

Size-Dependent Eshelby's Tensor for Embedded Nano-Inclusions Incorporating Surface/Interface Energies

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The classical formulation of Eshelby (Proc. Royal Society, A241, p. 376, 1957) for embedded inclusions is revisited and modified by incorporating the previously excluded surface/interface stresses, tension and energies. The latter effects come into prominence at inclusion sizes in the nanometer range. Unlike the classical result, our modified formulation renders the elastic state of an embedded inclusion size-dependent making possible the extension of Eshelby's original formalism to nano-inclusions. We present closed-form expressions of the modified Eshelby's tensor for spherical and cylindrical inclusions. Eshelby's original conjecture that only inclusions of the ellipsoid family admit uniform elastic state under uniform stress-free transformation strains must be modified in the context of coupled surface/interface-bulk elasticity. We reach an interesting conclusion in that only inclusions with a constant curvature admit a uniform elastic state, thus restricting this remarkable property only to spherical and cylindrical inclusions. As an immediate consequence of the derivation of modified size-dependent Eshelby tensor for nano-inclusions, we also formulate the overall size-dependent bulk modulus of a composite containing such inclusions. Further applications are illustrated for size-dependent stress concentrations on voids and opto-electronic properties of embedded quantum dots. [DOI: 10.1115/1.1781177]

1 Introduction

Eshelby's linear elastic solution of an embedded inclusion, [1], has a distinguished place in the history of mechanics, materials science, and solid-state physics. Characterized by its insightful thought experiments, Eshelby's classic solution of the embedded inclusion has been fruitfully used in diverse areas and problems of physical sciences, e.g., localized thermal heating, residual strains, dislocation-induced plastic strains, phase transformations, overall or effective elastic, plastic and viscoplastic properties of composites, damage in heterogeneous materials, quantum dots, microstructural evolution; to name just a few. In this work, we seek to modify the classical elasticity original solution of an embedded inclusion to include surface/interface energies, tension and stresses. In the following we will simply use the word "surface" to signify both the free surface of a void in a material or the interface of a solid inclusion with that of the surrounding host matrix. As has been done tacitly in most elastic problems, the original elastic solution of the embedded inclusion ignored surface energies of the inclusion—for fairly good reasons. Surface energies only enter physics when surface to volume ratio becomes appreciable. For most technological problems (until recently) inclusions were of the order of microns and rarely were one concerned with nano-inclusions or related size effects. At the micron and higher length scales, the surface-to-volume ratios are negligible and indeed Eshelby's original assumptions hold true and so does his solution. In short, in the present work we seek to derive Eshelby's tensor in the context of coupled surface-bulk elasticity

that then can be utilized to capture at least part of the length scale effects likely to be prominent for embedded nano-inclusions.

The literature on Eshelby's tensor and related problems is indeed rich and extensive. While we can hardly do justice in our review of all pertaining work, attempt is made in Section 2 to identify some pertinent literature. To make this article self-contained, a brief description of Eshelby's main conclusions in the classical elasticity context are also reviewed. In Section 3, we formulate the general problem of an embedded inclusion incorporating surface energy and related terms. Some simple closed-form expressions can be obtained for inclusions of constant curvature (i.e., spherical and cylindrical shapes). That is the object of Section 4. The inhomogeneity problem is briefly discussed in Section 5 after which several applications of this work are presented in Section 6 closing finally with summary and conclusions in Section 7.

2 Background

By way of introduction, consider a localized arbitrarily shaped region (Ω) in a material undergoing a stress-free inelastic deformation. Such strains are referred to as either transformation strains, [1], or eigenstrains, [2]. Various physical examples of such strains are thermal expansion, dislocation mediated inelastic strain, swelling strain, magnetomechanical strains, lattice mismatch, and so forth. If the inclusion is removed from the material and allowed to relax (thus enacting the eigenstrain), no stress is generated. However, due to the presence of the matrix or surrounding material, the final relaxed elastic state of the inclusion admits a state of stress. When the material properties of the inclusion and the matrix are the same, the problem of determining the elastic state is often referred to as Eshelby's first problem. The scenario where the inclusion elastic properties are different than those of the matrix is Eshelby's second problem (in which case the inclusion is referred to as an "inhomogeneity"). This nomen-

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closure was introduced by Mura [2]. Eshelby's interior or exterior tensor (\mathbf{S} or \mathbf{D}) relates the eigenstrain ($\boldsymbol{\varepsilon}^*$) to the actual strain ($\boldsymbol{\varepsilon}$) in and out of the inclusion, [1,3,4]:

$$\boldsymbol{\varepsilon}(\mathbf{X}) = \mathbf{S}(\mathbf{X}) : \boldsymbol{\varepsilon}^*(\mathbf{X}) \quad \mathbf{X} \in \Omega \quad (1a)$$

$$\boldsymbol{\varepsilon}(\mathbf{X}) = \mathbf{D}(\mathbf{X}) : \boldsymbol{\varepsilon}^*(\mathbf{X}) \quad \mathbf{X} \notin \Omega \quad (1b)$$

Both boldfaced and index notation will be used as convenient. Eshelby's tensor, in classical elasticity context, depends solely on shape (i.e., aspect ratios) of the inclusions and is thus size-independent. Furthermore, for the family of ellipsoidal shaped inclusions (including spheres, cylinders, spheroids), this tensor is uniform within the interior of the inclusion. The latter fact greatly facilitates, for example, the calculation of effective properties of composites containing ellipsoidal inhomogeneities. For the sake of completeness, some additional details on classical Eshelby's tensor are recorded in Appendix A while an exhaustive account can be found in Refs. [1–4]. For nonuniform eigenstrains the Eshelby tensors are integral operators while for uniform eigenstrains numerical values can be established either analytically or numerically (depending upon the geometrical and material symmetry complications).

Since the original appearance of Eshelby's paper [1] several works have extended, modified and applied the concept of Eshelby's tensor to a diverse set of physical problems. There exist extensive reviews of this subject hence only selected representative papers are cited to establish appropriate context. We will, however, allude to some review articles; the references of which more or less contain an updated account of this topic:

(1) Anisotropy: Several works have modified the classic (originally isotropic) formulation to incorporate anisotropic behavior. Progress has largely been made only in the plane case. An excellent, but somewhat dated, account of these aspects is given in the now classic monograph by Mura [2]. Some more recent works, which also contain extensive list of references on this subject, are: Ru [5] who discusses arbitrary shaped inclusions in anisotropic half and full plane, Li and Dunn [6] address coupled field anisotropic inclusion problems, Pan and Yang [7] who present a semi-analytical method for application to embedded quantum dots and Faux and Pearson [8] who have also applied an anisotropic formulation to quantum dots.

(2) Inclusion shapes: Chiu [9] has considered parallelepiped inclusion. Rodin [10] considers the general polyhedral inclusion. So do Nozaki and Taya [11].

