# Elastic response of cubic crystals to biaxial strain: Analytic results and comparison to density functional theory for InAs

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The elastic energy of a biaxially strained material depends on both the magnitude and the plane of the applied biaxial strain, and the elastic properties of the material. We employ continuum-elasticity theory (CET) to determine general analytic expressions for the strain tensor, the Poisson ratio, and the elastic energy for materials with cubic crystal symmetry exposed to biaxial strain in arbitrary planes. In application to thin homogeneously strained films on a substrate, these results enable us to estimate the role of elastic energy for any substrate orientation. When calculating the elastic response to biaxial strain in an arbitrary plane by numerical methods, our analytic results make it possible to set up these calculations in a much more efficient way. This is demonstrated by density-functional theory calculations of the Poisson ratio and elastic energy upon biaxial strain in several planes for the case of InAs. The results are in good agreement with those of CET, but show additional nonlinear contributions already at moderate biaxial strain.

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## I. INTRODUCTION

Heterostructures of two materials with different lattice constants are of considerable technological importance. For the stability of these structures, the energy associated with elastic lattice distortions plays a major role. Apart from strained semiconductor heterostructures[1] that are in the main focus of this work, other related fields of technology where elastic energy is important are self-assembled semiconductor nanostructures,[2] thin metallic films,[3] and phase stability in metal superalloys.[4] One way to create a material under considerable biaxial strain is the heteroepitaxial or pseudomorphic growth of an overlayer on a substrate, implying that the lateral lattice spacing of the overlayer adapts to the substrate lattice.

The associated elastic energy is an important factor when analyzing the structural stability of the overlayer: When the elastic energy becomes too large, it is energetically more favorable to reduce the strain, e.g., by introducing misfit dislocations or by a structural phase transition from a smooth to a rough overlayer (see, e.g., Ref. 5). For moderate misfit strain, however, rather thick overlayers can be grown before an instability occurs. In this case, most of the strain energy is stored in regions of the overlayer that are already bulklike, and can be estimated by studying biaxial deformations of bulk materials. In the region near the interface, the character of the chemical bonds between the atoms is affected by the presence of the interface. This gives rise to effects unknown in bulk elasticity theory, e.g., excess interface stress, or oscillatory displacements[6] that decay to either side of the interface. However, it has been argued that deviations from bulk elastic behavior play a notable role only in films that are less than a few monolayers thick.[7] For example, for InAs films on GaAs(001), it has been shown by density-functional theory (DFT) calculations that the energy stored in thin films increases linearly (as predicted by elasticity theory) when the film is thicker than three monolayers.[8] In this paper, we concentrate on biaxial strain in bulk materials, exemplifying the elastic properties of thick heteroepitaxial or pseudomorphic films.

Theoretical investigations of strain effects in macroscopic systems are generally based on continuum-elasticity theory (CET), see, e.g., Ref. 9. Within this framework, Marcus *et al.*[10] presented a general scheme to calculate the elastic response upon biaxial deformations numerically. Analytic solutions in terms of the Miller indices of the strain plane have been worked out only for a few selected cases in systems with cubic symmetry,[11] and for thin films.[12] Our first goal is the derivation of general analytic expressions of the strain tensor, the Poisson ratio, and the elastic energy for cubic systems under biaxial strain within linear-response CET.

Deformations larger than a few percent are not uncommon in epitaxial or pseudomorphic overlayers, but their treatment goes beyond linear elasticity theory. In fact, quantitative agreement between the observed and the calculated wavelength of light emission from semiconductor heterostructure lasers could only be achieved by taking nonlinear elastic response into account.[13,14] Further examples where nonlinear effects play a role are piezoelectricity in semiconductor quantum wells,[15] the stability of epitaxial films of noble metals,[16] or structural transformation paths in metals.[17] Although CET can be extended to include nonlinear effects, a nonlinear treatment is in many cases hindered by the limited knowledge of the higher-order elastic constants. An alternative approach to nonlinear elastic effects are systematic numerical studies using, e.g., DFT. Until now such investigations were mainly applied to isotropic strain and biaxial strain in low-index planes. The second goal of this paper is therefore to establish a scheme through which such investigations of nonlinear contributions can be very efficiently extended to biaxial strain in high-index planes. As an example, we perform DFT calculations for the dependence of nonlinear elastic effects in InAs/GaAs heteroepitaxy on the substrate orientation.

