SIZE-DEPENDENT ELASTIC STATE OF EMBEDDED NANO-INCLUSIONS & QUANTUM DOTS

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Summary The classical formulation of Eshelby for embedded inclusions is revisited and modified to at least partially account for size-effects likely to be prominent at the nanoscale. Unlike the classical results, our modified formulations render the elastic state of an embedded inclusion size-dependent. Among others, applications to quantum dots are presented.

INTRODUCTION

The classical formulation of Eshelby [1] for embedded inclusions is revisited and modified to account for size-effects likely to be prominent at the nanoscale. In this two-pronged work, we firstly incorporate the previously excluded surface/interface stresses, tension and energies. The latter effects come into prominence at inclusion sizes in the nanometer range where surface-to-volume ratios are appreciable. Unlike the classical results, our modified formulations incorporating surface energies render the elastic state of an embedded inclusion size-dependent making possible the extension of Eshelby's original formalism to nano-inclusions.

Presuming that, at least for some material systems, the inherent long-wavelength assumption of elasticity is violated for inclusions in the nanometer range, we also derive a modified Eshelby tensor in the framework of second gradient elasticity with couple stresses. Closed-form expressions of the modified Eshelby's tensor(s) are presented for spherical and cylindrical inclusions.

We also present some simple illustrative examples of the present work i.e. size-dependent stress concentrations and size-dependent effective properties of composites containing nano-inclusions. However, 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 thus size-independent [2]. 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 aforementioned size effects are neglected. Limited empirical evidence is also presented to support our results.

SIZE-DEPENDENT ESHELBY'S TENSOR FOR NANOINCLUSIONS INCORPORATING SURFACE ENERGIES

Employing Gurtin et. al's [3] framework for surface/interface elasticity, surface & interface energies are coupled to conventional bulk elasticity formulation for inclusions [1]. New (inclusion) curvature related terms are introduced rendering the elastic state size-dependent. 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.

SIZE-DEPENDENT ESHELBY'S TENSOR FOR NANOINCLUSIONS INCORPORATING GRADIENT & COUPLE STRESS EFFECTS

Based entirely on simple group theoretic symmetry arguments and some associated continuum postulates, a second gradient elasticity theory with couple stresses can be constructed [4]. Based upon the Green's function for such a theory, the elastic state of inclusions is determined i.e. Eshelby's tensor is formulated and at least for spherical and circular cylindrical shapes explicitly derived. The results are size-dependent however, for the applications that the present authors are interested in (strains in embedded semiconductor quantum dots), these effects were found to be small in comparison to surface energy effects. The formal framework though, will be of immense use in polymeric or biological materials as well as metallic ones with large number of defects.

APPLICATIONS (QUANTUM DOTS, SIZE-DEPENDENT STRESS CONCENTRATIONS & EFFECTIVE PROPERTIES)

For sake of brevity only application to quantum dots is summarized here. As well known [2] strain impacts the band structure and hence optoelectronic properties of quantum dots. In Figures (1-2), we illustrate the error that may be incurred in the estimation of the band structure and emitted wavelength of an InGaN quantum dot embedded in a GaN matrix if the aforementioned size-effects are neglected. These errors far exceed the strict tolerances in optoelectronic applications. Note that this effect is of importance only in the size range of a few nanometers. Some limited empirical evidence appears to support our assertions.

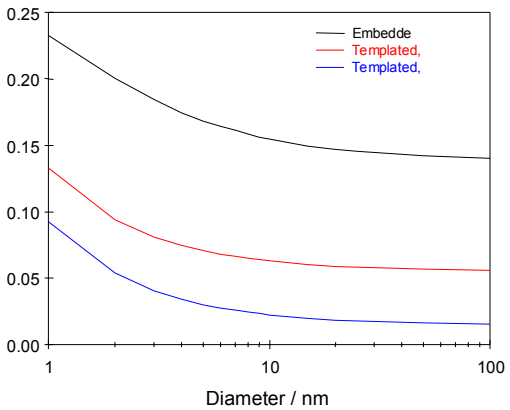

Figure 1:Size-dependent band structure shift due to surface energy effects

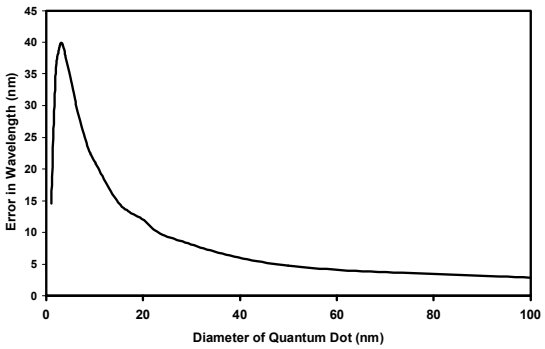

Figure 1:Size-dependent wavelength shift due to surface energy effects

References

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