(3) Bonding conditions of inclusion: The original assumption in Eshelby's work is that the inclusion is perfectly bonded to the matrix, i.e., the normal tractions are continuous and so are the displacements. Under certain conditions these conditions must be relaxed (e.g., grain boundary sliding, diffusive sliding, etc.). Various researchers have considered the imperfectly bonded inclusion, e.g., Furuhashi et al. [12], Ru and Schiavone [13], Zhong and Meguid [14], Qu [15,16] and Kouris et al. [17] to name a few.

(4) Coated inclusions: Frequently for technological reasons inclusions are embedded in a matrix with a coating (or which may be developed due chemical interaction with the matrix). A few representative works in this area are: Walpole [18], Luo and Weng [19], Cherkaoui et al. [20], among many others.

(5) Coupled problems: Due to possible applications in sensor and actuator technology, a large body of work has focused on coupled problems, e.g., magnetostrictive inclusions, piezoelectric media, etc. See, for example, the works by Taya [21], Ru [22], Deng and Meguid [23], Mikata [24], Li and Dunn [6], and Pan [25,26].

(6) Nonuniform eigenstrains: Sendekyj [27] and Moschovidis [28] considered general polynomial eigenstrains. Their work is useful for both nonuniform loadings as well as for taking into account interactions between inhomogeneities. Asaro and Barnett [29] and Mura and Kinoshita [30] addressed polynomial eigenstrains in an anisotropic media. Note also must be made of the

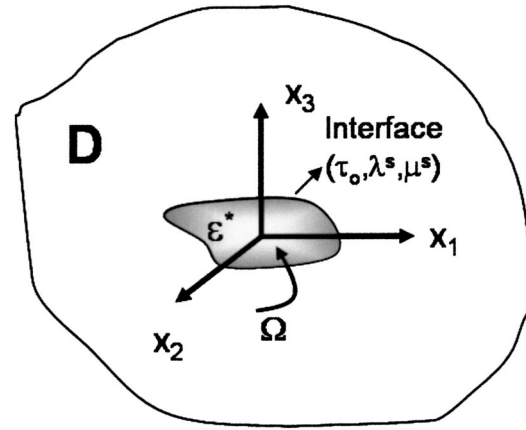


Fig. 1 Schematic of the problem

recent work of Rahman [31] who presents simplified calculations of Eshelby type tensors for polynomial eigenstrains.

(7) Enriched elasticity: the classical theory of elasticity itself has been modified in several ways. Micromorphic elasticity takes into account additional microdegrees-of-freedom such as independent rotations, dilations, and shears. An extensive account of these theories can be found in Eringen [32]. As far as inclusion problem are concerned, it appears that the only two solutions that exist are due to Cheng and He [33,34] who, respectively, solve the spherical and cylindrical inclusion problem. Based on the latter work, Sharma and Dasgupta [35] have formulated the overall properties of micropolar composites.

In addition to the aforementioned group of papers, several other works exist in the context of nonlinear behavior and of course in application areas (such as effective medium theories, phase transformations, stability, among others.). A review of those works is beyond the scope of this paper. The following monographs, review articles, books and references therein are recommended for the interested reader: Mura [2], Nemat-Nasser and Hori [36], and Markov and Preziosi [37], Weng et al. [38], Bilby et al. [39], and Mura et al. [40].

3 The General Size-Dependent Inclusion Problem in Coupled Bulk-Surface Elasticity

Consider, for now, an arbitrary shaped inclusion (Ω) embedded in an infinite amount of material. By definition of an inclusion, we suppose a prescribed stress-free transformation strain within the domain of the inclusion (Fig. 1). Consider the eigenstrain to be uniform. As a departure from the classical solution, we now require that the interface of the inclusion and the matrix be endowed with a deformation-dependent interfacial energy, Γ . The interfacial or surface energy is positive definite. This quantity is distinct from the bulk deformation-dependent energy due to the different coordination number of the surface/interface atoms, different bond lengths, angles, and a different charge distribution, [41]. Within the assumptions of infinitesimal deformations and a continuum field theory, the concept of surface stress and surface tension can be clarified by the following relation between interface/surface stress tensor, $\boldsymbol{\sigma}^s$, and the deformation-dependent surface energy, $\Gamma(\boldsymbol{\varepsilon}^s)$ by

$$\boldsymbol{\sigma}^s = \tau_o \mathbf{I}^2 + \frac{\partial \Gamma}{\partial \boldsymbol{\varepsilon}^s} \quad (2)$$

Where applicable, superscripts B and S indicate bulk and surface, respectively. Here, $\boldsymbol{\varepsilon}^s$ is the 2×2 strain tensor for surfaces or interfaces, \mathbf{I}^2 represents the identity tensor for surfaces while τ_o is

the deformation-independent surface/interfacial tension. It is worth pointing out that the concepts of surface tension, surface stress, and surface energy are often confused and used interchangeably. Only for liquids are all three the same. For solids, they are vastly different and must be carefully distinguished. See, for example, the excellent review article by Ibach [41]. A further source of confusion often is the sign of the surface stress. The latter can be negative but not the surface energy. Conceptual mistakes abound if one equates the surface stress to the surface energy. The determination of the surface tension and the surface elastic constants is often nontrivial and a discussion on this can be found elsewhere, e.g., Ibach [41], Miller and Shenoy [42], and Gurtin and Murdoch [43]. Some brief comments on this are also provided in Appendix C where the properties used in subsequent numerical calculations are listed.

Having introduced the essential concept of surface elasticity, the governing linearized isotropic equations can be written following Gurtin and co-workers, [44,45] who (along with previous works) can be credited for setting the theory of surface elasticity on a rational mechanics footing. The equilibrium and isotropic constitutive equations of bulk elasticity are written as usual:

$$\text{div } \boldsymbol{\sigma}^B = 0 \quad (3a)$$

$$\boldsymbol{\sigma}^B = \lambda \mathbf{I}^3 \text{Tr}(\boldsymbol{\varepsilon}) + 2\mu \boldsymbol{\varepsilon}. \quad (3b)$$

At the interface, the concept of surface or interface elasticity, [43–45], is introduced which is excluded in the classical elasticity formulation:

$$[\boldsymbol{\sigma}^B \cdot \mathbf{n}] + \text{div}_s \boldsymbol{\sigma}^S = 0 \quad (4a)$$

$$\boldsymbol{\sigma}^S = \tau_o \mathbf{I}^2 + 2(\mu^s - \tau_o) \boldsymbol{\varepsilon}^S + (\lambda^s + \tau_o) \text{Tr}(\boldsymbol{\varepsilon}^S) \mathbf{I}^2. \quad (4b)$$

