipeds. In section 3 we briefly discuss the H-measure and show how it can be used to calculate the elastic energy for infinite splitting. In section 4 we discuss the results.

2 Elasticity Formulation

We want to compute the elastic energy of a two-phase system consisting of particles embedded coherently in a matrix. Both phases are taken to be linearly elastic with cubic symmetry and identical elastic constants. In reduced notation, these constants are given by the stiffness values C_{11} , C_{12} and C_{44} . The anisotropy factor is

$$\Delta = C_{11} - C_{12} - 2C_{44}$$

and is taken to be negative.

For a dilatational misfit strain ϵ_0 between the particle and matrix phases, Khachaturyan et al. [1] have shown that the elastic energy of the system is

$$E_{el} = \frac{1}{2} \int_{\mathbf{k}} B(\mathbf{n}) |\widehat{\chi}(\mathbf{k})|^2 (d^3k / (2\pi)^3) \quad (1)$$

where

$$\widehat{\chi}(\mathbf{k}) = \int_{\mathbf{x}} \chi(\mathbf{x}) e^{-i\mathbf{k}\cdot\mathbf{x}} d^3x \quad (2)$$

is the Fourier transform of the characteristic function $\chi(\mathbf{x})$ describing the shape of the particle or particles, \mathbf{k} is a vector in Fourier space, and $\mathbf{n} = \mathbf{k}/|\mathbf{k}|$. Throughout the paper, we use boldface to denote a vector, e.g., $\mathbf{k} = (k_1, k_2, k_3)$ and we use hats to denote a function defined in Fourier space.

The elasticity kernel $B(\mathbf{n})$ is given by [1]

$$B(\mathbf{n}) = \frac{2\beta\epsilon_0^2}{C_{11}} \left[(C_{11} - C_{12}) - \frac{2\beta\Delta\gamma_1(\mathbf{n})}{2C_{11} - \Delta} - \frac{27\beta\Delta^2\gamma_2(\mathbf{n})}{(2C_{11} - \Delta)(2C_{11} - 2\Delta)} \right] \quad (3)$$

with

$$\begin{aligned} \beta &= C_{11} + 2C_{12}, \\ \gamma_1(\mathbf{n}) &= n_x^2 n_y^2 + n_x^2 n_z^2 + n_y^2 n_z^2 \end{aligned} \quad (4)$$

and

$$\gamma_2(\mathbf{n}) = n_x^2 n_y^2 n_z^2. \quad (5)$$

As noted in [1], γ_1 and γ_2 vanish for $\mathbf{n} = \{1, 0, 0\}$. Hence the elastic energy may be decomposed into a shape independent piece corresponding to the energy of a thin plate with a $\{1, 0, 0\}$ facet, plus a piece that depends explicitly on the shape function $\chi(\mathbf{x})$. Subtracting the first piece gives the elastic energy relative to a thin plate,

$$\Delta E_{el} = V E_1 [4I_1 + 54\Delta I_2 / (3C_{11} - 2\Delta)] \quad (6)$$

where V is the total volume of precipitate phase,

$$E_1 = -\frac{1}{2} \frac{\beta^2 \Delta \epsilon_0^2}{C_{11} (2C_{11} - \Delta)} \quad (7)$$

is a positive material constant. The shape function enters through the integrals

$$I_1 = \frac{1}{2} \int_{\mathbf{k}} \gamma_1(\mathbf{n}) |\widehat{\chi}(\mathbf{k})|^2 d^3k / (2\pi)^3 \quad (8)$$

and

$$I_2 = \frac{1}{2} \int_{\mathbf{k}} \gamma_2(\mathbf{n}) |\widehat{\chi}(\mathbf{k})|^2 d^3k / (2\pi)^3. \quad (9)$$

Dividing Eq. (6) by VE_1 gives a dimensionless measure of the elastic energy per unit volume,

$$\Delta E_{el}^* = \frac{\Delta E_{el}}{VE_1} = 4I_1 + 54\Delta I_2 / (3C_{11} - 2\Delta) \quad (10)$$

Khachaturyan et al. [1] evaluate the energy (10) for different particle configurations, including: (1) a spherical particle with total volume $8a^3$; (2) a cuboidal particle with dimensions $2a \times 2a \times 2a$; (3) a doublet consisting of two plates with dimensions $2a \times a \times 2a$ separated by a distance ζa in the x_2 direction; and (4) an octet of cubes with dimensions $a \times a \times a$ equally separated by ζa in all three spatial directions. The energy for the sphere is found analytically, while for the other three cases the Fourier transforms of the shapes are computed explicitly and the elastic energy is found by evaluating the integrals (8) and (9) numerically.