In the first part of this paper we introduce the strain tensor that is used to obtain the Poisson ratio and elastic energy for

 

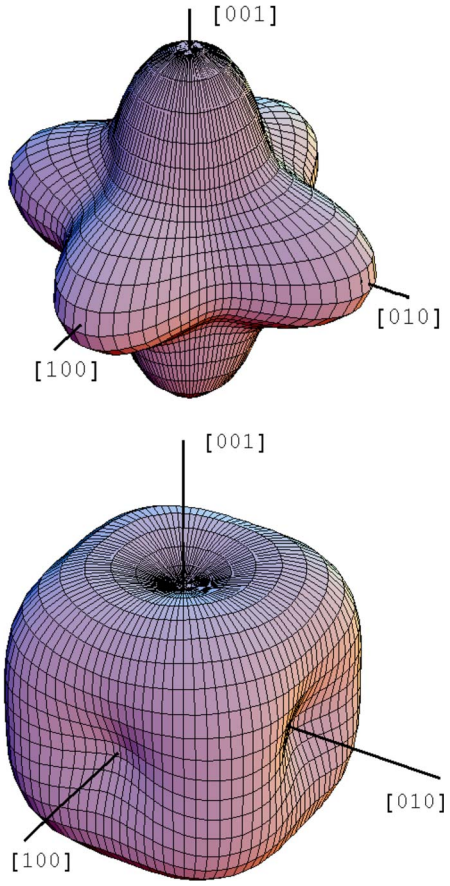


FIG. 1. (Color online) Dependence of the Poisson ratio (top) and the elastic-energy per volume (bottom) of InAs on the normal vector of the plane of biaxial strain.

cubic systems as given in the second part. The remainder of this paper is then devoted to a comparison of CET results and DFT calculations, along with a discussion of nonlinear elastic effects and the consideration of internal relaxations.

## II. BIAXIAL STRAIN-TENSOR

The free energy of isothermal elastic deformations of a medium is given by the elastic constants $c_{klmn}$ and the strain tensor $\varepsilon$ as

$$F(\varepsilon) = \frac{1}{2}\sum_{klmn} c_{klmn}\varepsilon_{kl}\varepsilon_{mn}. \tag{1}$$

Often the symmetries of crystal structures can be used to simplify the above expression[9] by specifying the strain tensor in the canonical coordinate system of the crystal, i.e., for $\mathbf{e}_x \| [100]$, $\mathbf{e}_y \| [010]$, and $\mathbf{e}_z \| [001]$. For structures with cubic symmetry the elastic energy reduces to[9]

$$F(\varepsilon) = \frac{c_{11}}{2}(\varepsilon_{xx}^2 + \varepsilon_{yy}^2 + \varepsilon_{zz}^2) + 2c_{44}(\varepsilon_{xy}^2 + \varepsilon_{xz}^2 + \varepsilon_{yz}^2) + c_{12}(\varepsilon_{xx}\varepsilon_{yy} + \varepsilon_{xx}\varepsilon_{zz} + \varepsilon_{yy}\varepsilon_{zz}), \tag{2}$$

where the elastic constants $c_{ij}$ are given in Voigt notation. The elastic response of a medium under external stress is determined by minimizing the free energy $F$ with respect to the directions with no external stress. The general analytic solutions for isotropic and for one-dimensional (uniaxial) external deformations yield the well-known bulk modulus and Poisson ratio, respectively. The Poisson ratio of elastically anisotropic materials depends on the direction of uniaxial strain. In analogy to the uniaxial case, one can define a Poisson ratio for isotropic two-dimensional deformations, that we will refer to as biaxial deformations, in compliance with most previous works. Similar to the uniaxial case, the elastic relaxation upon biaxial strain in a plane $(hkl)$ can be given in an orthogonal coordinate system of the deformation with two axes $(\mathbf{e}_1, \mathbf{e}_2)$ in the strain-plane $(hkl)$ and a third $(\mathbf{e}_3)$ along the direction of relaxation $[hkl]$. The relation to the canonical coordinates can be given by a matrix $\mathbf{T} = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)^{-1}$. The biaxial strain tensor $\varepsilon_s$ in this coordinate system of the deformation is

$$\varepsilon_s = \begin{pmatrix} \alpha_s & 0 & 0 \\ 0 & \alpha_s & 0 \\ 0 & 0 & -\nu\alpha_s \end{pmatrix}, \tag{3}$$