Here, λ and μ are the Lamé constants for the isotropic bulk material. Isotropic interfaces or surfaces can be characterized by surface Lamé constants λ^s , μ^s and surface tension, τ_o . \mathbf{n} is the normal vector on the interface. It is to be noted that only certain strain components appear within the constitutive law for surfaces due to the 2×2 nature of the surface stress tensor (i.e., strains normal to the surface are excluded). Thus, \mathbf{I}^2 represents the 2×2 identity tensor while \mathbf{I}^3 represents the same for bulk 2nd rank tensor. Tr indicates the trace operation. The square brackets in Eq. (4a) indicate the jump of the field quantities across the interface. In absence of surface terms, Eq. (4) reduce to the usual normal traction continuity equations of classical elasticity. “div_s” represent the surface divergence. To define this further and well as the role of surface identity tensor \mathbf{I}^2 (i.e., the 2×2 nature of surface tensors), it would be convenient to first recall certain projection tensors (\mathbf{P}^s) employed by Gurtin et al. [44]:

$$\mathbf{P}^s = \mathbf{I} - \mathbf{n} \otimes \mathbf{n}. \quad (5)$$

Here \mathbf{I} is the three-dimensional identity tensor and we have dropped the superscript “3.” This surface projection tensor maps tensor fields from bulk to surface and vice versa. For example, the surface strain tensor projected into such a tangent space would be written as $\boldsymbol{\varepsilon}^s = \mathbf{P}^s \boldsymbol{\varepsilon} \mathbf{P}^s$. This notion of projection tensor (and related tensor machinery of superficial and tangential tensors) elegantly allows one to mix bulk and surface tensors in the same equations. To clarify the notion of surface divergence, consider a vector \mathbf{v} . The surface gradient and surface divergence, then, take the following form, [44]:

$$\nabla_s \mathbf{v} = \nabla \mathbf{v} \mathbf{P}^s \quad (6)$$

$$\text{div}_s(\mathbf{v}) = \text{Tr}(\nabla_s \mathbf{v}).$$

Noting that the transformation strain is only nonzero within the inclusion domain ($\mathbf{x} \in \Omega$), we can write the bulk-constitutive law for the inclusion-matrix as follows:

$$\boldsymbol{\sigma}^B = \mathbf{C} : \{ \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^* H(z(\mathbf{x})) \}. \quad (7)$$

Here “ H ” is the Heaviside function and \mathbf{C} is the classic fourth-order stiffness tensor. We define $z(\mathbf{x})$ to be of the form

$$\begin{aligned} \{z(\mathbf{x}) > 0 | \mathbf{x} \in \Omega\} \\ \{z(\mathbf{x}) < 0 | \mathbf{x} \notin \Omega\}. \end{aligned} \quad (8)$$

Taking the divergence of Eq. (7) we obtain

$$\nabla \cdot \boldsymbol{\sigma}^B = \nabla \cdot (\mathbf{C} : \boldsymbol{\varepsilon}) - \nabla \cdot \{ \mathbf{C} : \boldsymbol{\varepsilon}^* H(z(\mathbf{x})) \} - \underbrace{[\boldsymbol{\sigma}^B \cdot \mathbf{n}]}_{\delta(\bar{z}(\mathbf{x}))} = \mathbf{0}. \quad (9)$$

It can be readily seen that the eigenstrain and the underlined term appear as a body force. Note that in classical elasticity the last underlined expression in Eq. (9), i.e., $[\boldsymbol{\sigma}^B \cdot \mathbf{n}]$ is typically omitted since the jump in the normal tractions is zero. $\delta(\cdot)$ is the Dirac delta function while $\bar{z}(\mathbf{x}) = 0$ defines the interface. However, taking cognizance of Eq. (4a), i.e., coupling interface elasticity with bulk elasticity, we must rewrite Equation (9) as

$$\nabla \cdot \boldsymbol{\sigma}^B = \nabla \cdot (\mathbf{C} : \boldsymbol{\varepsilon}) - \nabla \cdot \{ \mathbf{C} : \boldsymbol{\varepsilon}^* H(z(\mathbf{x})) \} + \underbrace{\delta(\bar{z}(\mathbf{x})) \text{div}_s \boldsymbol{\sigma}^S}_{\mathbf{0}} = \mathbf{0}. \quad (10)$$

Using the underlined term as representing a body force in conjunction with the elastic Green’s function, we can write the displacement field due to both the eigenstrain and the surface effect as

$$\begin{aligned} \mathbf{u} = & - \int_V \mathbf{G}^T(\mathbf{y} - \mathbf{x}) \cdot (\nabla \cdot \{ \mathbf{C} : \boldsymbol{\varepsilon}^* H(\mathbf{y}) \}) dV_y \\ & + \underbrace{\int_S \mathbf{G}^T(\mathbf{y} - \mathbf{x}) \cdot \text{div}_s \boldsymbol{\sigma}^S(\mathbf{y}) dS_y}_{\mathbf{0}} \end{aligned} \quad (11)$$

A more rigorous treatment of the interface conditions in Eq. (9)–(11) is provided in Appendix A. Here \mathbf{G} is the Green’s tensor for isotropic classical elasticity (Appendix B). The underlined term indicates the extra surface terms that we have incorporated in the present work. The first integral in Eq. (11) is simply the classical part. As customary, [1,36], we make use of Gauss theorem to cast Eq. (11) in a more attractive form:

$$\mathbf{u} = \int_V (\mathbf{C} : \boldsymbol{\varepsilon}^*) : (\nabla_x \otimes \mathbf{G}^T(\mathbf{y} - \mathbf{x})) dV_y + \underbrace{\int_S \mathbf{G}^T(\mathbf{y} - \mathbf{x}) \cdot \text{div}_s \boldsymbol{\sigma}^S(\mathbf{y}) dS_y}_{\mathbf{0}} \quad (12)$$

Here we have also used the rule that, $\nabla_x \mathbf{G}(\mathbf{y} - \mathbf{x}) = -\nabla_y \mathbf{G}(\mathbf{y} - \mathbf{x})$. Invoking the linearized strain-displacement law: $\boldsymbol{\varepsilon} = \text{sym}\{\nabla \otimes \mathbf{u}\}$, we can then write

$$\boldsymbol{\varepsilon} = \mathbf{S} : \boldsymbol{\varepsilon}^* + \text{sym} \left\{ \nabla_x \otimes \underbrace{\int_S \mathbf{G}^T(\mathbf{y} - \mathbf{x}) \cdot \text{div}_s \boldsymbol{\sigma}^S(\mathbf{y}) dS_y}_{\mathbf{0}} \right\}. \quad (13)$$

Here we have invoked the definition of the classical size-independent Eshelby tensor, [1,2], based on which the first (non-underlined) integral in Eq. (12) reduces to the classical expression in Eq. (1). The notation, $\text{sym}\{\cdot\}$, represents the symmetric part of a second-order tensor, \mathbf{A} , e.g.,

$$\text{sym}\{\mathbf{A}\} = \frac{1}{2} \{ \mathbf{A} + \mathbf{A}^T \}.$$

Further simplification does not appear feasible without additional assumptions regarding inclusion shape. Note now that Eq. (13) implicitly gives the modified Eshelby’s tensor for inclusions incorporating surface energies. This relation is implicit since the

surface stress depends on the surface strain, which in turn is the projection of the conventional strain ($\boldsymbol{\varepsilon}$) on the tangent plane of the inclusion-matrix interface. In the next section, using Eq. (13) we will derive explicit expressions for cylindrical and spherical inclusions. For now, however, it is worth noting some general features of the new Eshelby tensor.

