Chapter 19: Elastic Inclusions

CHAPTER 19: ELASTIC INCLUSIONS

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19.1 INTRODUCTION

A number of important problems in materials science involve a common situation: a small particle of elastic material (an inclusion) forms or is inserted into an elastic matrix in which it does not quite fit. The inclusion strains the matrix and is strained by it, and the resulting elastic misfit energy affects the equilibrium of the composite system. Common examples of problems that can be modeled by systems of elastic inclusions include phase transformations in crystalline solids, coherent films on solid surfaces, inhomogeneous plastic deformation, solutes and precipitates, vacancies, voids and cracks.

When a phase transformation happens in the interior of a crystalline solid it perturbs the size, shape and elastic moduli of the transformed volume. The result is an elastic strain in both the new phase and the transformed matrix, which is particularly large when the transformation product is coherent with the matrix. The associated elastic
energy contributes to the thermodynamic potential of the system; it affects both the conditions under which the transformation can occur and the shape and crystallographic habit of the product phase.

A second example is a coherent film on a solid surface. Since such a film continues the lattice of the solid its elastic energy and state of strain are identical to those that would be created by a hypothetical phase transformation in which the solid began in a uniform state whose volume included the volume of the film, and then underwent a phase transformation that created the film.

A third example is an inhomogeneous plastic deformation in the interior of a solid. Consider a polygranular solid under a load that causes the plastic deformation of a single grain in the interior. Since the deformed grain remains attached to its surroundings, it acquires an elastic strain and imparts a strain to the matrix around it. The deformed grain behaves just as if it had undergone a phase transformation that created the plastic strain. In fact, it is possible to model the introduction of a single dislocation in this way. The introduction of a dislocation shears the material beneath the glide plane of the dislocation by an amount equal to its Burgers' vector. The process can be modeled by replacing the material beneath the glide plane by an elastic inclusion that is sheared with respect to the parent matrix.

Still another example is a crack or void in a solid. While one does not normally think of a crack in a solid as an inclusion, it can be created by replacing a region of the solid with an empty space, or, equivalently, with an inclusion whose elastic constants are zero. This picture is not unphysical, since a crack or void is produced when lattice vacancies condense in a specific region to form an "inclusion" of vacancies. If the inclusion of vacancies is introduced when the solid is under load, the resulting stress and strain fields are precisely those of a crack or void of the same shape. This picture leads directly to Eshelby's energy-momentum tensor of elasticity, or, as it is more widely known in modern fracture mechanics, Rice's J-integral.

The analysis of phase transformations in elastic solids requires a solution to the problem of the elastic inclusion. The other problems that were described above can be approached in a number of different ways. The advantage of modeling them as elastic inclusions is that there is a substantial body of known solutions to the inclusion problem, due largely to the work of Eshelby and Khachaturyan.

A general method for the solution of inclusion problems was suggested by J.D. Eshelby, who recognized that it is always possible to achieve the final state of a constrained elastic inclusion through a sequence of operations that are individually simple. And, under the assumption of linear (infinitesimal) elasticity, the elastic strains and elastic energies of the individual steps add together to create the final state of the solid. We shall call the sequence the Eshelby cycle. Eshelby used this procedure to obtain solutions to a number of important problems. However, the mathematical methods he employed, which primarily involve the use of Green's functions in real space, are cumbersome, and yield mathematical expressions whose physical content is often
difficult to extract without a complete numerical solution.

Khachaturyan's original contribution was to recognize that many of these problems can also be solved by Fourier transform techniques, in which case the solutions are formally simpler and are relatively transparent in their physical implications. In particular, the Khachaturyan solution retains a simple form when the solid is elastically anisotropic (as most solids of physical interest are) and when the solid contains an arbitrary distribution of different shapes and types (as most solids of physical interest do). For that reason we shall follow the Khachaturyan method in this Chapter.

The inclusion problem is simplest when the difference between the elastic constants of the inclusion and the matrix can be ignored, in which case the inclusions are said to be homogeneous. The homogeneous case is sufficient to treat most interesting problems in phase transformations since the material contained in a coherent precipitate or new-phase volume is often sufficiently like that in the parent phase that the effect of changing elastic constants is a small perturbation. However, when the inclusion is a crack or a material that is distinctly different from the matrix the assumption of similar elastic constants is clearly inadequate. The solution that governs the behavior of an inhomogeneous inclusion is significantly more complicated, and we shall consider only a few special cases.

19.2 THE ESHELBY CYCLE

In the problem we wish to solve an elastic inclusion or distribution of inclusions sits in an elastic matrix in which it does not quite fit. The misfit strains both the inclusions and the surrounding matrix. We wish to find the equilibrium strain field and the elastic energy for an arbitrary type and spatial distribution of inclusions.

The elastic strain and elastic energy depend on the final state of the system, but do not depend on how that state was created. If we can identify a sequence of operations that leads to the appropriate final state, with steps that are, individually, simple enough to be mathematically tractable, then we can use this sequence to find the solution. A sequence of operations that was suggested by Eshelby is sufficient for this purpose when the system behaves as a linear elastic medium. We specifically describe the Eshelby cycle for the case of a single inclusion in a solid that is initially unstressed. For the present we also assume that the elastic constants of the inclusion and the matrix are homogeneous and that the surface energy of the inclusion can be ignored. The Eshelby cycle can be easily modified to include these effects.

Consider a linear elastic solid that is initially homogeneous and unstressed, and let an inclusion of arbitrary shape be introduced by the following sequence of operations.

1. Isolate the region within the solid that the inclusion will eventually fill, and cut it out.
This operation produces a relaxed solid that contains a void, and a separated
volume of relaxed material that has been removed from the void. The stress and strain
are zero in both bodies. If the interfacial energy is ignored the energy of the system does
not change.

2. Let the volume that has been cut out undergo a stress-free transformation that
changes it from the material of the matrix to that of the inclusion.

The transformation is straightforward if the inclusion differs from the matrix only
in its structure, but requires a chemical transmutation if the two differ in their chemical
content. The transformation generally involves a change in the size and shape of the
inclusion. We specify the size and shape change by the transformation strain, $\varepsilon^0$, which
is measured with respect to the relaxed state of the matrix.

After step 2 the inclusion is unstressed, but has the strain, $\varepsilon^0$. There is no change
in the elastic energy of the system; the work done is entirely chemical and, assuming
constant temperature, is the free energy change of the phase transformation.

3. Impose a set of surface tractions on the inclusion and return it to its original
size and shape.

Since the surface traction is just sufficient to reverse the transformation strain, $\varepsilon^0$,
the stress in the inclusion is

$$\sigma_{ij} = \sigma_{ij}^0 = -\lambda_{ijkl}\varepsilon_{kl}^0$$

The $\lambda_{ijkl}$ are the elastic constants of the inclusion, which are equal to those of the matrix
in the homogeneous case. The stress, $\sigma^0$, is called the transformation stress.

After step 3 the inclusion has stress $\sigma^0$, but the strain within it is zero since strain
is measured with respect to the original state of the matrix, and the inclusion has been
strained back into that state. Since the transformation stress is confined to the inclusion
at the end of this step, the elastic energy resides in the inclusion, and is

$$\delta F^e = \delta F^0 = \frac{V_i}{2} \lambda_{ijkl}\varepsilon_{ij}^0\varepsilon_{kl}^0 = -\frac{V_i}{2} \sigma_{ij}^0\varepsilon_{ij}^0$$

where $V_i$ is the volume of the inclusion after it has been deformed back into the strain-
free state. The energy, $\delta F^0$, is called the elastic self-energy of the inclusion and is
positive definite.