In our calculations, we use the trapezoidal rule in three dimensions, with a fine grid in a cube near the origin and a coarser grid away from the origin; this is efficient because the Fourier transforms of the shape functions involve terms of the form $\sin x/x$. Our numerical results have been tested both by refining the grid and increasing the size of the cube on which we use the finest grid size; they also compare well to the H-measure calculation for cubes presented below. Our calculations are also in agreement with [1], though we consistently find energies about 5% higher, for example we compute $\Delta E_{el}^* = 0.593$ for a single cuboidal particle while [1] report $\Delta E_{el}^* = 0.558$.

The elastic energies for a doublet of plates and an octet of cubes are shown in Figures 1 and 2. One finds that the elastic energy decreases on splitting from a cube to a doublet, and from a cube to an octet of cubes. Khachaturyan et al. postulate that this decrease would continue with further splitting, but they do not calculate it. They argue that splitting beyond the first generation is unlikely from surface energy considerations.

However, as mentioned in the introduction, recent mathematical techniques now allow one to explicitly compute the elastic energy associated with infinite splitting. This limit is important because it gives the total elastic driving force for particle refinement and inverse coarsening. We note that the results of Khachaturyan et al. predict about a 13% decrease in elastic energy in going from a cube to a doublet, and a 22% decrease from a cube to an octet.

Hence there is still a significant elastic contribution to the total energy after such transitions, and so one might expect further evolution of the microstructure to further reduce the elastic energy.

3 H-measures

H-measures were introduced independently by Tartar [5] and Gérard [6] as a way to extract macroscopic information from a sequence of functions that converges weakly to zero. In the present context the sequence of functions that we consider will be the sequence of shape functions as splitting proceeds; e.g the sequence of shape functions for two plates, four plates, eight plates, etc. By subtracting the average shape function from this sequence, we generate a new sequence that converges weakly to zero and so is consistent with the definition of the H-measure. The energy associated with the splitting particles in the limit can then be calculated from the H-measure, see Eq. (14) below.

We first present a simplified version of Tartar's result for the H-measures for periodic functions [5] appropriate to the present situation. Consider a sequence of scalar functions

$$u_j(\mathbf{x}) = \chi_{co}(\mathbf{x})v(j\mathbf{x}) \quad (11)$$

where $v(\mathbf{y})$ is periodic in \mathbf{y} with period P . The function v represents a periodic array of particles and χ_{co} is a cutoff function to keep the total particle volume finite. If v has average zero then u_j converges weakly to zero as $j \rightarrow \infty$; i.e., as the period of the array goes to zero. As a periodic function v has the Fourier expansion

$$v(\mathbf{y}) = \sum_{\mathbf{k} \in Z^3} v_{\mathbf{k}} e^{2\pi i \mathbf{k} \cdot \mathbf{y}}, \quad (12)$$

where \mathbf{k} is a vector in Fourier space and Z^3 is the integer lattice. The condition that v has zero average amounts to $v_0 = 0$. Then, the H-measure of the sequence u_j is

$$\mu(\mathbf{x}, \mathbf{k}) = \chi_{co}(\mathbf{x}) d\mathbf{x} \otimes \sum_{\mathbf{k}} |v_{\mathbf{k}}|^2 \delta_{\mathbf{k}/|\mathbf{k}|}. \quad (13)$$

A fundamental property of the H-measure is that for any continuous function $\Phi(\mathbf{k}/|\mathbf{k}|)$ defined on the unit sphere S^2 ,

$$\lim_{j \rightarrow \infty} \int_{R^3} \Phi\left(\frac{\mathbf{k}}{|\mathbf{k}|}\right) |\hat{u}_j|^2 = \int_{R^3} \int_{S^2} \Phi\left(\frac{\mathbf{k}}{|\mathbf{k}|}\right) d\mu(\mathbf{x}, \mathbf{k}) = \int_{R^3} \chi_{co} d\mathbf{x} \sum_{\mathbf{k} \neq 0} \Phi\left(\frac{\mathbf{k}}{|\mathbf{k}|}\right) |v_k|^2. \quad (14)$$

In the example of particle splitting it is clear that the sequence u_j corresponds to the shape functions of the splitting particles and the function Φ corresponds to the elastic energy kernel $B(\mathbf{n})$ (or $\gamma_1(\mathbf{n})$ and $\gamma_2(\mathbf{n})$). We now compute the H-measure in detail, first for splitting into a sequence of plates, and then for splitting into a sequence of cubes.