In terms of the surface projection tensor the surface divergence of the surface stress tensor can be written as

$$\text{div}_s \boldsymbol{\sigma}^s = \text{div}_s \{ \mathbf{C}^s \mathbf{P}^s \boldsymbol{\varepsilon} \mathbf{P}^s + \tau_o \mathbf{P}^s \}. \quad (14)$$

The surface divergence of surface stress tensor can only be uniform if the classical "bulk" strain as well as the projection tensor is uniform over the inclusion surface. Consider that, [44]:

$$\text{div}_s \mathbf{P}^s = 2\kappa \mathbf{n}. \quad (15)$$

Here κ is the mean curvature of the inclusion. For a general ellipsoid the curvature is nonuniform and varies depending upon the location at the surface. Only for the special cases of spherical and cylindrical shape is the mean curvature uniform hence leading us to conclude the following:

PROPOSITION: *Eshelby's original conjecture that only inclusions of the ellipsoid family admit uniform elastic state under uniform eigenstrains must be modified in the context of coupled surface/interface-bulk elasticity. Only inclusions that are of a constant curvature admit a uniform elastic state, thus restricting this remarkable property to spherical and cylindrical inclusions.*

4 Inclusions With Constant Curvature (Spheres and Cylinders)

Spherical and cylindrical inclusions are endowed with a constant curvature and thus according to the previous section must admit a uniform elastic state in coupled bulk-surface elasticity. The new Eshelby's tensor will, of course, be size-dependent because of the presence of curvature terms.

Due to the constant curvature, Eq. (13) can be simplified considerably. The surface divergence of the surface stress can be simply taken out of the differential and integral operators. The surface integral is converted into a volume integral and we can then write:

$$\boldsymbol{\varepsilon} = \mathbf{S} : \boldsymbol{\varepsilon}^* - \mathbf{C}^{-1} : \left(\text{sym} \left\{ \nabla_x \otimes \mathbf{C} : \underbrace{\int_V \nabla_x \otimes \mathbf{G}(\mathbf{y} - \mathbf{x}) dV_y}_{\text{}} \right\} \right) : 2\kappa^s \mathbf{I} \quad (16)$$

where scalar "s" is defined from the relation:

$$\begin{aligned} \boldsymbol{\sigma}^s &= s \mathbf{P}^s \\ \Rightarrow s &= \tau_o + (\lambda^s + \mu^s) \text{Tr}(\mathbf{P}^s \boldsymbol{\varepsilon} \mathbf{P}^s) \end{aligned} \quad (17)$$

In the underlined integral term we have multiplied and divided by the elastic stiffness tensor to conveniently cast the term enclosed in the curly brackets in terms of the classical Eshelby tensor. Additionally we have used the surface constitutive law (Eq. 4(b)). We can rewrite Eq. (16) in the following simpler form:

$$\boldsymbol{\varepsilon} = \mathbf{S} : \boldsymbol{\varepsilon}^* - (2\kappa s) \mathbf{C}^{-1} : (\mathbf{S} : \mathbf{I}). \quad (18)$$

Equation (18) can be made more explicit by noting that an isotropic fourth tensor, \mathbf{A} , displaying the symmetries characteristic of the elastic stiffness tensor can be written in terms of two scalars a_1 and a_2 as: $A_{ijkl} = a_1 \delta_{ij} \delta_{kl} + a_2 (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})$. It is then straightforward to show that, $\mathbf{A} : \mathbf{I} = (3a_1 + 2a_2) \mathbf{I}$ which, after substituting $\mathbf{C}^{-1} : \mathbf{I} = (1/3K) \mathbf{I}$ in Eq. (18) directly leads to the following for spherical inclusions:

$$\boldsymbol{\varepsilon} = \mathbf{S} : \boldsymbol{\varepsilon}^* - \frac{K^s}{3KR_o} (\mathbf{S} : \mathbf{I}) \text{Tr}(\mathbf{P}^s \boldsymbol{\varepsilon} \mathbf{P}^s) - \frac{2\tau_o}{3KR_o} (\mathbf{S} : \mathbf{I}). \quad (19)$$

Here we have used the fact that $\kappa = 1/R_o$ for spheres where R_o is the radius. K^s is defined by us to be the surface elastic modulus and is given as $2(\lambda^s + \mu^s)$ while K is the usual hydrostatic modulus, $\lambda + 2\mu/3$.

For an infinite circular cylindrical inclusion, in addition to the plane-strain conditions we have κ as $1/2R_o$ hence

$$\boldsymbol{\varepsilon} = \mathbf{S} : \boldsymbol{\varepsilon}^* - \frac{K'^s}{3K'R_o} (\mathbf{S} : \mathbf{I}) \text{Tr}(\mathbf{P}^s \boldsymbol{\varepsilon} \mathbf{P}^s) - \frac{\tau_o}{3K'R_o} (\mathbf{S} : \mathbf{I}). \quad (20)$$

Here K'^s is the plane-strain surface modulus, $\lambda^s + 2\mu^s$ while K' is $2(\lambda + \mu)/3$. Note that for the interior solution, Eshelby's interior tensor (\mathbf{S}) must be used while for exterior solution the corresponding exterior version (\mathbf{D}) is required.

Substituting the well-known components of the classical Eshelby tensors for both spherical and cylindrical shapes, [2], we obtain the following simple expressions for spherical and cylindrical inclusions subjected to a dilatational eigenstrain, $\boldsymbol{\varepsilon}_{11}^* = \boldsymbol{\varepsilon}_{22}^* = \boldsymbol{\varepsilon}_{33}^* = \boldsymbol{\varepsilon}^*$.