4. Re-insert the inclusion into the matrix.

Since the inclusion just fits into the hole left in the matrix neither the inclusion
nor the matrix is strained in this operation and, ignoring surface tension, no additional energy is introduced. However, the composite system does contain an inhomogeneous stress field, $\sigma(\mathbf{R})$. Defining the shape function, $\theta(\mathbf{R})$, by the relation

$$
\theta(\mathbf{R}) = \begin{cases} 
1 & \mathbf{R} \ni \{ \mathbf{R}_i \} \\
0 & \text{otherwise}
\end{cases}
$$

where $\{ \mathbf{R}_i \}$ is the set of points within the inclusion phase, the stress field can be written

$$
\sigma(\mathbf{R}) = \sigma^0 \theta(\mathbf{R})
$$

5. Remove the surface tractions on the inclusion.

The internal stress within the inclusion can then relax by deforming the inclusion and the surrounding matrix, which induces the strain field, $\varepsilon(\mathbf{R})$. The associated stress field is

$$
\sigma_{ij}(\mathbf{R}) = \sigma^0_{ij} \theta(\mathbf{R}) + \lambda_{ijkl} \varepsilon_{kl}(\mathbf{R})
$$

where we have again assumed homogeneous elastic constants. The work done during the relaxation is

$$
\delta F' = \int V \left[ \int_0^\infty \sigma_{ij} \varepsilon_{ij} \right] dV = \int V \left[ \sigma^0_{ij} \varepsilon_{ij} \theta(\mathbf{R}) + \frac{1}{2} \lambda_{ijkl} \varepsilon_{ij} \varepsilon_{kl} \right] dV
$$

where

$$
\delta F' \leq 0
$$

since the elastic relaxation is spontaneous.

Step 5 completes the Eshelby cycle; the inclusion and matrix are both in their final, relaxed states.

To simplify the discussion we have described the Eshelby cycle as if there were only a single, isolated inclusion. Note, however, that the cycle is unchanged if the "inclusion" is an arbitrary distribution of inclusions of the same type. We need only interpret the shape function, $\theta(\mathbf{R})$, so that it has the value 1 when $\mathbf{R}$ is within any of the inclusions, and the value zero otherwise. Moreover, as we shall show below, the same relations apply with a minor change of notation when the solid contains simultaneous distributions of several different types of inclusions.
19.3 THE MACROSCOPIC STRAIN

19.3.1 Boundary conditions; microscopic homogeneity

The strain field in a solid that contains homogeneous inclusions can be found by applying the condition of mechanical equilibrium (Cauchy's First Law) to the stress field given in equation 19.5 to obtain a general solution, and then fitting the solution to appropriate boundary conditions to obtain the particular solution that applies to the situation of interest. Since elastic strains are additive the solution for an arbitrary state of external stress can be found by solving for the stress-free case and adding the strain field due to the external stress. However, even the stress-free problem is often difficult to solve since it requires that the traction be zero everywhere on the external surface of the body, and we must find the particular solution to Cauchy's First Law that leads to zero traction on all free surfaces in the presence of the strain fields of the inclusions.

There are, however, two general cases in which the strain field can be determined in a straightforward and simple way through the Fourier transform method that was suggested by Khachaturyan. The first is when the inclusion is isolated and embedded in a matrix of comparatively large size (the isolated inclusion). The second is when a distribution of inclusions is present, but the distribution is macroscopically homogeneous in the sense that every part of the system is like every other when it is examined on a sufficiently gross scale. In either case the actual solid can be replaced by an equivalent one whose displacement field satisfies periodic boundary conditions, and Fourier transform solutions are applicable. Fortunately, these two situations provide good approximations for a great many problems in materials science.

First, consider the case of an isolated inclusion that is embedded in a matrix whose volume is comparatively very large. Since the elastic field of an inclusion decreases rapidly at distances that are large compared to the dimension of the inclusion (as it must since the relaxation energy cannot exceed the self-energy of the source) the associated displacement vanishes on a boundary that is very far away, and hence vanishes everywhere on the boundary of the matrix, whatever its shape. It follows that the boundary can be replaced by a traction-free boundary that encloses the same volume but has a simple shape without changing the strain field or strain energy associated with the inclusion. This regular volume can then be repeated periodically in space so that the displacement field is periodic and its Fourier transform is well-defined. Since the displacement is constant (its gradient is zero) on the boundaries of each cell of the periodic array, each cell of the array is a replica of the system with the appropriate strain field and elastic strain energy.

Second, consider the case in which the solid contains a distribution of small inclusions that is homogeneous in the macroscopic sense. In this case a boundary can be drawn around any macroscopic subvolume and, to within a fluctuation that vanishes with the volume, the strain field and strain energy are the same within each subvolume. However, the inclusions will generally cause a net average strain that introduces a monotonic term into the total displacement. While the strain field is approximately
periodic, the displacement field is not, and Fourier transform solutions are difficult to apply since they are based on the Fourier transform of the displacement field.

We can, however, define a periodic elastic displacement for a system with a macroscopically homogeneous distribution of inclusions in the following way. If the average strain is \( \bar{\varepsilon} \) then the displacement gradient, \( \nabla u \), has a non-zero average, \( \bar{u}_{ij} \). The total displacement field can then be written as the sum of a macroscopic displacement field and an internal displacement that whose average gradient vanishes:

\[
\mathbf{u}_i^T(R) = \bar{u}_{ij} \mathbf{R}_j + u_i(R)
\]

where \( u_i(R) \) is the internal displacement, whose gradient has zero average. The strain field is, then,

\[
\varepsilon_{ij}(R) = \bar{\varepsilon}_{ij} + \Delta \varepsilon_{ij}(R)
\]

where \( \delta \varepsilon_{ij}(R) \) is the strain introduced by the internal displacement field.

Since the internal displacement, \( \mathbf{u}(R) \), has zero mean gradient, it has a constant average value over the boundary of any macroscopic subvolume. A constant displacement has no mechanical consequence, and, by St. Venant's Principle, the influence of any oscillation in \( \mathbf{u}(R) \) is confined to a region near the boundary whose dimension is of the order of the wavelength of the oscillation, and is hence microscopically small. It follows that, to within a small surface effect, \( \mathbf{u}(R) \) can be assumed constant on the boundary of any macroscopic subvolume. If the solid is modeled as a periodic repetition of identical macroscopic subvolumes then \( \mathbf{u}(R) \) can be assumed periodic and its Fourier transform is well-defined.

The strain field of a macroscopically homogeneous distribution of inclusions can hence be found in two steps: the macroscopic (average) strain is computed and subtracted out, then periodic boundary conditions are imposed and used to find the internal strain, \( \Delta \varepsilon(R) \). The sum of the two is the total strain field. The strain field of an isolated inclusion can be found in the same way since the average strain vanishes in that case.

### 19.3.2 The macroscopic strain field

To compute the average strain in a stress-free solid that contains a homogeneous distribution of inclusions we use a theorem that determines the average stress within an elastic body. If the body force is negligible (we assume it is) Cauchy's First Law reads

\[
\sigma_{ij} = 0
\]

If the divergence of the stress is multiplied by the position vector, \( \mathbf{R} \), and integrated over the body the result is
\[
\int_V \sigma_{ij} R_k dV = \int_V [\sigma_{ij} R_k]_j dV - \int_V [\sigma_{ij} R_{kl}]_j dV \\
= \int_S [\sigma_{ij} R_k] n_j dS - \int_V \sigma_{ij} \delta_{jk} dV \\
= \int_S T R_k dS - \int_V \sigma_{ik} dV
\]

19.11

Since the integral on the left-hand side vanishes, the average stress within a body whose surface traction is \( T \) is

\[
\bar{\sigma}_{ij} = \frac{1}{V} \int_S T R_j dS
\]

19.12

If the boundary is free of traction,

\[
\bar{\sigma}_{ij} = 0
\]

19.13

It follows from equations 19.13 and 19.5 that

\[
\bar{\sigma}_{ij}(R) = 0 = \sigma^0_{ij} \bar{\theta} + \lambda_{ijkl} \bar{\varepsilon}_{kl}
\]

19.14

Hence the macroscopic strain is

\[
\bar{\varepsilon}_{kl} = \varepsilon^0_{kl} \bar{\theta} = \left[ \frac{V_i}{V} \right] \varepsilon^0_{kl}
\]

19.15

The macroscopic strain due to a distribution of inclusions is just the stress-free strain of the inclusion phase multiplied by its volume fraction.

The macroscopic strain vanishes as the volume fraction of the inclusion phase approaches zero, as in the case of the isolated inclusion.