where $\nu$ is the biaxial Poisson ratio. A more general treatment is possible with introducing commensurability constraints,[18,19] but we focus on the case of isotropic planar strain. The strain tensor $\varepsilon_s$ can be inserted into the expression for the free energy [Eq. (1)] after transforming $\varepsilon_s$ from the coordinate system of the deformation to the canonical coordinate system of the crystal. This is advantageous as it allows to use the well-known structure-specific expressions of the free energy in canonical coordinates. The above matrix $\mathbf{T}$ transforms the strain tensor $\varepsilon_s$ expressed in terms of $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ to the corresponding strain tensor $\varepsilon$ in canonical coordinates $\{\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z\}$. This yields the free energy

$$F(\varepsilon) = F(\mathbf{T}\varepsilon_s\mathbf{T}^T). \tag{4}$$

Together with the structure-specific free energy and the values of the elastic constants, Eq. (4) allows us to calculate the elastic response upon biaxial strain in arbitrary planes by determining the minimum of the elastic energy with respect to the biaxial Poisson ratio

$$\frac{\partial}{\partial\nu}F(\varepsilon) = 0. \tag{5}$$

A general procedure of transforming the strain tensor to canonical coordinates with a tensor-transformation law[20] was described in detail previously.[10] With this scheme Marcus[11] determined the elastic energy of cubic systems upon biaxial strain analytically for low-index planes and numerically for several high-index planes.

A rigorous analytic derivation requires the knowledge of the transformation matrix $\mathbf{T}$ that is not unique for a given strain plane due to the freedom to choose the in-plane vectors $\mathbf{e}_1$ and $\mathbf{e}_2$. But for the case of biaxial strain, i.e., for two orthogonal deformations of equal absolute value, the strain tensor is invariant under the particular choice of $\mathbf{e}_1$ and $\mathbf{e}_2$. In other words, the elastic response can be calculated uniquely for a given plane of a structure with any choice of $\mathbf{e}_1$ and $\mathbf{e}_2$, and thus depends solely on the elastic constants of the mate-

rial, its crystal structure, and the normal of the biaxial-strain plane $\mathbf{e}_3 \| [hkl]$. This was already noted by Marcus[11] for the elastic energy. Without loss of generality we choose an orthonormal deformation coordinate system that allows to easily derive a general transformation matrix $\mathbf{T}$, similar to Lee:[12]

$$\mathbf{e}_1 = \mathbf{e}_2 \times \mathbf{e}_3, \quad \mathbf{e}_2 = \frac{1}{n_2}\begin{pmatrix} kl \\ hl \\ -2hk \end{pmatrix}, \quad \mathbf{e}_3 = \frac{1}{n_3}\begin{pmatrix} h \\ k \\ l \end{pmatrix} \tag{6}$$

with the normalization $n_2 = \sqrt{k^2l^2 + h^2l^2 + 4h^2k^2}$ and $n_3 = \sqrt{h^2+k^2+l^2}$. This defines the transformation matrix $\mathbf{T}$ that allows us to transform the strain tensor from the coordinate system of the deformation to canonical coordinates

$$\varepsilon = \mathbf{T}\begin{pmatrix} \alpha_s & 0 & 0 \\ 0 & \alpha_s & 0 \\ 0 & 0 & -\nu\alpha_s \end{pmatrix}\mathbf{T}^T$$

$$= -\frac{\alpha_s}{h^2+k^2+l^2} \times \begin{pmatrix} \nu h^2 - (k^2+l^2) & hk(\nu+1) & hl(\nu+1) \\ hk(\nu+1) & \nu k^2 - (h^2+l^2) & kl(\nu+1) \\ hl(\nu+1) & kl(\nu+1) & \nu l^2 - (h^2+k^2) \end{pmatrix}. \tag{7}$$

Note, that the cubic symmetry of the crystal lattice enters the transformation matrix in the definition of the orthonormal deformation coordinate system in Eq. (6). Therefore the canonic representation of the strain tensor as given in Eq. (7) holds only for materials with cubic symmetry.

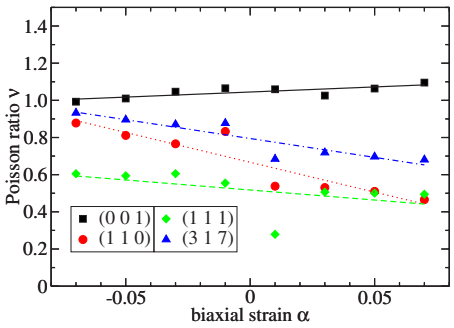


FIG. 2. (Color online) The Poisson ratio calculated with density-functional theory for biaxial strain in different planes (symbols) shows a linear dependency on the strain (lines).