Spherical inclusion (in spherical polar coordinates):

$$\varepsilon_{rr}(r) = \varepsilon_{\theta\theta}(r) = \varepsilon_{\phi\phi}(r) = \frac{3K^M \boldsymbol{\varepsilon}^* - 2\tau_o/R_o}{4\mu^M + 3K^M + 2K^s/R_o} \Big|_{r < R_o} \quad (21a)$$

$$\varepsilon_{rr}(r) = \left[\frac{3K^M \boldsymbol{\varepsilon}^* - 2\tau_o/R_o}{4\mu^M + 3K^M + 2K^s/R_o} \right] \frac{R_o^3}{r^3} \Big|_{r > R_o} \quad (21b)$$

$$\varepsilon_{\theta\theta}(r) = \varepsilon_{\phi\phi}(r) = - \left[\frac{3K^M \boldsymbol{\varepsilon}^* - 2\tau_o/R_o}{4\mu^M + 3K^M + 2K^s/R_o} \right] \frac{2R_o^3}{r^3} \Big|_{r > R_o}. \quad (21c)$$

Cylindrical inclusion (in cylindrical polar coordinates):

$$\varepsilon_{rr}(r) = \varepsilon_{\theta\theta}(r) = \frac{3K'^M \boldsymbol{\varepsilon}^* - \tau_o/R_o}{2\mu^M + 3K'^M + K'^s/R_o} \Big|_{r < R_o} \quad (22a)$$

$$\varepsilon_{rr}(r) = \left[\frac{3K'^M \boldsymbol{\varepsilon}^* - \tau_o/R_o}{2\mu^M + 3K'^M + K'^s/R_o} \right] \frac{R_o^2}{r^2} \Big|_{r > R_o} \quad (22b)$$

$$\varepsilon_{\theta\theta}(r) = - \left[\frac{3K'^M \boldsymbol{\varepsilon}^* - \tau_o/R_o}{2\mu^M + 3K'^M + K'^s/R_o} \right] \frac{R_o^2}{r^2} \Big|_{r > R_o} \quad (22c)$$

$$\varepsilon_{zz}(r) = 0. \quad (22d)$$

Wherever applicable, superscripts H and M will be used to represent inhomogeneity and matrix properties, respectively. The expressions (21)–(22) are exceptionally simple but clearly illustrate that elastic state is now size-dependent. The surface/interface tension is a residual strain-type term which, for example, should not impact the effective properties of composite. The effect of surface elasticity appears through K^s which (as shall be seen in Section 6(b)), leads to a size-dependent change in overall hydrostatic properties of a composite. By making the radius of the inclusion large we can trivially retrieve the known classical solution. Interestingly, although their treatment of a spherical precipitate was much more specialized, we can make contact with the results of Cahn and Larche [46]. Using an assumed displacement type method they (only taking into account surface tension) presented exactly the expression in Eq. (21a) with the surface elasticity effect (K^s) set to zero.

5 A Note on the Eshelby's 2nd Problem (Inhomogeneity)

Since the classical result for the strain within the inclusion is uniform for ellipsoids, Eshelby [1] was able to devise an elegant method to mimic an inhomogeneity by an inclusion containing a fictitious eigenstrain. The so-called equivalent inclusion method

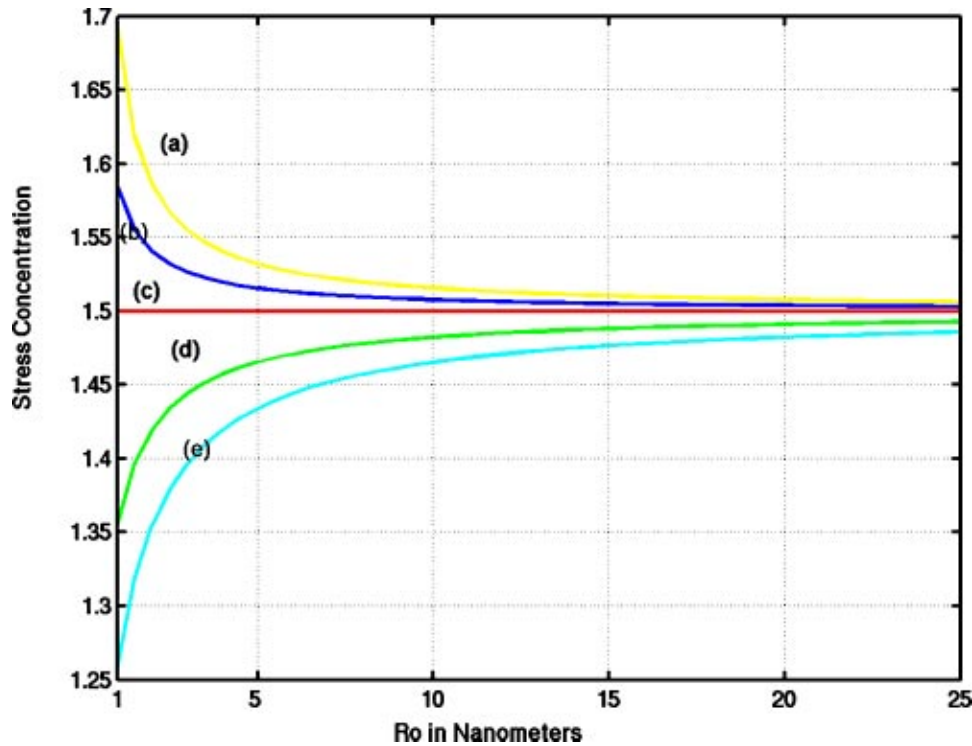


Fig. 2 Stress concentration as a function of surface properties and void radius. (a) Solution with surface modulus= $2K^s$, Al [1 0 0]. (b) Solution with surface modulus=nominal K^s for Al [1 0 0]. (c) Classical solution without surface effects, i.e., $K^s=0$. (d) Solution with surface modulus= $2K^s$ Al [1 1 1]. (e) Solution with surface modulus=nominal K^s , Al [1 1 1].

simply entails equating the elastic state of an inhomogeneity to that of an inclusion albeit with the aforementioned fictitious eigenstrain, i.e.,

$$\mathbf{C}^M : \{\boldsymbol{\varepsilon}^\infty + \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^*\} = \mathbf{C}^H : \{\boldsymbol{\varepsilon}^\infty + \boldsymbol{\varepsilon}\} \quad (23a)$$

$$\boldsymbol{\varepsilon} = \mathbf{S} : \boldsymbol{\varepsilon}^* \quad (23b)$$

$\boldsymbol{\varepsilon}^\infty$ is the externally applied strain. Since for spherical and cylindrical shapes the modified Eshelby's tensor with surface effects is also uniform, the equivalent inclusion method embodied in Eqs. 23(a,b) can be easily applied to study the size-dependent elastic state of inhomogeneities. Unlike the classical case, this fortuity, as was seen in Section 3, does not extend to ellipsoids. As an example, for a cylindrical inhomogeneity free of any external loading but containing a dilatational eigenstrain, the interior radial stress can be reduced to

$$\sigma_{rr} = 2(\mu^H + \lambda^H) \frac{-2\mu^M \boldsymbol{\varepsilon}^* - K'^s \boldsymbol{\varepsilon}^* / R_o - \tau_o / R_o}{2(\mu^M + \mu^H + \lambda^H) + K'^s / R_o} \quad (24)$$

6 Applications

The incorporation of surface size effects in the inclusion problem automatically reopens all the existing application areas of Eshelby tensor now extendable to the nanoscale. In the present paper we discuss three application areas: the first two are academic although classic in mechanics while the third is, currently, of immense technological importance.