Using equations 19.15 and 19.9 the internal stress field can now be written

\[
\sigma_{ij} = \sigma^0_{ij} (\theta(R) - \bar{\theta}) + \lambda_{ijkl} [\varepsilon_{kl}(R) - \bar{\varepsilon}_{kl}] = \sigma^0_{ij} \Delta \theta(R) + \lambda_{ijkl} \Delta \varepsilon_{kl}(R)
\]

19.16

Equation 19.16 shows that the internal stress field, \( \sigma_{ij}(R) \), is induced by the inclusion distribution, \( \Delta \theta(R) \), and relaxed by the internal strain field, \( \Delta \varepsilon(R) \). Since the displacement that yields \( \Delta \varepsilon(R) \) can be assumed constant on the boundary of any macroscopic subvolume of the system, we can employ periodic boundary conditions and
use the Fourier transform to find the internal strain, and add the macroscopic strain to complete the solution.

19.3.3 The internal strain

If equation 19.16 is substituted into Cauchy's First Law the result is

$$\sigma_{ij, j} = 0 = \sigma_{ij}^0 \Delta \theta_{ij} + \lambda_{ijkl} \Delta \epsilon_{kl, ij}$$  \hspace{1cm} 19.17

where we have used the homogeneity of the elastic constants. The internal displacement field is, therefore, the solution to the partial differential equation,

$$\sigma_{ij}^0 \Delta \theta_{ij} = -\lambda_{ijkl} \epsilon_{kl, ij} = -\lambda_{ijkl} \epsilon_{kl, ij}$$  \hspace{1cm} 19.18

The condition of mechanical equilibrium determines the stress field, and hence the strain field, to within an additive constant. The additive constant to the strain is its average value, which is given by equation 19.15.

Given the inclusion distribution, $\Delta \theta(R)$, we find the internal displacement field, $u(R)$, by replacing the solid by one of equal volume with regular boundaries and imagining that this volume is periodically repeated through space. We can then solve for the Fourier transform of the displacement field. The Fourier transform, $\phi(k)$, of a function, $\phi(R)$, is defined by the integral,

$$\phi(k) = \frac{1}{V} \int_V \phi(R) e^{-ik \cdot R} dV$$  \hspace{1cm} 19.19

where, for simplicity, we assume that the periodically repeated volume, $V$, is cubic

$$V = L_x L_y L_z$$  \hspace{1cm} 19.20

and the vectors, $k$, have the form

$$k = k_x e_x + k_y e_y + k_z e_z$$  \hspace{1cm} 19.21

and have values that are confined to the first Brillouin zone of the assumed period:

$$-\frac{\pi}{L_i} \leq k_i \leq \frac{\pi}{L_i}$$  \hspace{1cm} 19.22

The inverse transform can be found by multiplying both sides of eq. 19.19 by the factor $\exp(ik \cdot R) d^3k/(2\pi)^3$ and integrating over the first Brillouin zone. Using the identity
\[
\frac{1}{(2\pi)^3} \int_k e^{ik(R-R')} d^3k = V \delta(R-R')
\]

where \( \delta(R) \) is the Dirac delta function, the result is

\[
\phi(R) = \frac{1}{(2\pi)^3} \int_k \phi(k)e^{ikR} d^3k
\]

Taking the gradient of both sides of eq. 19.24 yields the result

\[
\nabla \phi(R) = \left[ \frac{\partial \phi(R)}{\partial R} \right] = \frac{1}{(2\pi)^3} \int_k ik \phi(k)e^{ikR} d^3k
\]

from which it follows that the Fourier transform of the gradient of \( \phi(R) \) is obtained by simple multiplication:

\[
\nabla \phi(k) = ik \phi(k)
\]

Repeating the process, the Fourier transform of the second derivative is, in tensor notation,

\[
[\nabla \nabla \phi(k)]_{ij} = \phi_{ij}(k) = -k_i k_j \phi(k)
\]

Using the identities 19.19-19.27 to take the Fourier transform of both sides of eq. 19.18 leads to the equation

\[
i_0 \sigma_{ij}^0 k_j \Delta \theta(k) = \lambda_{ijkl} k_i k_j u_i(k)
\]

which is an algebraic equation for the Fourier components of the displacement field. To solve equation 19.28 we define the second-order tensor, \( \Omega^e \), by the inverse relation

\[
[\Omega^e]^{-1}_{il} = \lambda_{ijkl} e_j e_k
\]

where \( e = k/|k| \) is a unit vector in the direction of \( k \). The tensor \( \Omega^e \) appears often in the elastic theory of inclusions, and is called the Green’s tensor or the elastic tensor for the inclusion problem. Substituting equation 19.29 into 19.28 yields

\[
i_0 \sigma_{ij}^0 k_j \Delta \theta(k) = |k|^2 [\Omega^e]^{-1}_{il} u_i(k)
\]

If both sides of 19.30 are now multiplied by \( [\Omega^e]_{mj} \) and summed over the index, \( i \), the result is

\[
u_m(k) = i[\Omega^e]_{mj} \sigma_{ij}^0 \left( \frac{k_j}{|k|^2} \right) \Delta \theta(k)
\]
Hence the $k^{th}$ Fourier component of the displacement gradient is

$$u_{mn}(k) = ik_n u_m(k) = -\varepsilon_{n \Omega_m^c} \sigma_{ij}^0 e_j \Delta \theta(k)$$  \hfill 19.32

where $\varepsilon$ is a unit vector in the direction of $\mathbf{k}$, and the internal strain field that satisfies the conditions of mechanical equilibrium has the Fourier components

$$\Delta \varepsilon_{mn}(k) = \frac{1}{2} \left[ u_{ml}(k) + u_{lm}(k) \right] = -\frac{1}{2} \left[ \varepsilon_{n \Omega_m^c} + \varepsilon_{m \Omega_n^c} \right] \sigma_{ij}^0 e_j \Delta \theta(k)$$  \hfill 19.33

Equation 19.33 holds when $k \neq 0$. When $|k| = 0$ the vector $\varepsilon$ is undefined. However, since

$$\theta(k = 0) = \int_V \theta(R) dV = V \bar{\theta}$$  \hfill 19.34

and

$$\Delta \theta(k=0) = \theta(0) - \bar{\theta} = 0$$  \hfill 19.35

it is consistent to set

$$\Delta \varepsilon_{mn}(0) = 0$$  \hfill 19.36

Where there is a reason to do so the Fourier component of the strain field at $k = 0$ can be taken to be

$$\varepsilon_{ij}(0) = V \bar{\varepsilon}_{ij} = V \varepsilon_{ij}^0 = \varepsilon_{ij}^0 \theta(0)$$  \hfill 19.37

The equilibrium strain field is, then,

$$\varepsilon_{ij}(R) = \bar{\varepsilon}_{ij} - \frac{1}{2(2\pi)^3} \int_k \left[ \varepsilon_{n \Omega_m^c} + \varepsilon_{m \Omega_n^c} \right] \sigma_{ij}^0 e_j \Delta \theta(k) e^{ik \cdot R} d^3 k$$

$$= \bar{\varepsilon}_{ij} - \frac{1}{2(2\pi)^3} \int_k \left[ \varepsilon_{n \Omega_m^c} + \varepsilon_{m \Omega_n^c} \right] \sigma_{ij}^0 e_j \theta(k) e^{ik \cdot R} d^3 k$$  \hfill 19.38

where the prime on the second integral has the meaning that a differential volume of $k$-space around the origin ($k = 0$) is to be excluded (if the material is periodic with period, L, the minimum admissible magnitude of $k$ is $2\pi/L$ in any case).

**19.3.4 The strain as an integral over the unit sphere**

Equation 19.38 can be further simplified into an integral over the unit sphere in Fourier space. Note that the only term in the kernel of the integral in 19.38 that depends on the magnitude of the wave vector, $k$, is the product, $\theta(k) \exp[-ik \cdot R]$. In terms of the
spherical coordinates $k, \theta, \phi$, the differential volume element in Fourier space is

$$\frac{d^3k}{(2\pi)^3} = \frac{k^2 \sin(\theta)}{(2\pi)^3} dkd\theta d\phi = \frac{1}{2\pi^2} k^2 dk d\omega$$  \hspace{1cm} (19.39)

where

$$d\omega = \frac{1}{4\pi} \sin(\theta) d\theta d\phi$$  \hspace{1cm} (19.40)

is the element of solid angle. Using these relations the strain can be rewritten as

$$\epsilon_{ij}(R) = \bar{\epsilon}_{ij} + \int_\omega \Delta \epsilon_{ij}(e) \theta(e) d\omega$$  \hspace{1cm} (19.41)

where the integral is taken over the unit sphere,

$$\Delta \epsilon_{ij}(e) = -\frac{1}{2} \left[ e_i \Omega_{jm}^e + e_j \Omega_{im}^e \right] \sigma_{mn}^0 e_n$$  \hspace{1cm} (19.42)

and $\theta(e)$ is the weight of the shape function in the direction of $e$,

$$\theta(e) = \frac{1}{2\pi^2} \int_s \theta(ke) e^{ik(e \cdot R)} k^2 dk$$  \hspace{1cm} (19.43)

where the integral again excludes the infinitesimal volume element around $k = 0$.