3.1 Splitting into plates

We consider splitting into a sequence of plates with habit planes in a $(0, 1, 0)$ orientation. We denote the oscillating part of the shape function as follows. Consider a periodic function p with period $2aL$ such that on the interval $[-aL, aL]$,

$$p(x) = \begin{cases} 1 & \text{for } |x| \leq a \\ 0 & \text{otherwise} \end{cases}. \quad (15)$$

The function $p(jx_2)$ represents an infinite array of plates with $(0, 1, 0)$ habit and with period $\frac{2aL}{j}$. The variable L is a dimensionless cluster size, and $\zeta = L - 1$ is a dimensionless particle separation. If we define

$$\chi_{(c_1, c_2)}(\eta) = \begin{cases} 1 & \text{for } c_1 \leq \eta \leq c_2 \\ 0 & \text{otherwise} \end{cases} \quad (16)$$

then the sequence of *splitting* particles is represented by

$$\chi_j(x_1, x_2, x_2) = \chi_{co}(\mathbf{x}) p(jx_2) \quad (17)$$

where the cutoff function is

$$\chi_{co}(\mathbf{x}) = \chi_{(-a, a)}(x_1) \chi_{(-aL, aL)}(x_2) \chi_{(-a, a)}(x_3). \quad (18)$$

Introduce the average characteristic function

$$\chi_\infty = \frac{1}{L} \chi_{(-a, a)}(x_1) \chi_{(-aL, aL)}(x_2) \chi_{(-a, a)}(x_3). \quad (19)$$

Then, because $p(x_2) - \frac{1}{L}$ has zero average over a period $2aL$, $\chi_j - \chi_\infty$ converges weakly to zero. Noting that the calculation of $\Delta E_{el}^*(\chi_j)$ involves the integrals I_1 and I_2 given in Eqs. (8) and (9), we compute for $i = 1, 2$

$$\begin{aligned} \int_{\mathbf{k}} \gamma_i(\mathbf{n}) |\chi_j - \widehat{\chi_\infty} + \chi_\infty|^2 d^3 k &= \int_{\mathbf{k}} \gamma_i(\mathbf{n}) |\chi_j - \widehat{\chi_\infty}|^2 d^3 k + \int_{\mathbf{k}} \gamma_i(\mathbf{n}) |\widehat{\chi_\infty}|^2 d^3 k \\ &\quad + 2\text{Re} \left(\int_{\mathbf{k}} \gamma_i(\mathbf{n}) (\chi_j - \widehat{\chi_\infty}) \widehat{\chi_\infty} d^3 k \right). \end{aligned} \quad (20)$$

One can show that the cross-term vanishes as $j \rightarrow \infty$ because $\chi_j - \widehat{\chi_\infty}$ approaches zero weakly in this limit, and both γ_i and $\widehat{\chi_\infty}$ are sufficiently smooth. See [5] for details. Hence

$$\Delta E_{el}^*(\chi_j) = \Delta E_{el}^*(\chi_j - \chi_\infty) + \Delta E_{el}^*(\chi_\infty) \quad (21)$$

as $j \rightarrow \infty$, where the energy associated with $\chi_j - \chi_\infty$ can be computed using H-measures and the energy associated with χ_∞ can be computed numerically as in [1].

We compute the H-measure from the Fourier series coefficients of

$$v(x_2) = p(x_2) - \frac{1}{L} \quad (22)$$

following Eqs. (12)-(14). However we notice immediately that because the oscillations are only in x_2 , this Fourier series has components only in k_2 . Hence the H-measure (13) of the sequence $\chi_j - \chi_\infty$ is

$$\mu = \chi_{co}(\mathbf{x}) d\mathbf{x} \otimes \sum_k |v_k|^2 \delta_{\mathbf{k}/|\mathbf{k}|} = \chi_{co}(\mathbf{x}) d\mathbf{x} \otimes \frac{1}{L} \delta_{(0,1,0)} \quad (23)$$

from Plancherel's theorem. Hence from Eq. (14)

$$\lim_{j \rightarrow \infty} \int_{\mathbf{k}} \gamma_i(\mathbf{n}) |\chi_j - \widehat{\chi_\infty} + \chi_\infty|^2 d^3 k = 0 \quad (24)$$

because $\gamma_i(0, 1, 0) = 0$. This result is a manifestation of the result that $\Delta E_{el}^* = 0$ for an infinitely thin plate with a $(0, 1, 0)$ habit. Note however that while the energy computed from the H-measure vanishes, the energy associated with particle splitting has a non-zero contribution from χ_∞ , see Eq. (21). This energy depends on the cluster size L , and is plotted in Figure 1 along with the energy for splitting into two plates. Note that as $L \rightarrow \infty$, the elastic energy associated with infinite splitting goes to zero.

3.2 Splitting into cubes

We next consider splitting into sequences of cubes. In this case the splitting is in all three spatial dimensions, so we represent the splitting particles by

$$\chi_j(x_1, x_2, x_3) = \chi_{co}(\mathbf{x})p(jx_1)p(jx_2)p(jx_3) \quad (25)$$

where the cutoff function is

$$\chi_{co}(\mathbf{x}) = \chi_{(-aL, aL)}(x_1)\chi_{(-aL, aL)}(x_2)\chi_{(-aL, aL)}(x_3) \equiv \chi_{(-aL, aL)^3}(x_1, x_2, x_3) \quad (26)$$

and where p is given by Eq. (15). Note that the average characteristic function in this case is

$$\chi_\infty = \frac{1}{L^3}\chi_{(-aL, aL)}(x_1)\chi_{(-aL, aL)}(x_2)\chi_{(-aL, aL)}(x_3) \quad (27)$$

such that $\chi_j - \chi_\infty$ converges weakly to zero. As in the previous case, we want to compute $\Delta E_{el}^*(\chi_j) = \Delta E_{el}^*(\chi_j - \chi_\infty) + \Delta E_{el}^*(\chi_\infty)$ as $j \rightarrow \infty$, using H-measures for the first term and numerical integration for the second.