(a) Size-Dependent Stress Concentration at a Spherical Void. Consider a spherical void under an applied hydrostatic tension. Based upon the preceding expressions (using Eshelby's exterior tensor and equivalent inclusion method), the stress concentration can then be derived to be

$$S.C. = \left. \frac{\sigma_{\theta\theta}}{\sigma_\infty} \right|_{r=R_o} = 1 + \frac{1}{2} \left(\frac{1 - 2K^s/3K^M R_o}{1 + K^s/2\mu^M R_o} \right) \quad (25)$$

In this section we have set $\tau_o=0$, to study the effect of surface elastic constant, K^s . Results can then also be presented independent of loading conditions since the surface tension is a residual stress type of effect. Note that Eq. (25) trivially gives 1.5 as the stress concentration for the classical elasticity case when either surface modulus is small or void radius is relatively large (typically > 25 nm). The numerical results are presented for Aluminum using free-surface properties computed by previous researchers ([42]—using molecular dynamics simulations). The surface properties are highly dependent upon crystallographic direction while ours is an isotropic formulation. The object of this section, however, is to simply use some realistic values to illustrate the physical effect. The stress concentration of the spherical cavity under hydrostatic tension is plotted as a function of the cavity radius R_o in Fig. 2 for two different set of surface properties (corresponding to [1 0 0] Al and [1 1 1] Al). To investigate a broader range of surface properties, curves of surface modulus twice that of Al [1 0 0] and Al [1 1 1] are also shown. The parameters as obtained from manipulation of data from Miller and Shenoy [42] are: [1 0 0], $\lambda^s = 3.48912$ N/m, $\mu^s = -6.2178$ N/m $\Rightarrow K^s = -5.457$ N/m, while for [1 1 1], they are: $\lambda^s = 6.842$ N/m, $\mu^s = -0.3755$ N/m $\Rightarrow K^s = 12.932$ N/m. As depicted in Fig. 2, surface effects cause the stress concentration to reduce (increase) with decreasing pore size when $K^s > 0$ ($K^s < 0$). The classical case (without surface effects) corresponds to $K^s = 0$ and is, as expected, independent of pore size. Below a critical void radius the void will sinter. This effect is closely related to the residual surface tension and is not investigated here.

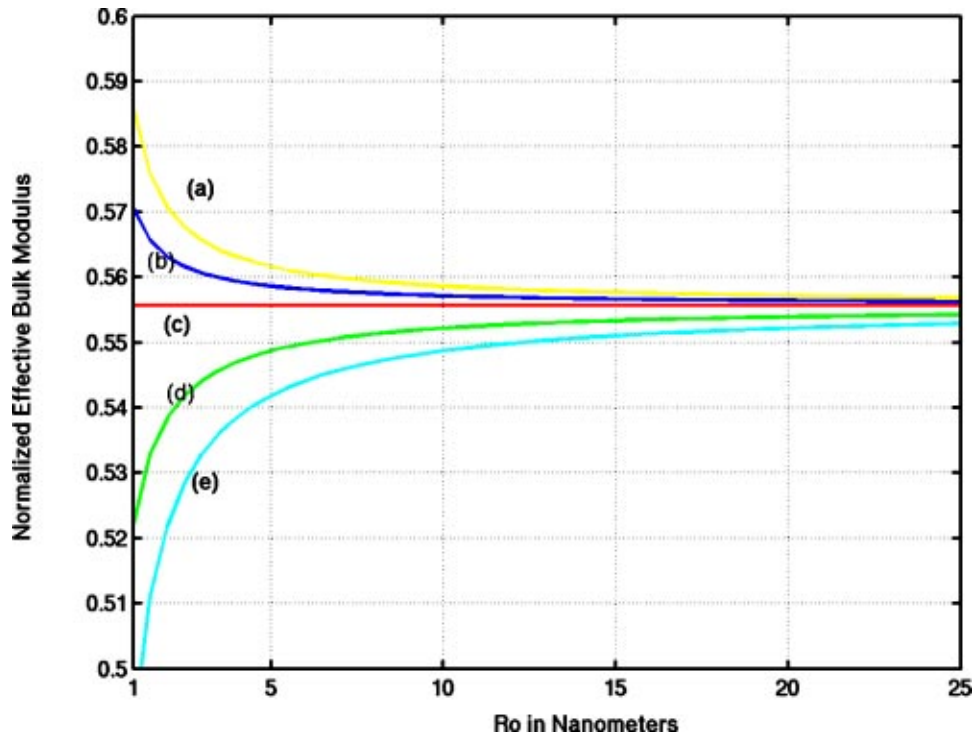


Fig. 3 Size-dependent effective hydrostatic modulus with surface effects versus void radius normalized with the matrix bulk modulus: (a) solution with surface modulus= $2K^s$, Al [1 0 0]; (b) solution with surface modulus=nominal K^s for Al [1 0 0]; (c) classical solution without surface effects, i.e., $K^s=0$; (d) solution with surface modulus= $2K^s$ Al [1 1 1]; (e) solution with surface modulus=nominal K^s , Al [1 1 1]

(b) Size-Dependent Overall Properties of Composites

One of the applications of this work is that surface effects can now be easily included in the determination of effective elastic properties of a composite. Here, as an example, a nanocomposite of Aluminum populated with a finite volume fraction of spherical voids is considered. Let the volume fraction of the inhomogeneities be denoted by “ c .” To take into account interactions between various inhomogeneities, we embed the single inhomogeneity (void) in a concentric spherical volume of matrix material with finite radius “ $R_M > R_o$.” Then, “ c ” is simply R_o^3/R_M^3 . This is nothing but the classical spherical assemblage system, [36]. Using the interior and exterior Eshelby’s tensor we can compute the displacement fields to be

$$u = \begin{cases} Pr, & 0 \leq r \leq R_o \\ Q + \frac{T}{r^2}, & R_o \leq r \leq R_M \end{cases} \quad (26)$$

$$Q = \frac{\sigma^\infty(4\mu^M + 3K^H)}{3K^M(4\mu^M + 3K^H) - 4c\mu^M[3\Delta K + 2K^s/R_o]}$$

$$\Delta K = K^M - K^H, \quad T = \frac{3\Delta KR_o^3}{4\mu^M + 3K^H} Q, \quad P = Q + T/R_o^3.$$

Here we have used the kinematical relations ($\varepsilon_{rr} = \partial u / \partial r$; $\varepsilon_{\theta\theta} = \varepsilon_{\phi\phi} = u/r$). The overall applied stress is related to the total average strain via the effective bulk modulus as

$$\sigma^\infty = K^{\text{eff}} \langle \varepsilon \rangle. \quad (27)$$

As is well known, [36], the average strain can be completely determined through the surface integral of the displacement on the boundary of sphere R_M , i.e.,

$$\langle \varepsilon \rangle = \frac{1}{V} \int_{S_M} u \mathbf{n} \otimes \mathbf{n} dS. \quad (28)$$