The integral (19.41) has a simple physical interpretation. The kernel is the internal strain due to an element of the inclusion distribution that is perpendicular to the direction $e$ multiplied by the weight of the inclusion distribution in the direction $e$. The integral sums this product for all directions.

Note that $\Delta \epsilon_{ij}(e)$ depends on the nature of the inclusion, through its dependence on the transformation stress, $\sigma^0$, and on the elastic properties of the matrix, through its dependence on the tensor, $\Omega^e$, but is independent of the shape and distribution of the inclusions. The function $\theta(e)$, on the other hand, depends on the inclusion distribution through its dependence on $\theta(ke)$ and on the shape and volume of the matrix through the limits on the integral, but is independent of the nature of the inclusion and the matrix. It follows that the shape function, $\theta(e)$, can be found in general for a given inclusion distribution in a matrix of given geometry. The internal strain function, $\Delta \epsilon_{ij}(e)$, can be found for a particular combination of inclusion and matrix phase, irrespective of their geometry.
19.4 **THE ELASTIC ENERGY: SIMILAR COHERENT INCLUSIONS**

Let the solid contain a distribution of homogeneous inclusions of a given type, and let its boundary be free of traction. Assuming constant temperature the elastic energy is the elastic contribution to the Helmholtz free energy. From the Eshelby cycle the elastic energy is

\[ \delta F^e = \delta F^0 + \delta F^r \]

where \( \delta F^0 \) is the self-energy of the inclusion distribution and \( \delta F^r \) is the relaxation energy. The self-energy is

\[ \delta F^0 = -\frac{V_i}{2} \sigma_{ij}^0 \epsilon_{ij}^0 \]

where \( V_i \) is the total inclusion volume.

**19.4.1 Evaluation of the relaxation energy**

The relaxation energy, \( \delta F^r \), can be phrased as a simple integral in the following way:

\[ \delta F^r = \int_V \left\{ \int_0^\varepsilon \sigma_{ij} d\epsilon_{ij} \right\} dV = \int_V \left\{ \sigma_{ij}^0 \epsilon_{ij}(R) + \frac{1}{2} \lambda_{ijkl} \epsilon_{ij} \epsilon_{kl} \right\} dV \]

The second integral in equation 19.46 can be split into an integral over the inclusion volume, \( V_i \), and an integral over the matrix volume, \( V_m \). Since the stress in the matrix is

\[ \sigma_{ij} = \lambda_{ijkl} \epsilon_{kl} \]

the matrix contribution to the elastic energy is

\[ \frac{1}{2} \int_{V_m} \sigma_{ij} \epsilon_{ij} dV = \frac{1}{2} \int_{V_m} \left\{ \sigma_{ij} (\bar{\epsilon}_{ij} + \Delta \epsilon_{ij}) \right\} dV \]

\[ = \frac{1}{2} \int_{V_m} \sigma_{ij} \bar{\epsilon}_{ij} dV + \frac{1}{2} \int_{V_m} \sigma_{ij} u_{ij} dV \]

\[ = -\frac{1}{2} \int_{V_i} \sigma_{ij} \bar{\epsilon}_{ij} dV + \frac{1}{2} \int_{V_m} \sigma_{ij} u_{ij} dV \]

where the first integral on the right in last form is taken over the volume of the inclusions. To derive it, we have used the fact that the mean stress vanishes: \( \bar{\sigma}_{ij} = 0 \).
We now calculate the work done in creating the internal strain in the matrix,

\[
\frac{1}{2} \int_{V_n} \sigma_{ij} u_{ij} \, dV = \frac{1}{2} \int_{V_n} \{ (\sigma_{ij} u_i)_j - \sigma_{ij} u_i \} \, dV
\]

\[
= \frac{1}{2} \left\{ \int_S \sigma_{ij} u_i n_j \, dS + \int_S \sigma_{ij} u_i n_j \, dS \right\}
\]

\[
= \frac{1}{2} \int_S \sigma_{ij} u_i n_j \, dS
\]

19.49

where \( S \) is the external surface of the solid and \( S_i \) is the surface of the inclusion (which may be the disconnected surface of many discrete inclusion particles). The third form on the right-hand side follows from the fact that the boundary is free of traction.

The displacement, \( u \), is continuous across the surfaces of the inclusions, and the condition of mechanical equilibrium at that interface (neglecting the interfacial tension) is

\[
\sigma_{ij}^m n_j = \sigma_{ij}^i n_j
\]

19.50

where the superscripts \( m \) and \( i \) distinguish the matrix from the inclusion, and \( n \) is the outward normal vector to the matrix. Since the outward normal to the inclusion is \( \hat{n}_i = -n_m \),

\[
\frac{1}{2} \int_{V_n} \sigma_{ij} u_{ij} \, dV = \frac{1}{2} \int_{S_i} \sigma_{ij}^i u_i n_j \, dS = -\frac{1}{2} \int_{S_i} \sigma_{ij}^i u_i n_j \, dS
\]

\[
= -\frac{1}{2} \int_{V_i} \sigma_{ij} \Delta \varepsilon_{ij} \, dV
\]

19.51

Using eq. 19.51 in 19.48 we have

\[
\frac{1}{2} \int_{V_n} \sigma_{ij} \varepsilon_{ij} \, dV = -\frac{1}{2} \int_{V_i} \{ \sigma_{ij} (\varepsilon_{ij} + \Delta \varepsilon_{ij}) \} \, dV = -\frac{1}{2} \int_{V_i} \sigma_{ij} \varepsilon_{ij} \, dV
\]

19.52

Using this in eq. 19.46,

\[
\delta F' = \int_V \left\{ \sigma_{ij}^0 \varepsilon_{ij} \theta(R) + \frac{1}{2} \lambda_{ijkl} \varepsilon_{ij} \varepsilon_{kl} \right\} \, dV
\]
\[ = \int_{V_i} \left\{ \sigma_{ij}^0 \epsilon_{ij} + \frac{1}{2} \lambda_{ijkl} \epsilon_{ij} \epsilon_{kl} \right\} dV - \frac{1}{2} \int_{V_i} \sigma_{ij}^0 \epsilon_{ij} dV \]

\[ = \int_{V_i} \left\{ \sigma_{ij}^0 \epsilon_{ij} + \frac{1}{2} \lambda_{ijkl} \epsilon_{ij} \epsilon_{kl} \right\} dV - \frac{1}{2} \int_{V_i} \left[ \sigma_{ij}^0 \epsilon_{ij} + \lambda_{ijkl} \epsilon_{ij} \epsilon_{kl} \right] dV \]

\[ = \frac{1}{2} \int_{V_i} \sigma_{ij}^0 \epsilon_{ij} dV \quad 19.53 \]

Or, substituting for the strain,

\[ \delta F^r = \frac{V_i}{2} \sigma_{ij}^0 \epsilon_{ij} + \frac{1}{2} \int_{V_i} [\sigma_{ij}^0 u_{ij}] dV \quad 19.54 \]

where the integral is taken over the volume of the inclusions and \( u_{ij} \) is the gradient of the internal displacement.

### 19.4.2 Fourier transform solution for the relaxation energy

The final form of the integral on the right-hand side of equation 19.53 (or 19.54) has a simple form, but is extremely difficult to solve directly for any case other than the isolated, ellipsoidal inclusion studied by Eshelby. The reason is that the strain within the inclusion depends on the details of the transformation and the precise distribution of the inclusion phase. Substituting the Fourier transform solution for the displacement gradient, equation 19.32, leads to an expression for the relaxation energy that appears more complex, but is much simpler to interpret and use because it re-phrases the kernel of the integral as a product of energy and shape-dependent terms.