## III. ELASTIC RESPONSE

With the elastic energy of Eq. (2) and the canonic strain tensor of Eq. (7), the elastic response of a system with cubic symmetry upon a biaxial deformation can be determined by minimizing the elastic energy with respect to the Poisson ratio $\nu$, according to Eq. (5). The resulting Poisson ratio and elastic energy upon biaxial strain in the $(hkl)$ plane depend only on the elastic constants $c_{ij}$, the strain plane $(hkl)$, the biaxial strain $\alpha_s$, and the volume of strained material $V$:

$$\nu = 2\frac{c_{12}(h^4+k^4+l^4) + (c_{11}+c_{12}-2c_{44})(h^2k^2+h^2l^2+k^2l^2)}{c_{11}(h^4+k^4+l^4) + 2(c_{12}+2c_{44})(h^2k^2+h^2l^2+k^2l^2)} =: \nu^{(0)}, \tag{8}$$

$$F(\alpha^s) = \frac{(c_{11}+2c_{12})[(c_{11}-c_{12})(h^4+k^4+l^4) - (c_{11}-c_{12}-6c_{44})(h^2k^2+h^2l^2+k^2l^2)]}{c_{11}(h^4+k^4+l^4) + 2(c_{12}+2c_{44})(h^2k^2+h^2l^2+k^2l^2)}\alpha_s^2 V. \tag{9}$$

These analytic results hold for arbitrary biaxial strain and every material with cubic symmetry. Materials are usually called elastically isotropic if $2c_{44}=c_{11}-c_{12}$, i.e., if the Poisson ratio for uniaxial strain is independent of the direction of strain. The above equations show that for such materials the Poisson ratio for biaxial strain is independent of the strain plane, too. Note, that the analytic results of both, the Poisson ratio and the elastic energy are identical for values of $(hkl)$ with constant ratio $m$ given by

$$m = \frac{h^4+k^4+l^4}{h^2k^2+h^2l^2+k^2l^2} \tag{10}$$

like, e.g., (110), (211), and (321). The analytic Poisson ratios for (100) and (110) from Eq. (8) are identical to those given in previous works.[9,11,21] In a comparison of the elastic-energy upon biaxial strain in Fe, Cu, V, and Ni as obtained previously by Marcus,[11] and our analytic expression with the same elastic constants, we find identical results for (100), (110), and (111), but different values for (211), (311), (310), (321), and (331). These differences arise from the bending of the film-substrate system that was considered in Ref. 11 but is absent in the bulk systems studied in this work. For high-index strain planes, the substrate bending leads to finite values of the off-diagonal elements of the strain tensor in the coordinate system of the deformation [Eq. (3)]. From a comparison of our results with those of Marcus,[11] we find that the substrate bending of a film-substrate system can lower the elastic energy density by up to approximately 20%.

The cubic symmetry of the crystal structure is reflected in the invariance of the biaxial Poisson ratio and the elastic energy under a permutation of the Miller indices of the strain normal. This symmetry is also apparent in Fig. 1 that shows a polar plot of both quantities as a function of the normal

vector of the biaxial strain-plane. These figures were obtained by multiplying the normalized vector $(hkl)$ with $\nu$ or $F$ as obtained from Eqs. (8) and (9), respectively, using the experimentally observed elastic constants of InAs as given in Ref. 22. Figure 1 illustrates the relationship between the elastic relaxation and the elastic energy. Biaxial strain in a plane perpendicular to an elastically soft direction, e.g., (001), allows for a relatively large relaxation along the plane normal with relatively small elastic energy.

## IV. DFT CALCULATIONS

The results presented in the previous sections now enable us to establish an efficient scheme for numerical investigations of the elastic response to biaxial strain in arbitrary planes. Frequently, calculations of bulk elastic properties are done with simulation cells that are chosen such that the strain plane is spanned by two basis vectors of the simulation cell. [For strain in, e.g., the (111) plane, one could use a bulk simulation cell with $\mathbf{e}_1 \| [11\bar{2}]$, $\mathbf{e}_2 \| [1\bar{1}0]$, and $\mathbf{e}_3 \| [111]$.] This choice allows one to easily apply biaxial strain by scaling those two basis vectors that span the strain plane. But the number of atoms in such a simulation cell depends on the plane of biaxial strain and, for high-index planes, becomes very large and eventually hard to handle in DFT calculations. The strain tensor in canonical coordinates [Eq. (7)], however, determines the strained unit cell and the atomic coordinates for biaxial deformations in any plane. This reduces the required simulation cell to a single conventional unit cell of the investigated cubic material. The determination of the biaxial Poisson ratio for a certain strain $\alpha$ in some chosen plane $(hkl)$ then reduces to scaling the atomic coordinates and the cell vectors of a conventional cubic unit cell according to the strain tensor, and minimizing the elastic energy with respect to $\nu$.