Here, \mathbf{n} is the normal vector on the outer surface. The average strain field is obtained as

$$\langle \varepsilon \rangle = 3 \left(Q + \frac{3K^M}{4\mu^M} Q - \frac{1}{4\mu^M} \right) \sigma^\infty \quad (29)$$

from which the effective hydrostatic modulus is deduced to be

$$K^{\text{eff}} = \frac{1}{3 \left(Q + \frac{3K^M}{4\mu^M} Q - \frac{1}{4\mu^M} \right)}. \quad (30)$$

The overall hydrostatic modulus of the composite is size and surface-property-dependent (via “ Q ” which in turn depends on “ K^s ” weighted by the inhomogeneity curvature). The size effect is illustrated in Fig. 3, where the normalized effective hydrostatic modulus is plotted against the void radius for a constant volume fraction of $c=0.5$. The effective hydrostatic modulus with surface effects, shown in Fig. 3, is normalized by the hydrostatic modulus of the matrix material without voids. As can be observed, at small length scales, the size of inhomogeneities (at constant volume fraction) can cause a change in the macroscopic behavior of a composite. Asymptotically, as the inhomogeneity (void) size is increased, the surface effects begin to diminish and the normalized modulus approaches the classical solution.

(c) Size-Dependent Strain and Emission Wavelength in Quantum Dots. Quantum dots (QDs) have recently been the focus of several experimental and theoretical researchers due to the promise of improved and new opto-electronic properties, [47]. QDs are typically embedded in another semiconductor material

with differing elastic constants and lattice parameter. The ensuing elastic relaxation within the QD is well known to impact their opto-electronic properties. Several works, of varying sophistication (both analytical and numerical), have focused on the calculation of the strain state in buried quantum dots and the subsequent impact on opto-electronic properties (see, for example, the following works appearing in the mechanics literature: [48,49]). It would be of interest to see how much error (in strain and electronic

properties) is incurred when surface effects are neglected considering that quantum dots are often “fabricated” in the sub 10-nm regime. An electronic property of interest in quantum dots is its bandgap, which in turn affects its emission wavelength. Using a simple effective mass theory, the deformation potential theory, [50], and the size effects from the present work, the shift in quantum dot emission wavelength due to surface effects can be written as

$$\Delta\lambda = \frac{hc(a_c + a_v)[\varepsilon^{cl} - \varepsilon^s(R_o)]}{\left(E_g^\infty + \frac{h^2(m_e^*m_{lh}^*)}{8\pi^2R_o^2(m_e^* + m_{lh}^*)} + (a_c + a_v)\varepsilon^s(R_o)\right) \left(E_g^\infty + \frac{h^2(m_e^*m_{lh}^*)}{8\pi^2R_o^2(m_e^* + m_{lh}^*)} + (a_c + a_v)\varepsilon^{cl}\right)}. \quad (31)$$

Here, h is Planck’s constant while m^* is the effective mass of the carriers (“ e ” is electron and “ lh ” is light hole). E_g^∞ is the bulk band gap of the material while $(a_c + a_v)$ represents the dilatational deformation potential. ε^{cl} is the classical strain and $\varepsilon^s(R_o)$ is the size-dependent strain from the present work that includes surface effects. Note that for the purposes of band structure calculations, the eigenstrain must be subtracted from the compatible strain. The second term on the denominator of Eq. (31) is the usual quantum confinement effect, [51]. As an example, we have used an In_{32}GaN quantum dot system embedded in a GaN matrix. The error in wavelength calculation is shown in Fig. 4. Numerical constants are listed in Appendix C. We have used a simple first-order approximation (Eq. (31)) to capture the wavelength shift and while a more sophisticated treatment is possible (following, say, Ref. [49]) the present expression in Eq. (31) suffices to provide a measure of the severity of surface effects on the opto-electronic properties.

As patent from Fig. 4 the error in wavelength calculation by neglecting the surface size effect is appreciable in certain size ranges. For large QD size, as expected, the classical and the new results are indistinguishable. For very small QD sizes, while surface effects are appreciable so are the quantum confinement effects (which scale as $1/R^2$) and hence dominate. In the “mid-regime” (still at the nanoscale), surface effects have the most impact. To be specific, in this particular material system, a maximum wavelength shift of ~ 40 nm (for a diameter of ~ 3 nm) is observed which is large enough to cause a shift of colors and indeed exceeds the strict optoelectronic design tolerances.

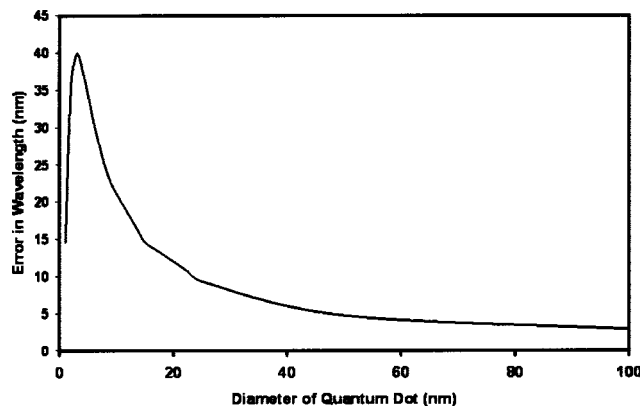


Fig. 4 Size-dependent wavelength shift due to surface elastic effects

7 Summary and Conclusions

To summarize, we have modified Eshelby’s classical approach towards inclusions and inhomogeneities to incorporate the effect of surface energies via the continuum field formulation of surface elasticity. As a consequence, the elastic state of inclusions is rendered size-dependent making possible the establishment of scaling laws that are valid at the nanoscale. Eshelby’s original conjecture that only inclusions of the ellipsoid family admit uniform elastic state under uniform eigenstrains must be modified in the context of coupled surface/interface-bulk elasticity. Only inclusions that are of a constant curvature admit a uniform elastic state, thus restricting this remarkable property only to spherical and cylindrical inclusions. The modified size-dependent Eshelby tensor for the spherical and circular cylindrical shape is explicitly calculated in the present work.

Apart from the formal contribution, by way of illustration, the size-dependent stress concentration on a spherical void was demonstrated. Taking advantage of the fact that the modified Eshelby tensor is uniform for the spherical shape, we are also able to derive the exact size-dependent hydrostatic modulus of a heterogeneous solid. Perhaps the most technologically important application of the present work lies in arena of quantum dots and wires. While physicists routinely take into account the impact of strain on band structure and opto-electronic properties, the strain calculations are typically based upon classical elasticity and are size-independent. In the present work, a first-order calculation clearly shows that large errors in both the band structure and the emitted wavelength can be incurred if the surface size effects are neglected.

There are several limitations of the present work and a few are worth mentioning. They point naturally to future extensions:

(1) Isotropic behavior was assumed throughout. This is a rather dubious assumption when one is concerned with surfaces and interfaces. Unfortunately, matters are unlikely to be analytically tractable once the assumption of isotropy is abandoned. Numerical formulation of the coupled-surface bulk elasticity may be necessary to remove this restriction.