Using the identity,

\[ \int_{V} \sigma_{ij}^0 u_{ij} dV = \int_{S} \sigma_{ij}^0 u_{ij} n_j dS = \sigma_{ij}^0 u_{ij} \int_{S} n_j dS = 0 \quad 19.55 \]

since the displacement, \( u \), is constant on the external boundary, which is closed, we have,

\[ \int_{V} \sigma_{ij}^0 u_{ij} dV = \int_{V} \sigma_{ij}^0 u_{ij} \theta(R) dV = \int_{V} \sigma_{ij}^0 u_{ij} \Delta \theta(R) dV \]

\[ = \int_{V} \sigma_{ij}^0 \left[ \int_{k} u_{ij} \gamma_{ij}(k) \frac{d^3k}{(2\pi)^3} \right] \left[ \int_{k'} \Delta \theta(k') e^{i(k \cdot R)} \frac{d^3k'}{(2\pi)^3} \right] dV \]

\[ = \int \int \sigma_{ij}^0 u_{ij} \gamma_{ij}(k) \Delta \theta(k') \left[ \int_{V} e^{i(k \cdot R)} dV \right] \frac{d^3k'}{(2\pi)^3} \frac{d^3k}{(2\pi)^3} \]
\[ V \int_{k,k'} \sigma^0_{ij} u_{ij} (k) \Delta \theta (k') \delta (k + k') \frac{d^3 k}{(2\pi)^3} \frac{d^3 k'}{(2\pi)^3} \]

\[ = V \int_k \sigma^0_{ij} u_{ij} (k) \Delta \theta (-k) \frac{d^3 k}{(2\pi)^3} \quad 19.56 \]

where we have used the identity

\[ \int_V e^{i(k+k') \cdot R} dV = V \delta (k + k') \quad 19.57 \]

Introducing eq. 19.32 for the Fourier transform of the displacement gradient, \( u_{ij}(k) \), and the identity, \( \Delta \theta (-k) = \Delta \theta^* (k) \), we have

\[ \int_{V_i} \sigma^0_{ij} u_{ij} dV = -V \int_k e_i \sigma^0_{ij} \Omega^e_{jk} \sigma^0_{kl} e_l \Delta \theta (k) \frac{d^3 k}{(2\pi)^3} \]

\[ = -V \int_k B(e) \| \Delta \theta (k) \|^2 \frac{d^3 k}{(2\pi)^3} \quad 19.58 \]

where the elastic energy function, \( B(e) \), is defined as

\[ B(e) = e_i \sigma^0_{ij} \Omega^e_{jk} \sigma^0_{kl} e_l \quad 19.59 \]

The relaxation energy is, hence,

\[ \delta F^r = V \int_{V_i} \sigma^0_{ij} \varepsilon_{ij} + \frac{1}{2} \int_{V_i} [\sigma^0_{ij} u_{ij}] dV \]

\[ = V \frac{1}{2} \sigma^0_{ij} \varepsilon_{ij} + \frac{1}{2} \int_{V_i} \sigma^0_{ij} u_{ij} dV \]

\[ = \frac{V}{2} \sigma^0_{ij} \varepsilon_{ij} \theta^2 - V \int_k B(e) \| \Delta \theta (k) \|^2 \frac{d^3 k}{(2\pi)^3} \quad 19.60 \]

### 19.4.3 Fourier transform solution for the total elastic energy

Given equations 19.44, 19.45 and 19.60 the total elastic energy of a macroscopically homogeneous distribution of inclusions is

\[ \delta F^e = \delta F^0 + \delta F^r \]
\[
\begin{align*}
\frac{V}{2} \sigma^0_{ij} \varepsilon^0_{ij} \bar{\theta} + \frac{V}{2} \sigma^0_{ik} \varepsilon^0_{ik} \bar{\theta}^2 - \frac{V}{2} \int B(e) |\Delta \theta(k)|^2 \frac{d^3 k}{(2\pi)^3} \\
= \frac{V}{2} \lambda_{ijkl} \varepsilon^0_{ij} \varepsilon^0_{kl} (1 - \bar{\theta}) - \frac{V}{2} \int B(e) |\Delta \theta(k)|^2 \frac{d^3 k}{(2\pi)^3} 
\end{align*}
\]

Note that the first term in the final form of this equation is positive definite. Since the relaxation energy must be negative, the second term must be negative, so the integral is positive. Since \( \delta F^e \) is positive, the value of the integral must be smaller than the lead term.

The total elastic energy can be written as a single Fourier integral. To do this we use the identity

\[
\int_{k} |\Delta \theta(k)|^2 \frac{d^3 k}{(2\pi)^3} = \int_{V} \Delta \theta(R)^2 \frac{dV}{V} \\
= \int_{V} [\theta(R)^2 - 2\bar{\theta}\theta(R) + \bar{\theta}^2] \frac{dV}{V} \\
= \bar{\theta}(1 - \bar{\theta})
\]

in equation 19.61, yielding

\[
\delta F^e = \frac{V}{2} \int_{k} B_{0}(e) |\Delta \theta(k)|^2 \frac{d^3 k}{(2\pi)^3} 
\]

where the total energy function

\[
B_{0}(e) = -\sigma^0_{ij} \varepsilon^0_{ij} - B(e) = -\sigma^0_{ij} \varepsilon^0_{ij} - \varepsilon_{ij} \sigma^0_{ij} \mathbf{\Xi} \sigma^0_{ij} \\
= -\sigma^0_{ij} \left[ \varepsilon^0_{ij} + \Delta \varepsilon_{ij}(e) \right] = \lambda_{ijkl} \varepsilon^0_{ij} \left[ \varepsilon^0_{ij} + \Delta \varepsilon_{ij}(e) \right]
\]

The equation 19.63 for the total elastic energy has a simple physical interpretation. The kernal of the integral is the product of a function, \( B_e(e) \), that depends on the nature of the inclusion and the matrix, but is independent of the inclusion shape, and a structure factor, \( I(\theta(k)^2) \), that depends only on the inclusion shape. The equation can be rewritten as an integral over the unit sphere, as in equation 19.41:

\[
\Delta F_{el} = \frac{V}{2} \int_{e} B_{0}(e) S(e) d\omega
\]
where

\[ S(e) = \frac{1}{2\pi^2} \int \theta(ke)^2 k^2 dk \]  

\[ 19.66 \]

In this equation \( B_\alpha(e) \) is the contribution to the elastic energy from an element of inclusion that is normal to the direction, \( e \), and \( S(e) \) is the "weight" of the inclusion distribution in that direction.

The equations given in this section permit the relatively straightforward computation of the elastic energy of an arbitrary distribution of like, homogeneous inclusions. The function \( B(e) \) depends only on the nature of the matrix and the inclusion, and need be found only once for a given combination of matrix and inclusion. The function \( S(e) \) depends on the distribution of inclusions, but is a universal function for a given spatial distribution. We shall describe some of the applications of the equation below; it can be to compute the elastic energies, shapes and habit planes of precipitates, solutes or second-phase particles, the total energy of interacting distributions of like particles, and the change of energy of a distribution of second-phase particles during precipitation or coarsening.

### 19.5 Mixtures of Coherent Inclusions

Let a solid contain a distribution of different inclusions, all of which are approximately homogeneous with the matrix in their elastic constants. The different inclusions may be different phases, may be different variants of the same phase, or may simply be distinct inclusions of the same kind, in which case the analysis is used to obtain a simple expression for the interaction energy between the inclusions.

Returning to the Eshelby cycle, the self-energy of a distribution of distinct inclusions is (eq. 19.2)

\[ \delta F^0 = -\sum \frac{V^\alpha}{2} \sigma_{ij}^{\alpha0} \varepsilon_{ij}^{\alpha0} = -\frac{V}{2} \sum \bar{\theta}^\alpha \sigma_{ij}^{\alpha0} \varepsilon_{ij}^{\alpha0} \]

\[ \quad = \frac{V}{2} \sum \lambda_{ijkl} \varepsilon_{ij}^{\alpha0} \varepsilon_{kl}^{\alpha0} \bar{\theta}^\alpha \]  

\[ 19.67 \]

where \( \sigma^{\alpha0} \) and \( \varepsilon^{\alpha0} \) are the transformation stress and strain for an inclusion of the \( \alpha \)th kind, \( V^\alpha \) is the total volume of inclusions of the \( \alpha \)th kind, and \( \bar{\theta}^{\alpha} \) is their volume fraction.

