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Is there an elastic anomaly for a (001) monolayer of InAs embedded in GaAs?

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When a coherently grown (001)-oriented layer of InAs is embedded in a GaAs host, the coherency [redacted] theory to be $\epsilon_\perp=7.3\%$. Brandt, Ploog, Bierwolf, and Hohenstein, [Phys. Rev. Lett. **68**, 1339 (1992)] [redacted] report on an investigation into whether a first-principles local-density total energy minimization shows such an elastic anomaly in the monolayer limit. We find that it does not.

When a layer of material with cubic lattice parameter a_0 is grown coherently in a host with cubic lattice parameter $a_h \neq a_0$, the buried layer undergoes a distortion of its lattice parameter c perpendicular to the plane of the layer in response to the distortion of its lattice parameter parallel to the [redacted] bulk energy as a function of all the structural degrees of [redacted] harmonic continuum elasticity theory (see, e.g., Ref. 1). For [redacted] to (001), the perpendicular strain $\epsilon_\perp=(c-a_0)/a_0$ is related[1] to [redacted]

$$\epsilon_\perp = -2\frac{C_{12}}{C_{11}}\epsilon_\parallel, \qquad (1)$$

[redacted] For example, with the measured[2] $C_{11}=0.8329$ and $C_{12}=0.4526$ (Tdyn/cm^2) for InAs, Eq. (1) predicts $\epsilon_\perp=7.27\%$ for a layer of InAs buried in GaAs.

Recently, Brandt *et al.*[3] examined the strain of buried (001) layers of InAs in GaAs experimentally, via a high- [redacted] sponding to $\epsilon_\perp=12.46\%$, much greater than the prediction of [redacted] plied to a *three* monolayer film of InAs revealed a lattice [redacted] ness of the embedded layer. Regarding (1), we can expect the [redacted] strains; however, the lattice mismatch between GaAs and InAs ($\approx 7\%$) is not sufficient to cause a substantial departure [redacted] from harmonicity. Regarding (2), it was previously shown[4] that for certain interface orientations nonuniform atomic relaxations near an interface can be large. But for (001)-oriented interfaces the allowed relaxations all lie parallel to [001], and the nonuniformity of these interplanar relaxations [redacted] these do not substantially alter the applicability of the simple picture provided by continuum elasticity theory. Regarding [redacted] been untested in semiconductor layers.[5] One might imagine, [redacted] small, interaction between them might substantially alter the [redacted] theory.

In view of the unprecedented result of Brandt *et al.*,[3] we tested the validity of Eq. (1) via an atomistic, nonharmonic, first-principles theory of the relaxations of such a system to [redacted] determine whether it would reveal the breakdown ostensibly demonstrated in the experiment. Our first-principles results in no way depend upon Eq. (1) or the approximations on which it is based. We found good agreement with Eq. (1) and no theoretical evidence for such a breakdown, in spite of [redacted]

Our tests improve on harmonic continuum elasticity [redacted] proach by a discrete atomistic approach, still limited to [redacted] valence-force-field (VFF) model, which uses a description in terms of microscopic quantities, the two-body bond [redacted] tions to the total energy, not just the elastic contribution [redacted] mation (LDA). With the total energy represented as a func- [redacted]

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to it are treated on the same quantum-mechanical footing. This avoids all the potential pitfalls discussed above, and can be regarded as giving the best available theoretical estimate

[redacted]

In the first step, we applied the VFF model, with the

[redacted]

structure containing an embedded (001)-oriented layer of InAs in a GaAs host, all confined to the GaAs lattice constant in the (001) plane. We found values ranging from $\epsilon_\perp=7.09\%$ with 1 monolayer (ML) of InAs, to $\epsilon_\perp=7.17\%$ with 10 ML.[9] This demonstrates good agreement with the prediction of Eq. (1) and shows no evidence of anomalously large distortion in the ultrathin limit.

We note that in a recent paper Massies and Grandjean[10] used a one-dimensional variant of the VFF model to investigate the behavior of monolayer-height InAs surface islands

[redacted]

ever, the clear agreement of our bulk three-dimensional VFF calculations with continuum elasticity theory demonstrates that this comparison of a one-dimensional model of surface relaxation with bulk strain is inappropriate.

The inability of the VFF model to reproduce the

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tions were performed using the LDA in the form of the

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stants of zinc-blende GaAs and InAs were determined by fitting to a Birch equation of state[15] the total energies from seven calculations with differing lattice constants. The fit gives the values (Å) 5.60±0.005 (5.65) for GaAs and 6.02

[redacted]

overestimation in our calculated $\epsilon_\perp$.