(2) Analytical formulas were restricted to the spherical and cylindrical shape. This limits our ability to study the effect of shape on the size-dependent elastic state of nano-inclusions. Derivation of the modified Eshelby tensor for the general ellipsoid (which surely must proceed numerically) would be a useful extension of the present work.

(3) It would be also of interest to see the behavior of nonsmooth inclusion shapes, e.g., parallelepipeds. Polyhedral inclusions with vertices essentially possess zero curvature everywhere except at the corners where singularities exist.

(4) Slip, twist, and wrinkling of surfaces/interfaces were ignored. One can expect some interesting physics to emerge from inclusion of such effects. Slip and twist of elastic interfaces were

recently included by Gurtin et al. [44] to supplement the original formulation, [45]. These notions are closely linked to the concept of coherency-incoherency and their discussion in relation to Eshelby's problems is relegated to a future work.

Acknowledgments

The present work greatly benefited from the comments by an anonymous reviewer. In particular, the rigorous treatment of Eqs. (9) and (16) and the note in Appendix A is a direct consequence of reviewer's suggestion.

Appendix A

Interfacial Conditions in Equations (9)–(11). The form of the underlined term in Eq. (9), i.e., the jump in traction across the inclusion-matrix interface, can be justified by considering the stress balance law in the following form:

$$\text{div } \boldsymbol{\sigma} = \int_S f(\mathbf{y}) \delta(\mathbf{x} - \mathbf{y}) dS_y = \mathbf{0} \quad (32)$$

Equation (32) defines a stress field perturbed by a force spread over the interface. An arbitrary trial function $\mathbf{w}(\mathbf{x})$ is introduced. Upon multiplication of this trial function with Eq. (32), integration over the volume and subsequent use of Gauss theorem yields

$$\int_S \{[\boldsymbol{\sigma}(\mathbf{x})] \cdot \mathbf{n}\} \cdot \mathbf{w}(\mathbf{x}) dS_x - \int_V \{\text{div } \boldsymbol{\sigma}(\mathbf{x})\} \cdot \mathbf{w}(\mathbf{x}) dS_x + \int_S \mathbf{f}(\mathbf{y}) \cdot \mathbf{w}(\mathbf{y}) dS_y = 0. \quad (33)$$

Since, $\mathbf{w}(\mathbf{x})$ is completely arbitrary, Eq. (33) implies (a) the usual balance law within the bulk of the continuum, $\text{div } \boldsymbol{\sigma} = \mathbf{0}$ and (b) the identification of the interface force with the jump in the normal tractions, i.e., $\mathbf{f} = -[\boldsymbol{\sigma}] \cdot \mathbf{n}$.

Table 1 Numerical values used in Fig. 4

Property	Value
E_g^∞ (eV)	1.94 [52]
m_e^*	0.18 [53]*
m_{ih}^*	0.8 [54]*
$a_c + a_v$ (eV)	8.3 Chin et al. [55]*
μ^M (Gpa)	67
K^M (Gpa)	102
K^H (Gpa)	168
μ^H (Gpa)	95
K^s (J/m ²)	161.73 [♠]
τ_o (J/m ²)	1.33 [♠]

*Linearly interpolated between InN and GaN using proportion of In concentration.

[♠]Estimated approximately using Gurtin and Murdoch's [43,45] analogy to membrane theory of Tiersten [56]. A transition from bulk constants to interface/surface properties can be made by the following transformation: $\{\mu^s, \lambda^s\} \rightarrow \{\mu^h, 2\lambda\mu^h/(\lambda + \mu)\}$. Here, h is the thickness over which surface/interface elasticity behavior differs from the bulk. Our molecular dynamics simulations indicate that such behavior is typically confined to about 1–2 lattice spacing. For the interface, we have assumed this value to be 5 Angstroms.

[♠]Interfacial tension for this material combination is not known. Conventional EAM potentials are not useful for Nitride structures (especially for surface property evaluation). Generally, however, it is well known that depending upon the degree of coherency the interfacial tension varies from 0.7 J/m² to 2 J/m². Our estimation proceeded as follows. For an indium concentration of zero, the interfacial tension is also zero while it should be the maximum for 100% In (which is completely incoherent with respect to GaN). Assuming tentatively a maximum interfacial tension of 2 J/m² for 100% In, we obtain 1.33 J/m² by simple proportion for the current composition of 32%.

Appendix B

Green's Function for Elasticity and Eshelby's Classical Tensor. The Green's function for elasticity $\mathbf{G}(\mathbf{y} - \mathbf{x})$ is the fundamental solution to the Kelvin's solution of a point load in an infinite solid. It is given by (for isotropic materials)

$$\mathbf{G}(\mathbf{y} - \mathbf{x}) = \frac{1}{16\pi\mu(1-\nu)|y-x|} \left\{ (3-4\nu)\boldsymbol{\delta} + \frac{(\mathbf{y}-\mathbf{x}) \otimes (\mathbf{y}-\mathbf{x})}{|y-x|^2} \right\}. \quad (34)$$

Substituting this expression in the first integral of Eq. (12) yields, [2]:

$$\varepsilon_{ij}(x) = \frac{1}{8\pi(1-\nu)} [\Psi_{kl,klj} - 2\nu\Phi_{kk,ij} - 2(1-\nu)(\Phi_{ik,kj} + \Phi_{jk,ki})] \quad (35)$$

where ψ and Φ are biharmonic and harmonic potentials of the inclusion shape (Ω). They are given as

$$\Psi_{ij}(\mathbf{x}) = \int_{\Omega} |\mathbf{x} - \mathbf{y}| \varepsilon_{ij}^*(\mathbf{y}) d^3\mathbf{y} \quad (36)$$

$$\Phi_{ij}(\mathbf{x}) = \int_{\Omega} \frac{1}{|\mathbf{x} - \mathbf{y}|} \varepsilon_{ij}^*(\mathbf{y}) d^3\mathbf{y} \quad (37)$$

Equation (35) can then be cast into the more familiar expression of Eq. (1a,b)

$$\begin{aligned} \boldsymbol{\varepsilon}(\mathbf{x}) &= \mathbf{S}(\mathbf{x}) : \boldsymbol{\varepsilon}^* \quad \mathbf{x} \in \Omega \\ \boldsymbol{\varepsilon}(\mathbf{x}) &= \mathbf{D}(\mathbf{x}) : \boldsymbol{\varepsilon}^* \quad \mathbf{x} \notin \Omega. \end{aligned} \quad (38)$$

Mura's book [2] contains detailed listing of \mathbf{S} and \mathbf{D} tensor for various inclusion shapes (spheres, cylinders, ellipsoids, and cuboids).

Appendix C

Numerical Constants for Wavelength Shift Calculation

The numerical values used in the calculation of Fig. 4 are listed in Table 1.

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