After the inclusions have been introduced and allowed to relax the stress field is

\[ \sigma_{ij}(R) = \sum \sigma_{ij}^{\alpha0} \theta^\alpha (R) + \lambda_{ijkl} \varepsilon_{kl}(R) \]  

\[ 19.68 \]
where \( \theta^\alpha(R) \) is the shape function for the \( \alpha \)th inclusion and \( \varepsilon_{ij}(R) \) is the strain field. Since the body is free of traction the average stress is zero; hence the average strain is (eq. 19.15)

\[
\bar{\varepsilon}_{ij} = \varepsilon_{ij}^{\alpha} \bar{\theta}^\alpha = \sum_\alpha \frac{\varepsilon_{ij}^{\alpha} \bar{\theta}^\alpha}{V} \varepsilon_{ij}^{\alpha} = \sum_\alpha \left( \frac{V^\alpha}{V} \right) \varepsilon_{ij}^{\alpha} = 19.69
\]

and, as in the previous section, the total strain is

\[
\varepsilon_{ij}(R) = \bar{\varepsilon}_{ij} + u_{ij}(R) = 19.70
\]

where the average value of the internal displacement gradient, \( u_{ij}(R) \), is zero.

19.5.1 The Khachaturyan-Shatalov Equation

It follows from equation 19.53 that the elastic energy due to relaxation of the inclusions is

\[
\delta F^r = \int_V \left[ \sum_\alpha \sigma_{ij}^{\alpha} \varepsilon_{ij} \theta^\alpha(R) + \frac{1}{2} \lambda_{ijkl} \varepsilon_{ij} \varepsilon_{kl} \right] dV = 19.71
\]

We evaluate the two terms individually. First, using eq. 19.69 and the definition of the transformation stress, eq. 19.1,

\[
\delta F^r = \int_V \left[ \sum_\alpha \sigma_{ij}^{\alpha} \varepsilon_{ij} \theta^\alpha + \frac{1}{2} \lambda_{ijkl} \varepsilon_{ij} \varepsilon_{kl} \right] dV = \int_V \left[ \sum_\alpha \sigma_{ij}^{\alpha} \bar{\varepsilon}_{ij} \bar{\theta}^\alpha + \frac{1}{2} \lambda_{ijkl} \bar{\varepsilon}_{ij} \bar{\varepsilon}_{kl} \right] dV = 19.72
\]

To evaluate the second term on the right in 19.70 we proceed as in the previous section to obtain the Fourier components of the displacement gradient. If we follow through the derivation of eq. 19.32, to adapt it for the multi-inclusion case we need only replace the term \( \sigma^\theta A\theta(k) \) by a sum over the inclusions, giving
\[ u_{mln}(k) = ik_n u_m(k) = -e_n \Omega_{mn}^\epsilon \left[ \sum_\alpha \sigma^{0\alpha}_{ij} \Delta \theta^\alpha(k) \right] e_j \]  
19.73

Then

\[ \delta F_2^r = \int \frac{1}{2} \left[ \sum_\alpha \sigma^{0\alpha}_{ij} u_{ij} \Delta \theta^\alpha(R) + \frac{1}{2} \lambda_{ijkl} u_{ij} u_{kl} \right] dV \]

\[ = \int \frac{1}{2} \left[ \sum_\alpha \sigma^{0\alpha}_{ij} u_{ij} \Delta \theta^\alpha(R) + \frac{1}{2} \lambda_{ijkl} u_{ij} u_{kl} \right] dV \]

\[ = V \int \frac{1}{2} \left[ \sum_\alpha \sigma^{0\alpha}_{ij} u_{ij} \Delta \theta^\alpha(k) + \frac{1}{2} \lambda_{ijkl} u_{ij} u_{kl} \right] d^3k \]

The second term in the integrand can be evaluated with the help of eq. 19.73. Using eq. 19.29 and the symmetry of the tensors \( \lambda, \sigma \) and \( \Omega^\epsilon \),

\[ \frac{1}{2} \lambda_{ijkl} u_{ij} u_{kl}(k)^* = \frac{1}{2} \lambda_{ijkl} u_{ij}(k) u_{ij}(k)^* \]

\[ = \frac{1}{2} \lambda_{ijkl} e_j \Omega^\epsilon_{jm} \left[ \sum_\alpha \sigma^{0\alpha}_{mn} \Delta \theta^\alpha(k) \right] e_n e_k \Omega^\epsilon_{kp} \left[ \sum_\beta \sigma^{0\beta}_{pq} \Delta \theta^\beta(k) \right] e_q \]

\[ = \frac{1}{2} \left[ \Omega^\epsilon_{il} \right]^{-1} \Omega^\epsilon_{lm} \left[ \sum_\alpha \sigma^{0\alpha}_{mn} \Delta \theta^\alpha(k) \right] e_n \Omega^\epsilon_{ip} \left[ \sum_\beta \sigma^{0\beta}_{pq} \Delta \theta^\beta(k) \right] e_q \]

\[ = \frac{1}{2} \left[ \sum_\alpha \sigma^{0\alpha}_{mn} \Delta \theta^\alpha(k) \right] e_n \Omega^\epsilon_{ip} \left[ \sum_\beta \sigma^{0\beta}_{pq} \Delta \theta^\beta(k) \right] e_q \]

\[ = \frac{1}{2} \sum_{\alpha, \beta} e_n \sigma^{0\alpha}_{mn} \Omega^\epsilon_{mp} \sigma^{0\beta}_{pq} e_q \Delta \theta^\alpha(k) \Delta \theta^\beta(k) \]  
19.75

Now using 19.73 in the first term in the integrand, we have

\[ \delta F_2^r = -\frac{V}{2} \sum_{\alpha, \beta} \int \left[ e_i \sigma^{0\alpha}_{ij} \Omega^\epsilon_{jk} \sigma^{0\beta}_{kl} e^*_l \Delta \theta^\alpha(k) \Delta \theta^\beta(k) \right] \frac{d^3k}{(2\pi)^3} \]

19.76

Summing eqs. 19.75 and 19.79 gives the relaxation energy:
\[ \delta F^r = \int_v \left[ \sum_{\alpha} \sigma_{ij}^{\alpha \alpha} \varepsilon_{ij}^{\alpha \alpha} \theta_{ij}^{\alpha \alpha} + \frac{1}{2} \lambda_{ijkl} \varepsilon_{ij}^{\alpha \alpha} \varepsilon_{kl}^{\alpha \alpha} \right] dV \]

\[ = \frac{V}{2} \sum_{\alpha, \beta} \sigma_{ij}^{\alpha \alpha} \varepsilon_{ij}^{\alpha \alpha} \bar{\theta}_{ij}^{\alpha \alpha} \bar{\theta}_{ij}^{\alpha \alpha} - \frac{V}{2} \sum_{\alpha, \beta} \left\{ \int_k e_i \sigma_{ik}^{\alpha \alpha} \Omega e_{\beta}^{\alpha \alpha} e_{ij} \Delta \theta_{ij}^{\alpha \alpha}(k) \Delta \theta_{ij}^{\alpha \alpha}(k) \frac{d^3 k}{(2\pi)^3} \right\} \]

\[ = \frac{V}{2} \sum_{\alpha, \beta} \sigma_{ij}^{\alpha \alpha} \varepsilon_{ij}^{\alpha \alpha} \bar{\theta}_{ij}^{\alpha \alpha} \bar{\theta}_{ij}^{\alpha \alpha} - \frac{V}{2} \sum_{\alpha, \beta} \left\{ \int_k B_{ij}^{\alpha \alpha}(e) \Delta \theta_{ij}^{\alpha \alpha}(k) \Delta \theta_{ij}^{\alpha \alpha}(k) \frac{d^3 k}{(2\pi)^3} \right\} \]

\[ = -\frac{V}{2} \sum_{\alpha, \beta} \lambda_{ijkl} \varepsilon_{ij}^{\alpha \alpha} \varepsilon_{kl}^{\alpha \alpha} \bar{\theta}_{ij}^{\alpha \alpha} \bar{\theta}_{ij}^{\alpha \alpha} - \frac{V}{2} \sum_{\alpha, \beta} \left\{ \int_k B_{ij}^{\alpha \alpha}(e) \Delta \theta_{ij}^{\alpha \alpha}(k) \Delta \theta_{ij}^{\alpha \alpha}(k) \frac{d^3 k}{(2\pi)^3} \right\} \]

where, by analogy to eq. 19.56, the elastic energy function, \( B_{ij}^{\alpha \alpha}(e) \), is

\[ B_{ij}^{\alpha \alpha}(e) = e_i \sigma_{ij}^{\alpha \alpha} \Omega e_{\beta}^{\alpha \alpha} \]