In this case, the fact that splitting is in all three spatial dimensions implies that the H-measure will be supported on all unit vectors $\mathbf{k}/|\mathbf{k}|$, where $\mathbf{k} = (k_1, k_2, k_3)$ runs through the integer lattice. To find μ , we compute the Fourier series coefficients of

$$v(\mathbf{x}) = p(x_1)p(x_2)p(x_3) - \frac{1}{L^3}.$$

This yields $v_0 = 0$ and

$$v_{\mathbf{k}} = \frac{1}{\pi^3 k_1 k_2 k_3} \sin\left(\frac{\pi k_1}{L}\right) \sin\left(\frac{\pi k_2}{L}\right) \sin\left(\frac{\pi k_3}{L}\right) \quad (28)$$

for $\mathbf{k} \neq 0$. Hence from Eq. (13),

$$\mu(\mathbf{x}, \mathbf{k}) = \chi_{co} d\mathbf{x} \otimes \sum_{k_1, k_2, k_3 \in \mathbb{Z}} \frac{1}{\pi^6 k_1^2 k_2^2 k_3^2} \sin^2\left(\frac{\pi k_1}{L}\right) \sin^2\left(\frac{\pi k_2}{L}\right) \sin^2\left(\frac{\pi k_3}{L}\right) \delta_{\mathbf{k}/|\mathbf{k}|}. \quad (29)$$

Applying Eq. (14) to the integrals (8) and (9), we find (for $i = 1, 2$)

$$\begin{aligned} \lim_{j \rightarrow \infty} \frac{1}{2} \int_{\mathbf{k}} \gamma_i(\mathbf{n}) |\chi_j - \chi_\infty|^2 d^3 k / (2\pi)^3 = \\ \frac{1}{(2\pi)^3 V} \int_{R^3} \chi_{co} d\mathbf{x} \sum_{k_1, k_2, k_3 \in \mathbb{Z}} \frac{\gamma_i(\mathbf{k}/|\mathbf{k}|)}{\pi^6 k_1^2 k_2^2 k_3^2} \sin^2\left(\frac{\pi k_1}{L}\right) \sin^2\left(\frac{\pi k_2}{L}\right) \sin^2\left(\frac{\pi k_3}{L}\right) \delta_{\mathbf{k}/|\mathbf{k}|}. \end{aligned} \quad (30)$$

This gives $\Delta E_{el}^*(\chi_j - \chi_\infty)$. It is also straightforward to compute $\Delta E_{el}^*(\chi_\infty)$; indeed but for a scaling by L this is identical to the calculation for the elastic energy of a cube. The results are shown in Figure 2 as a function of cluster size L . Also plotted is the elastic energy associated with splitting into an octet of cubes. Note that in this case, as $L \rightarrow \infty$, the elastic energy approaches the elastic energy of a single cube, consistent with elasticity scaling for this self-similar splitting geometry.

4 Discussion

In this paper, we have extended the calculation of Khachaturyan et al. [1] to calculate the elastic driving force for a cuboidal particle to split into both an infinitely fine laminate and an infinitely fine dispersion of cubes. While Khachaturyan et al. use an explicit shape function to compute the elastic energy of a cube, two plates and eight cubes, we compute the limiting energy by calculating the H-measure associated with a sequence of splitting particles. We then find the elastic energy in the limit of infinite splitting by using the elastic energy kernel of [1] together with the results of Tartar [5].

The calculation of the H-measures for particle splitting naturally separates the elastic energy into two pieces, denoted $\Delta E_{el}^*(\chi_\infty)$ and $\Delta E_{el}^*(\chi_j - \chi_\infty)$. The first term is associated with the average characteristic function for the particle cluster. Essentially the cluster is considered as a homogeneous but diffuse particle, with strength proportional to the ratio of particle volume to cluster volume. One then calculates the energy directly from Eq. (1) using the shape function for the cluster, scaled by its strength. The second term gives the energy associated with the (zero average) rapid oscillations. This contribution to the energy is calculated directly from the H-measure of the sequence using Eq (14).