In this section we apply this scheme exemplarily to biaxially strained InAs in the ZnS structure that plays a major role in the self-assembled growth of quantum dots (see, e.g., Ref. 23 for a recent review). The analytic results obtained in the previous section are compared to self-consistent total-energy calculations using DFT.[24] We use norm-conserving pseudopotentials,[25] Monkhorst-Pack **k**-point meshes,[26] and the local-density approximation for the exchange-correlation functional. The calculations for all planes of biaxial strain $(hkl)$ were performed with a single ZnS unit cell with eight atoms in total, displaced according to the strain tensor [Eq. (7)] for the corresponding $(hkl)$. An energy cutoff of 20 Ry and a $5\times5\times5$ folding of one **k** point in the center of the Brillouin zone turned out to be sufficient to converge the value of $\nu^{(0)}$ (see below) to a remaining error of about 1%.

An additional issue for the case of the chosen ZnS lattice is that biaxial strain can lift the equivalence of the atomic bonds inside the unit cell. This causes the atoms to relax their relative position and is well known from the calculation of the elastic constants $c_{44}^{(0)}$ and $c_{44}$ (see Ref. 27). To investigate the role of such internal relaxations under biaxial deformations, we performed two kinds of DFT calculations: In the first set, we scaled the unit cell and the position of the atoms according to the strain tensor and computed the total energy without relaxing. In the second set, we additionally relaxed the positions of the atoms in the unit cell until the absolute value of the change in the total energy was less than 0.3 meV. The procedure is similar to numerically calculating $c_{44}^{(0)}$ and $c_{44}$, respectively, and will be referred to as "unrelaxed" and "relaxed" in the following.

TABLE I. The Poisson ratios $\nu^{(0)}$ of InAs under biaxial strain in selected planes as obtained from continuum-elasticity theory (CET) are in good agreement with DFT calculations.

| | no internal relaxation | | | internal relaxation | | |
|---|---|---|---|---|---|---|
| | CET $\nu^{(0)}$ | DFT $\nu^{(0)}$ | DFT $\nu^{(1)}$ | CET $\nu^{(0)}$ | DFT $\nu^{(0)}$ | DFT $\nu^{(1)}$ |
| (0 0 1) | 1.09 | 1.05 | +0.55 | 1.09 | 1.04 | +0.55 |
| (1 1 0) | 0.34 | 0.40 | −1.23 | 0.67 | 0.67 | −3.21 |
| (1 1 1) | 0.20 | 0.29 | −1.51 | 0.57 | 0.55 | −0.92 |
| (1 1 3) | 0.54 | 0.60 | −1.77 | 0.81 | 0.78 | −1.65 |
| (3 1 7) | 0.58 | 0.63 | −1.56 | 0.83 | 0.79 | −2.03 |
| (3 7 15) | 0.52 | 0.57 | −1.65 | 0.79 | 0.77 | −2.10 |

In both cases, we determined the biaxial Poisson ratio $\nu$ numerically with DFT calculations for different values of the strain $\alpha_i$. To address the case of InAs/GaAs heteroepitaxy with about 6.9% lattice mismatch, we have chosen $\alpha_i \in \{\pm0.07, \pm0.05, \pm0.03, \pm0.01\}$. For each $\alpha_i$, we calculated the total energy of the strained InAs unit cell at $\nu(\alpha_i) = \nu_a \pm j0.05$, where $\nu_a$ is the analytic result and $j=0,\ldots,5$. The elastic energy $E_{\mathrm{el}}$ is given by the difference in total energies of strained and unstrained unit cell. From our DFT calculations we find that the elastic energy for a particular strain $\alpha_i$ is well described by

$$E_{\mathrm{el}}(\alpha_i,\nu) = E_{\mathrm{el}}^{(0)}(\alpha_i) + E_{\mathrm{el}}^{(1)}(\alpha_i)\nu + E_{\mathrm{el}}^{(2)}(\alpha_i)\nu^2. \tag{11}$$

The minimum of the elastic energy with respect to $\nu$ yields the elastic response $\nu_i(\alpha_i)$ upon this particular strain $\alpha_i$. The Poisson ratios for different biaxial strain in different planes $(hkl)$ as obtained from our DFT calculations are shown in Fig. 2.