The total elastic energy is, then,

\[ \delta F^r = \delta F^0 + \delta F^r \]

\[ = \frac{V}{2} \sum_{\alpha, \beta} \lambda_{ijkl} \varepsilon_{ij}^{\alpha \alpha} \varepsilon_{kl}^{\alpha \alpha} \bar{\theta}_{ij}^{\alpha \alpha} \bar{\theta}_{ij}^{\alpha \alpha} - \frac{V}{2} \sum_{\alpha, \beta} \left\{ \int_k B_{ij}^{\alpha \alpha}(e) \Delta \theta_{ij}^{\alpha \alpha}(k) \Delta \theta_{ij}^{\alpha \alpha}(k) \frac{d^3 k}{(2\pi)^3} \right\} \]

Eq. 19.79 is the \textit{Khachaturyan-Shatalov Equation}. Note that, like eq. 19.61, eq. 19.79 divides the elastic energy into two contributions: a configuration-independent term that depends only on the volume fraction of the inclusions, and a configuration-dependent term that depends on the precise shape and distribution of the inclusions.

\subsection*{19.5.2 Alternate forms for the elastic energy}

There are three alternative ways to write eq. 19.79 that are often useful.

First, the energy can be written as a single integral. Using the identity

\[ V \bar{\theta}_{ij}^{\alpha \alpha} \left[ \delta_{ij}^{\alpha \alpha} - \bar{\theta}_{ij}^{\alpha \alpha} \right] = \int_v \left[ \Delta \theta_{ij}^{\alpha \alpha}(r) \Delta \theta_{ij}^{\alpha \alpha}(r) \right] dV = \int_k \left[ \Delta \theta_{ij}^{\alpha \alpha}(k) \Delta \theta_{ij}^{\alpha \alpha}(k) \right] \frac{d^3 k}{(2\pi)^3} \]

We can re-write eq. 19.76 in the formally simpler form

\[ \delta F^r = \frac{V}{2} \sum_{\alpha, \beta} \left\{ \int_k B_{ij}^{\alpha \alpha}(e) \Delta \theta_{ij}^{\alpha \alpha}(k) \Delta \theta_{ij}^{\alpha \alpha}(k) \frac{d^3 k}{(2\pi)^3} \right\} \]
where \( B_0^{\alpha\beta}(e) \) is the total energy function

\[
B_0^{\alpha\beta}(e) = \lambda_{ijkl} e_{ij} e_{kl} - B_{ijkl}^{\alpha\beta} (e) = \lambda_{ijkl} e_{ij} e_{kl} - \epsilon \sigma_{ijkl}^{\alpha\beta} \Omega_{ijkl}^{\alpha\beta} \epsilon_{l}
\]

Note that all the directional dependence of \( B_0^{\alpha\beta}(e) \) is contained in \( B_{ijkl}^{\alpha\beta}(e) \). The two differ through a constant, additive term.

Second, a slight change in notation allows us to replace \( \Delta \theta^\alpha(k) \) by \( \theta^\alpha(k) \). Since

\[
\Delta \theta^\alpha(k) = \int_V \left[ \theta^\alpha(r) - \bar{\theta}^\alpha \right] e^{i(k \cdot r)} dV = \begin{cases} \theta^\alpha(k) & k \neq 0 \\ 0 & k = 0 \end{cases}
\]

we may write the elastic energy as

\[
\delta F^e = \frac{V}{2} \sum_{\alpha,\beta} \left[ \int k \left[ B_0^{\alpha\beta}(e) \theta^\alpha(k) \theta^\beta^*(k) \right] \frac{d^3k}{(2\pi)^3} \right]
\]

where the prime on the integral has the meaning that an elementary volume about \( k = \theta \) is to be excluded.

### 19.5.3 Inclusion interactions in real space

Third, and most usefully, it is possible to write the configuration-dependent interaction (eq. 19.79) as a sum of two-body interactions in real space. To accomplish this we begin by using eq. 19.83 in 19.79 to obtain:

\[
\delta F^e = \frac{V}{2} \sum_{\alpha,\beta} \lambda_{ijkl} e_{ij} e_{kl} \bar{\theta}^\alpha \left[ \delta_{\alpha\beta} - \bar{\theta}^\beta \right] - \frac{V}{2} \sum_{\alpha,\beta} \left[ \int k B_0^{\alpha\beta}(e) \theta^\alpha(k) \theta^\beta^*(k) \right] \frac{d^3k}{(2\pi)^3}
\]

We then recognize that the inclusion distribution is actually a distribution of discrete inclusions in which inclusions of type \( \alpha \) (\( \alpha = 1,2,3,\ldots \)) are located (centered) at the positions, \( R_i^\alpha, (I = 1,2,3,\ldots) \). It follows that the shape function of the \( \alpha^\text{th} \) particle type, \( \theta^\alpha(r) \), is the sum of the shape functions of the individual particles:

\[
\theta^\alpha(r) = \sum_{I=1}^{N_{\alpha}} \theta^\alpha_I (r - R_i) \]

where \( \theta^\alpha_I (r - R_i) \) is the shape function of the inclusion of type \( \alpha \) centered at \( R_i \). The Fourier transform of the shape function is, then

\[
\theta^\alpha(k) = \sum_{I=1}^{N_{\alpha}} \theta^\alpha_I (k) e^{-i(k \cdot R_i)}
\]
Substituting this result into eq. 19.85 gives

$$
\delta F^e = \frac{V}{2} \sum_{\alpha, \beta} \lambda_{ijkl} e_{ij}^{\alpha \beta} \theta^{\alpha \beta} \left[ \delta_{\alpha \beta} - \overline{\delta}_{\alpha \beta} \right]
$$

$$
- \frac{V}{2} \sum_{\alpha, \beta} \sum_{k} \left\{ \int d^3 k \left[ B^\alpha (e) \theta^\alpha (k) \theta^{\beta \ast} (k) e^{-\frac{1}{2} (k \cdot \mathbf{r}^\alpha - \mathbf{r}^\beta)} \right] \frac{d^3 k}{(2\pi)^3} \right\}
$$

19.88

The terms in this summation for which $\alpha = \beta$ and $I = J$ give the elastic energy of the individual inclusions, that is, the energy $a_n$ of type $\alpha$ at position $R_i$ would have if it were present all by itself:

$$
\delta F^e_{\alpha} (R_i^\alpha) = \frac{V}{2} \lambda_{ijkl} e_{ij}^{\alpha \alpha} \theta^{\alpha \alpha} (1 - \overline{\theta}^{\alpha \alpha}) - \frac{V}{2} \sum_{k} \left[ \int B^\alpha (e) \theta^\alpha (k) \theta^{\alpha \ast} (k) e^{-\frac{1}{2} (k \cdot \mathbf{r}^\alpha - \mathbf{r}^\alpha)} \right] \frac{d^3 k}{(2\pi)^3}
$$

19.89

where

$$
B^\alpha (e) = e_{ij}^{\alpha \alpha} O_{jk} e_{kl}^{\alpha \alpha} e_j
$$

19.90

Eq. 19.89 is identical to eq. 19.61 with a slight change in notation. Using eq. 19.89,

$$
\delta F^e = \sum_{\alpha, R_i} \delta F^e_{\alpha} (R_i^\alpha) - \frac{V}{2} \sum_{\alpha, \beta, R_i^\alpha \neq R_j^\beta} \lambda_{ijkl} e_{ij}^{\alpha \beta} \theta^{\alpha \beta} \theta^{\alpha \beta}
$$

$$
- \frac{V}{2} \sum_{\alpha, \beta, R_i^\alpha \neq R_j^\beta} \left\{ \int \left[ B^\alpha (e) \theta^\alpha (k) \theta^{\beta \ast} (k) e^{-\frac{1}{2} (k \cdot \mathbf{r}^\alpha - \mathbf{r}^\beta)} \right] \frac{d^3 k}{(2\pi)^3} \right\}
$$