The elastic energies of the two geometries considered— splitting into plates and splitting into cubes —show very different behavior in the H-measure limit. Consider first splitting into plates. As expected, the energy $\Delta E_{el}^*(\chi_\infty)$ equals the energy of a single cube at zero particle separation (i.e. the cluster size is identical to the particle size), and decreases as

the separation increases. This decrease is inversely proportional to the cluster size as the splitting only occurs in one direction. However, the energy $\Delta E_{el}^*(\chi_j - \chi_\infty)$ associated with oscillations is always zero. This is because the H-measure for particle splitting is non-zero only when $\mathbf{n} = \mathbf{k}/|\mathbf{k}| = (0, 1, 0)$, the direction of the splitting, and both γ_1 and γ_2 (Eqs. (8) and (9)) vanish for this \mathbf{n} . Essentially we recover in this infinite splitting limit the result that a thin plate with a $(0, 1, 0)$ facet is the optimal elastic energy shape.

Consider next splitting into cubes. Here again, $\Delta E_{el}^*(\chi_\infty)$ equals the energy of a single cube at zero particle separation and decreases as the separation increases. In this case, the decrease is inversely proportional to the cluster size cubed, as splitting occurs in all three directions. More interestingly, the energy $\Delta E_{el}^*(\chi_j - \chi_\infty)$ associated with the H-measure does not vanish, but instead is an increasing function of cluster size. At very large cluster sizes, this H-measure energy is identical to the energy of a single particle, as expected from elasticity scaling. We note that the total energy associated with a sequence of cube splitting has a minimum at a finite cluster size, and so is similar in behavior to splitting into octets. We find for octets $\Delta E_{el}^* = 0.467$ at a cluster size of 1.37 (equivalently, a separation of 0.37), while for the infinite splitting limit the minimum $\Delta E_{el}^* = 0.349$ at a cluster size of 1.39. Thus, infinite splitting into cubes provides at most about a 25% decrease below the elastic energy of an octet.

As noted by Khachatryan et al. [1], the elastic energy decrease upon splitting is countered by the increase in surface energy. It seems reasonable that the small gain in elastic energy associated with splitting beyond an octet of cubes will not be sufficient to overcome the increased surface energy. A more intriguing possibility is splitting into a laminate of plate-shaped particles, as the elastic energy can be decreased to zero for such a microstructure. It is interesting to note that such a microstructure has been observed in some simulations using isotropic elasticity but with different elastic constants for the two phases [7]. In contrast, splitting has been observed in other other simulations using anisotropic homogeneous elasticity as considered here [8].

Finally, we note that the simplest alternative to particle splitting is particle ‘plating,’

in which a cube undergoes a morphological transition in which two sides lengthen while the third side shrinks. Khachatryan et al. [1] consider such a possibility, though they do not calculate the elastic energy of a plate with flat sides (their ‘platelet’ has the shape of a circular disk). The results of such a calculation for a plate with dimensions $2a\eta \times \frac{2a}{\eta} \times 2a\eta$ are shown in Figure 3 as a function of η . Following [1] we also calculate the critical size for the transition from a cube to a plate; this is shown in Figure 4. We scale by a length $r_0 = \sigma/E_1$, where σ is surface energy and E_1 is the elastic energy given by Eq. (7). Of particular interest is the value $(a/r_0)|_{\eta=1} = 4.39$. This compares to critical values of $(a/r_0) = 13$ for splitting from a cube to a doublet, and $(a/r_0) = 25$ for splitting from a cube to an octet, see [1]. Hence, at least on energetic grounds, the formation of plates seems more likely than particle splitting.