For the first-principles calculations of the properties of

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more than adequate to converge the structural features of the interface and the GaAs layer to match those with much thicker layers. We minimized the SL total energy with respect to all structural degrees of freedom, subject to the co-

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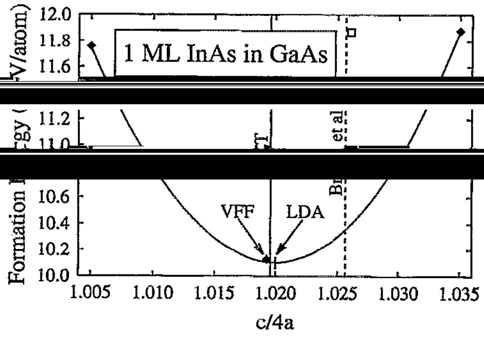

FIG. 1. Formation energy of the atomically relaxed eight-layer structure containing 1 monolayer of InAs vs its $c/4a$ ratio. Filled diamonds denote direct first-principles LDA results; the curve is a cubic fit to those points. The minimum of the fit curve is marked by a vertical tick, labeled "LDA." The diamond symbol labeled "VFF" lies at the $c/4a$ value predicted by the VFF model. The solid vertical line, labeled "CET," marks the prediction of

[redacted]

the InAs layer has $\epsilon_\perp=12.5\%$, illustrating the large energy penalty incurred if the strain is concentrated in the InAs layer.

was used to find the equilibrium c/a_h ratio. While the symmetry of the structure permits additional relaxations beyond

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Our results are illustrated for the single-monolayer case

[redacted]

recent pseudopotential calculation by Shiraishi and Yamaguchi.[16] However, correspondence with one of the authors[17] has clarified that their results do not, in fact, show evidence of an elastic anomaly in the monolayer limit.

[redacted]

measured shift in the lattice.[9] Because the VFF model provides a sufficiently accurate reproduction of the structural

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permitting more precise determination of the individual spacings, suggests that they should be able to detect excess In, at least in the two larger amounts we have suggested.[20]

[redacted]

ratio of the two expanded spot-row spacings in different

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[110] or along [1̄10]—in one case increasing the ratio, and in the other case decreasing it. Thus it would be possible to compare such images as another test for excess In. To our

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of InAs to be distributed among three layers, with 75% in the

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nately, the samples used for this study were not characterized by HREM, so it is not clear whether they would exhibit the

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ment to help determine whether the experimental results of Brandt *et al.*[3] could be a consequence of excess In in the

[redacted]

mental findings, and further work to attempt to resolve the

[redacted]

received under Subcontract No. XR-1-11236-1 from the National Renewable Energy Laboratory. Work [illegible]

[redacted]

gratefully acknowledged. We thank the reviewer for pointing

[redacted]

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[1] D. M. Wood and A. Zunger, Phys. Rev. B 40, 4062 (1989); A. Zunger and D. M. Wood, J. Cryst. Growth 98, 1 (1989).

[2] [redacted] Vol. 17, Pt. A.

[3] O. Brandt, K. Ploog, R. Bierwolf, and M. Hohenstein, Phys. Rev. Lett. **68**, 1339 (1992).

[4] R. G. Dandrea, J. E. Bernard, S.-H. Wei, and A. Zunger, Phys. Rev. Lett. [redacted]

[6] P. N. Keating, Phys. Rev. **145**, 637 (1966).

[7] R. M. Martin, Phys. Rev. B **1**, 4005 (1970).

[redacted]

[9] For consistency with Ref. 3, we calculate $\epsilon_\perp$ from the theoretical c/a ratio of the unit cell, attributing all of the c-axis expansion to the InAs layer. With actual layer spacings, $\epsilon_\perp$ increases by less than 0.5 percentage points [redacted] generally at bulk semiconductor interfaces (Ref. 4).

[redacted]

[12] N. Troullier and J. L. Martins, Phys. Rev. B **43**, 1993 (1991).

[redacted]

[15] F. Birch, Phys. Rev. **71**, 809 (1947); J. Geophys. Res. **57**, 227 (1952).

[16] K. Shiraishi and E. Yamaguchi, Phys. Rev. B **42**, 3064 (1990).

[17] Reference 3 cites results of Ref. 16 as evidence of theoretical support for [redacted] InAs in GaAs (2.55 Å). However, Dr. Shiraishi has informed us that the [redacted] blende GaAs bond length. Their calculated bond length for the embedded layer is 2.49 Å, corresponding to $\epsilon_\perp=4.6\%$.

[redacted]

with the overall shift. Further, application of the method (Ref. 19) to [redacted]

[21] C. Giannini, L. Tapfer, S. Lagomarsino, J. C. Boulliard, A. Taccoen, B. [redacted] (1993).