19.91

or, in a simpler notation,

$$
\delta F^e = \sum_{\alpha, R_i} \delta F^e_{\alpha} (R_i^\alpha) + \frac{V}{2} \sum_{\alpha, \beta, R_i^\alpha \neq R_j^\beta} \overline{V}^\alpha \beta + \frac{V}{2} \sum_{\alpha, \beta, R_i^\alpha \neq R_j^\beta} V^\alpha \beta (R_i^\alpha - R_j^\beta)
$$

19.92

where

$$
\overline{V}^\alpha \beta = O_{ij} e_{ij}^{\alpha \beta} \theta^{\alpha \beta} \theta^{\alpha \beta} = -\lambda_{ijkl} e_{ij}^{\alpha \beta} \theta^{\alpha \beta} \theta^{\alpha \beta}
$$

19.93

and

$$
V^\alpha \beta (R_i^\alpha - R_j^\beta) = - \int \left[ B^\alpha (e) \theta^\alpha (k) \theta^{\beta \ast} (k) e^{-\frac{1}{2} (k \cdot \mathbf{r}^\alpha - \mathbf{r}^\beta)} \right] \frac{d^3 k}{(2\pi)^3}
$$

19.94
19.5 EXTERNAL STRESS

To this point we have assumed that there is no traction on the external surface of the solid. We now impose traction. The traction introduces an elastic stress and strain which, given linear elasticity, simply adds to the internal stress and strain of the inclusions. For simplicity we shall assume the external stress is uniform; the generalization to an inhomogeneous external stress is straightforward, but complicates the equations.

19.5.1 The elastic energy

Since the external stress and strain add to whatever internal stress and strain fields are already present, when a traction is imposed on a solid that contains inclusions the increment to the elastic energy is simply the elastic energy of the external stress field; the elastic interaction energy between the external and internal stress fields is zero. This can be shown by computing the increase in elastic energy when the external field is imposed. Let $\sigma$ and $\varepsilon$ be the internal stress and strain in the traction-free system. An external traction introduces the strain, $\varepsilon^e$, and the stress

$$\sigma^e_{ij} = \lambda_{ijkl} \varepsilon^e_{kl}$$

19.95

To find the increment to the elastic energy due to the external stress, let the stress be imposed on a solid that contains a distribution of inclusions. The increase in free energy is due to the elastic work done:

$$\delta F^e = \int_v (\sigma_{ij} + \sigma^e_{ij}) \varepsilon^e_{ij} dV$$

$$= \int_v \int_0^{\varepsilon^e_{ij}} (\sigma_{ij} + \lambda_{ijkl} (\varepsilon^e_{kl} - \varepsilon_{kl})) d\varepsilon^e_{ij} dV = \int_v \int_0^{\varepsilon^e_{ij}} (\sigma_{ij} + \lambda_{ijkl} \varepsilon^e_{kl}) d\varepsilon^e_{ij} dV$$

$$= \int_v \left[ \sigma_{ij} \varepsilon^e_{ij} + \frac{1}{2} \lambda_{ijkl} \varepsilon^e_{ij} \varepsilon^e_{kl} \right] dV = \int_v \left[ \sigma_{ij} \varepsilon^e_{ij} + \frac{1}{2} \sigma^e_{ij} \varepsilon^e_{kl} \right] dV$$

19.96

The first term on the right in 19.96 vanishes, since the internal stress field, $\sigma$, that was present prior to the external load is in equilibrium with no external traction,

$$\int_v \left[ \sigma_{ij} \varepsilon^e_{ij} \right] dV = \int_v \left[ \left\{ \sigma_{ij} u^i_j \right\}_j - \sigma^e_{ij} u^i \right] dV$$

$$= \int_v \sigma_{ij} u^i_j n_j dV = 0$$

19.97
Hence, from 19.96

$$
\delta F^e = \frac{1}{2} \int_V \sigma_{ij}^{e} \varepsilon_{ij}^{e} dV
$$

19.98

which is just the elastic energy of the external stress field.

Eq. 19.98 shows that there is no elastic interaction between external and internal stress fields when the strain is the controlled variable. However, we cannot infer from this result that the external stress field has no effect on the equilibrium of the inclusions. The interaction becomes real and important when the external stress, $\sigma$, is controlled. To see this we need to compute the change in the Gibbs free energy, which controls equilibrium in that case

19.5.2 The Gibbs free energy

To compute the Gibbs free energy associated with the inclusions let them form in a solid that is under a given external stress, imposed by a suitable reservoir. The inclusions strain the solid, and the resulting surface displacement does work on the reservoir. The change in the Gibbs free energy is the total energy change, solid plus reservoir, with the reservoir traction fixed.

The total energy change, system plus reservoir, is

$$
\delta G^e = \delta F^e + \delta W^{rev} = \delta F^e + \int_S \sigma_{ij}^{e} u_{j} n_{i}^{rev} dS
$$

$$
= \delta F^e - \int_S \sigma_{ij}^{e} u_{j} n_{i} dS
$$

$$
= \delta F^e - \int_V \sigma_{ij}^{e} \varepsilon_{ij}^{e} dV
$$

19.99

Where $\delta F^e$ is the increase in the elastic free energy of the solid due the inclusions. The equation on the second line follows because the outward normal to the reservoir at the solid boundary is the negative of the outward normal to the solid, and the closed, external boundary of the reservoir is assumed undisplaced ($u=0$).

As in the previous section we write

$$
\varepsilon_{ij}(R) = \varepsilon_{ij} + \delta u_{i,j}
$$

19.100

where the internal displacement, $\delta u$, vanishes on the boundary. It follows that
\[ \delta G^e = \delta F^e - \int \sigma_{ij}^e (\epsilon_{ij} + \delta u_{ij}) dV \]

\[ = \delta F^e - V \sigma_{ij}^e \epsilon_{ij} - \int_s \sigma_{ij}^e \delta u n_j dS \]

\[ = \delta F^e - V \sigma_{ij}^e \epsilon_{ij} = \delta F^e - \sum_\alpha V^\alpha \sigma_{ij}^{\alpha} \epsilon_{ij}^{\alpha} \]  

Eq. 19.101

The second term in eq. 19.101 gives the interaction between the average strain and the internal stress. Note that the interaction depends only on the average strain, or, equivalently, on the volume fractions of the various inclusions, and is independent of the precise configuration of the inclusions. The inclusion distribution affects the elastic energy, \( \delta F^e \), but not the interaction term. It follows that an external stress does not affect the preferred shape of the inclusion.

However, an external stress will ordinarily have an important influence on the relative populations of inclusion type if more than one type (or crystallographic variant) is possible. Eq. 19.101 shows that inclusions with different transformation strain, \( \epsilon^\phi \), make different contributions to the Gibbs free energy. When the external stress is controlled the evolution of the system is governed by the minimization of the Gibbs free energy. This is accomplished by increasing the volume fraction of those inclusions whose transformation strains are favorably oriented with respect to the external stress, that is, the inclusions for which

\[ \sigma_{ij}^{\alpha} \epsilon_{ij}^{\alpha} \geq 0 \]  

Eq. 19.102

An important example of the influence of an external stress on the inclusion distribution is the effect of an external stress on the relative density of distinct variants of a transformed phase or precipitate phase. As a specific example consider a tetragonal transformation product that forms coherently in a cubic matrix, such as a particle of \( \alpha \) (bct) martensite in a \( \gamma \) (fcc) matrix of steel, or a coherent carbide or nitride precipitate in an \( \alpha \) (bcc) matrix. The transformation strain, \( \epsilon^\phi \), that creates the inclusion has three distinct variants that correspond to the three possible \( <100> \) directions that may be selected for the tetragonal axis of the transformed particle. The three variants have transformation strain tensors that differ in the magnitude of the principle strains along the three \( <100> \) axes, and make different contributions to the Gibbs free energy if the external traction is different on the three \{100\} planes. The relative fractions of the three variants is, hence, changed if the inclusions are formed or allowed to coarsen under an appropriate external load. A similar result follows for any transformation product whose transformation strain has a deviatoric component; the transformed particle has several distinct variants whose relative free energies are changed by the imposition of an appropriate external stress.