Acknowledgments

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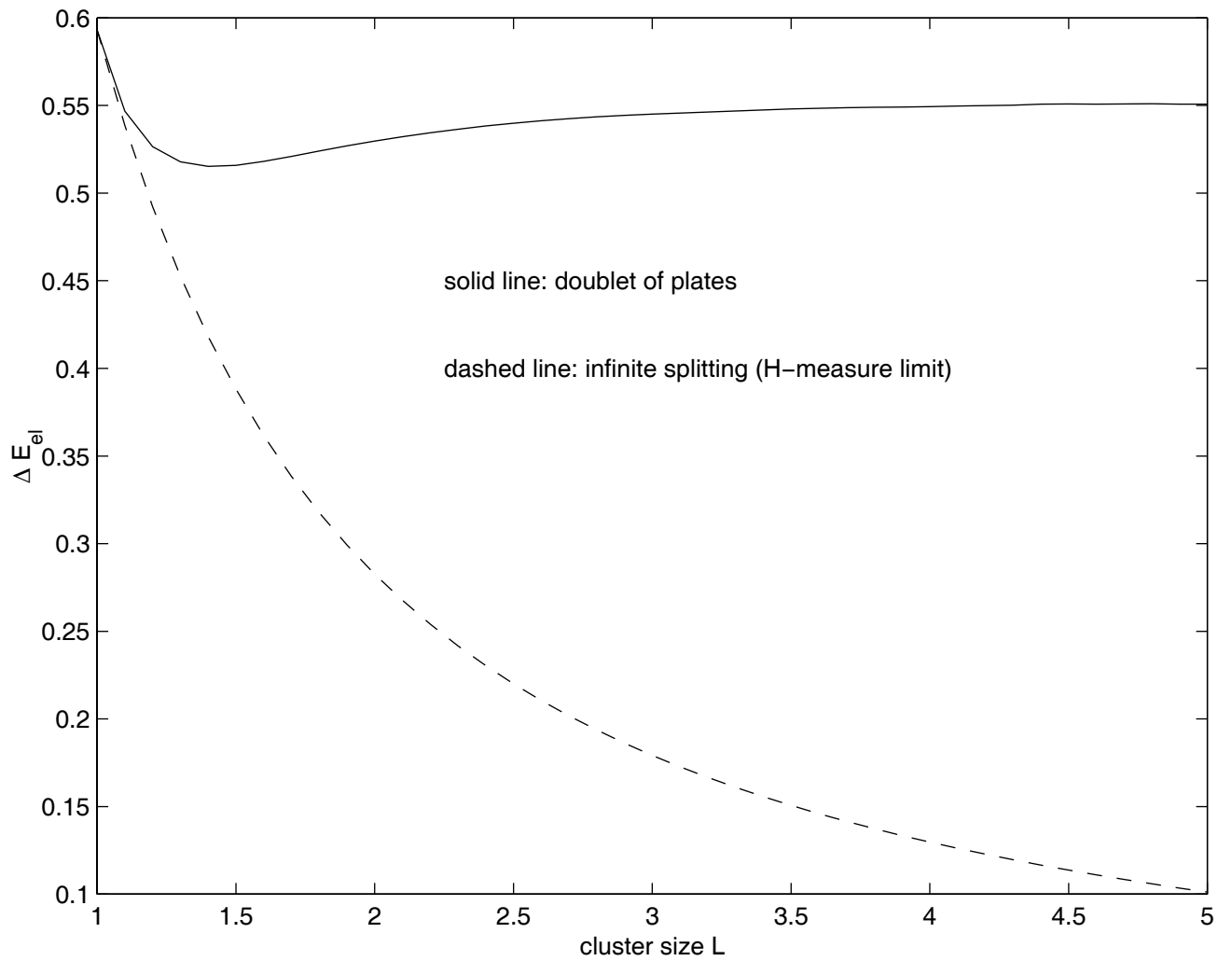


Figure 1: The elastic energy ΔE_{el} plotted against cluster size L for a doublet of plates and in the H-measure limit of infinite splitting into plates.

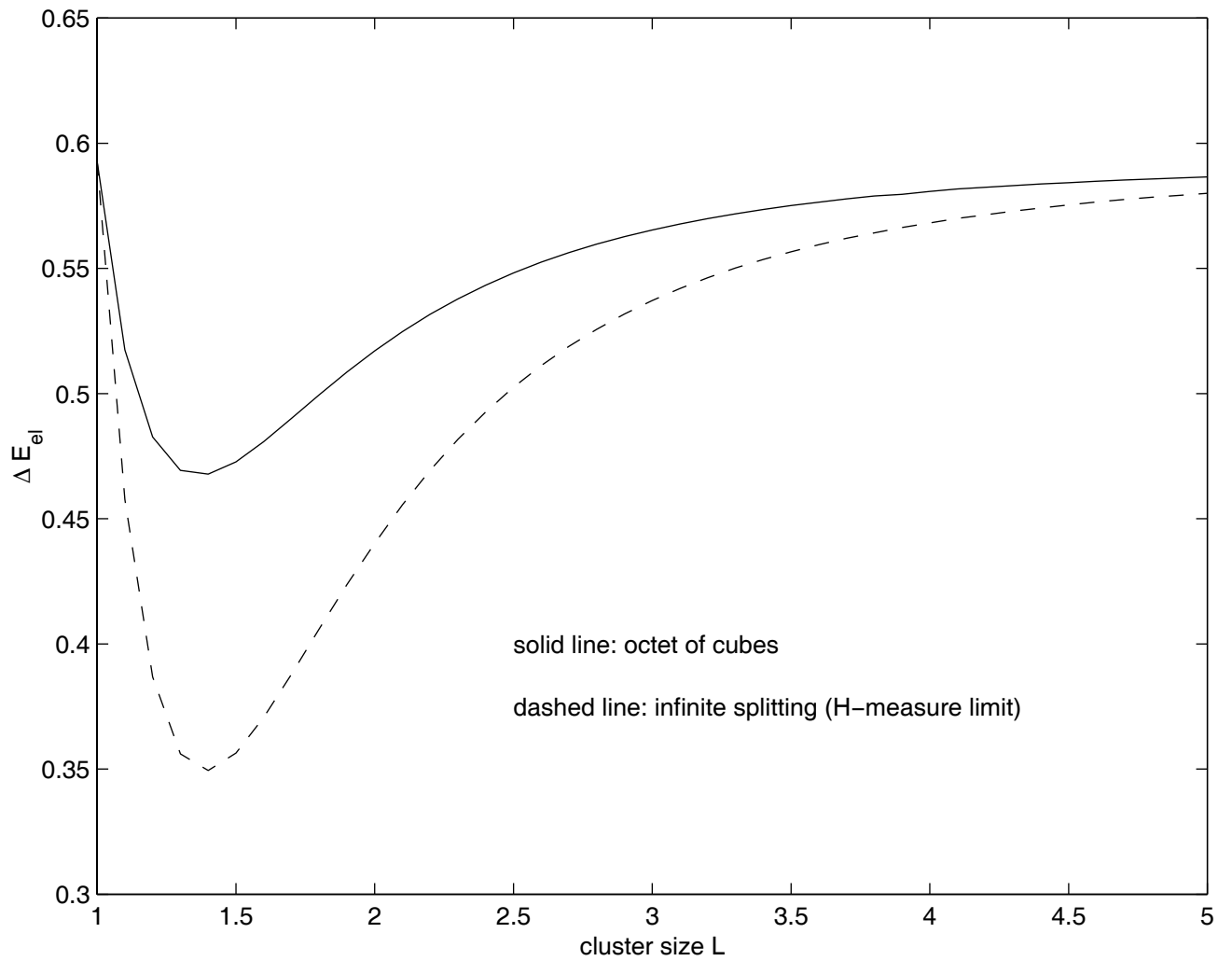


Figure 2: The elastic energy ΔE_{el} plotted against cluster size L for an octet of cubes and in the H-measure limit of infinite splitting into cubes.

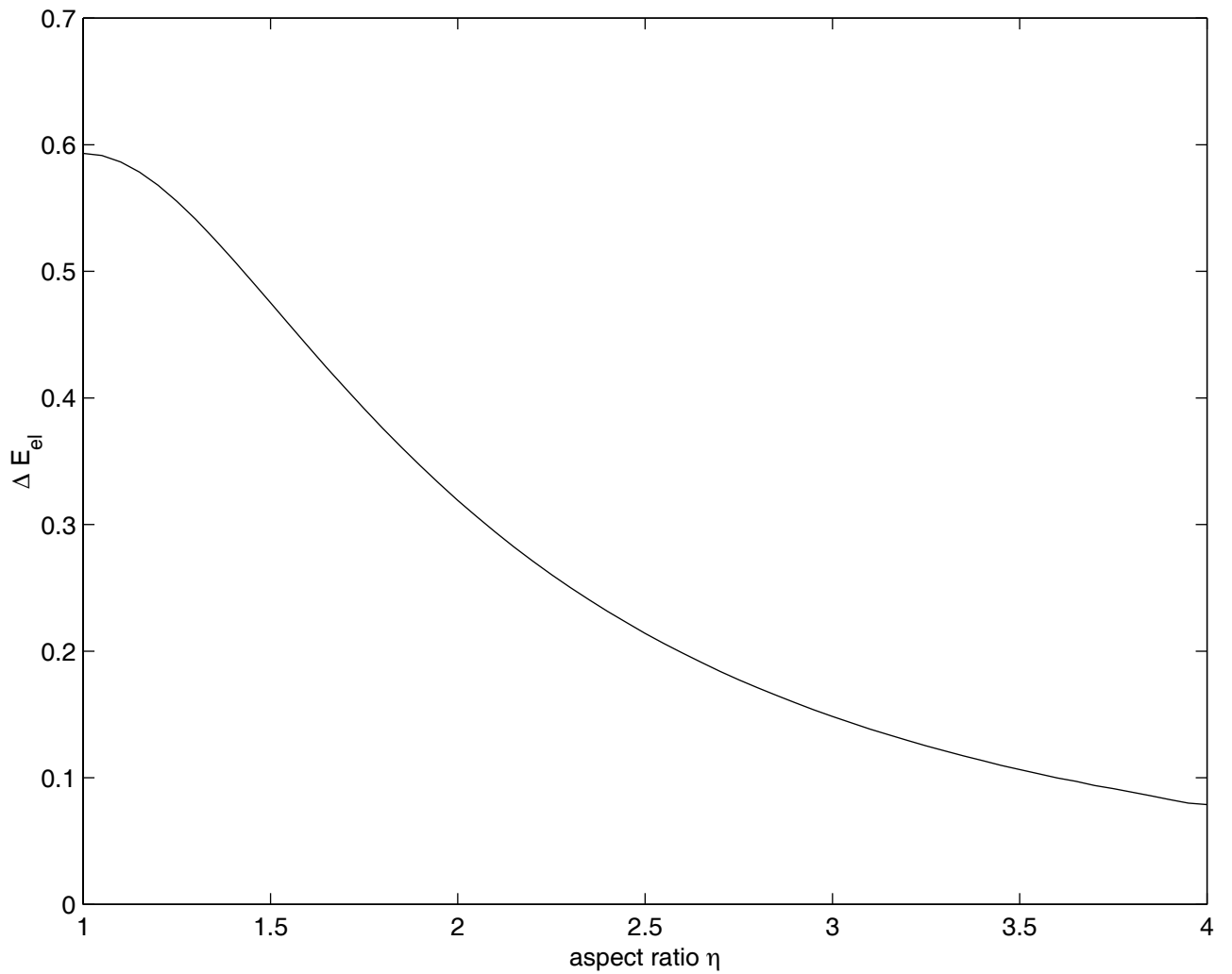


Figure 3: The elastic energy ΔE_{el} plotted against aspect ratio η for a single plate with dimensions $2a\eta \times 2a/\eta^2 \times 2a\eta$.

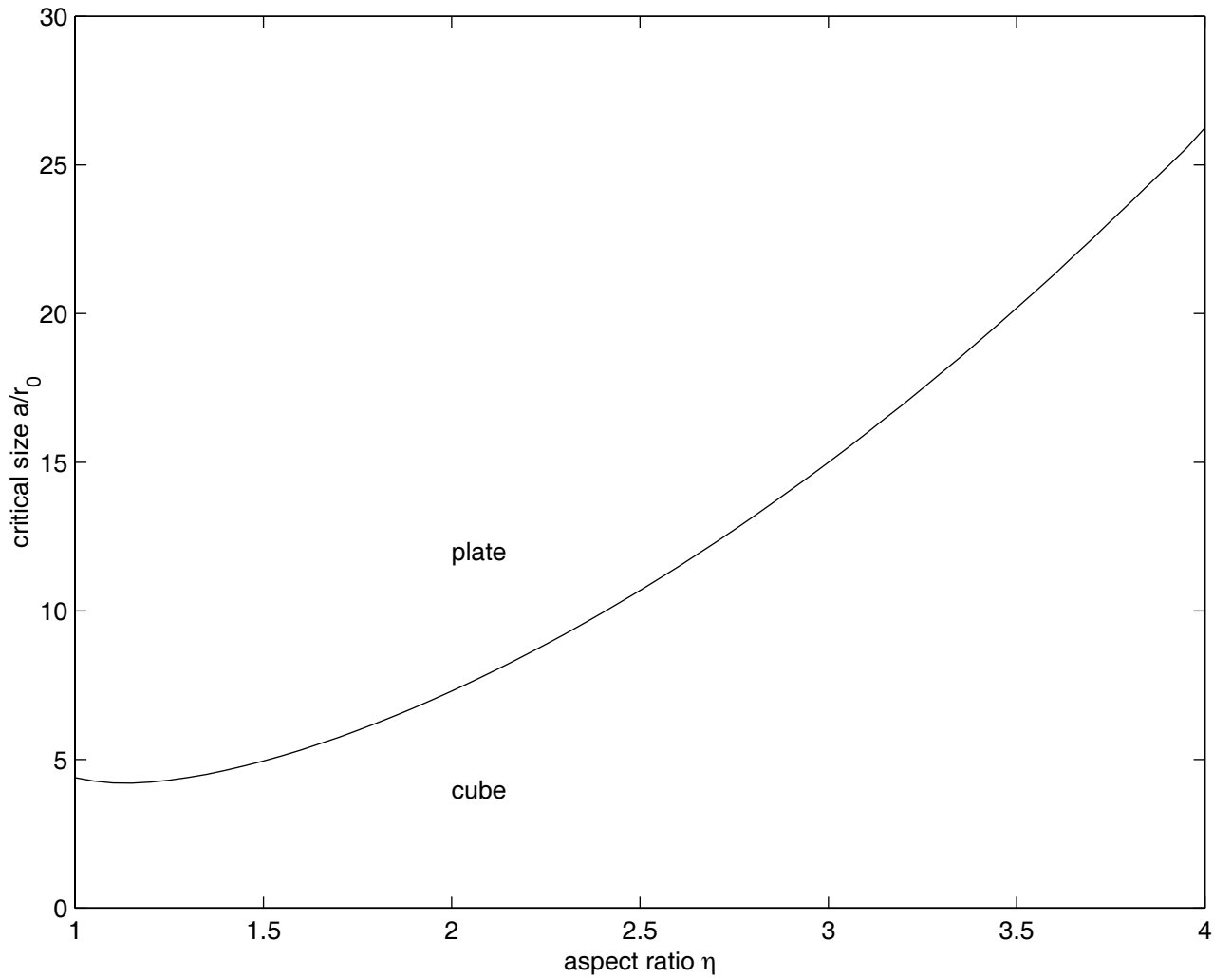


Figure 4: The critical size a/r_0 for transition from a cube with dimensions $2a \times 2a \times 2a$ to a plate with dimensions $2a\eta \times 2a/\eta^2 \times 2a\eta$ plotted against aspect ratio η . The parameter $r_0 = \sigma/E_1$ is a length scale, where σ is the surface energy and E_1 is the elastic energy given by Eq. (7).