For a quantitative comparison with CET we performed a linear fit of the DFT results according to

$$\nu(\alpha) = \nu^{(0)} + \nu^{(1)}\alpha. \tag{12}$$

Note, that the slope $\nu^{(1)}$ indicates a nonlinear elastic response that is not captured by the continuum-elasticity theory approach presented in the previous sections. Within the validity of the linear CET approach, different strain dependencies of the elastic constants in Eq. (8) could give rise to the different slopes $\nu^{(1)}$ observed in Fig. 2: The negative slopes of all but one curve in Fig. 2 are likely due to the role of $c_{44}$ in Eq. (8) and its strain dependence. The shear strain described by $c_{44}$ is absent for biaxial strain in the (001) plane, and indeed a positive slope of the Poisson ratio is found for this plane.

The biaxial Poisson ratio $\nu^{(0)}$ that corresponds to linear elastic response as obtained from DFT calculations is compiled with the analytic result from Eq. (8) in Table I for

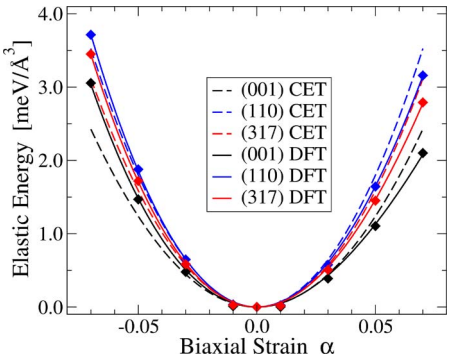


FIG. 3. (Color online) The elastic energy per volume [$E_{el}$ of Eq. (13)] of InAs upon biaxial strain in selected planes as obtained from DFT (points and full lines) shows considerable nonlinear response [$E_{el}^{(3)}$ in Eq. (13)] that is not captured by linear CET (dashed lines).

different strain planes (*hkl*). The consideration of internal relaxations in the analytic expressions obtained from CET by employing $c_{44}$ or $c_{44}^{(0)}$ in Eq. (8) is compared to DFT calculations without and with relaxation of the internal degrees of freedom, respectively. For both cases, we also provide the value of $\nu^{(1)}$ that leads to nonlinear elastic response and is not apparent in the CET calculations. In both cases, i.e., with and without internal relaxations, the Poisson ratios of the investigated planes of biaxial strain as obtained from CET are in good agreement with DFT calculations. This confirms that the consideration of internal relaxation in CET can be controlled by choosing either $c_{44}$ or $c_{44}^{(0)}$. Note, that the analytic results were obtained with the experimentally observed elastic constants of InAs (Ref. 22) that differ slightly from the corresponding DFT results.

The elastic energy densities with internal relaxations are shown in Fig. 3. According to Eqs. (11) and (12), the elastic-energy densities calculated with DFT were found to be well described by

$$E_{el}(\alpha) = E_{el}^{(2)}\alpha^2 + E_{el}^{(3)}\alpha^3. \tag{13}$$

The numerical values of $E_{el}^{(2)}$ and $E_{el}^{(3)}$ as obtained from our DFT calculations are compiled in Table II for different strain planes (*hkl*), together with the analytic result from CET by employing $c_{44}$ or $c_{44}^{(0)}$ in Eq. (9). For the case of InAs studied here, the Poisson ratio varies between the smallest and the largest value by a factor of five, whereas the range of elastic energy densities is about 30%.

TABLE II. The elastic energy density $E_{el}^{(2)}$ of InAs under biaxial strain in selected planes as obtained from continuum-elasticity theory (CET) are in good agreement with DFT calculations. (Values given in eV/Å$^3$.)

| | no internal relaxation | | | internal relaxation | | |
|---|---|---|---|---|---|---|
| | CET $E_{el}^{(2)}$ | DFT $E_{el}^{(2)}$ | DFT $E_{el}^{(3)}$ | CET $E_{el}^{(2)}$ | DFT $E_{el}^{(2)}$ | DFT $E_{el}^{(3)}$ |
| (0 0 1) | 0.50 | 0.52 | −1.40 | 0.50 | 0.52 | −1.40 |
| (1 1 0) | 0.90 | 0.88 | −2.83 | 0.72 | 0.70 | −0.83 |
| (1 1 1) | 0.90 | 0.95 | −3.12 | 0.76 | 0.78 | −1.88 |
| (1 1 3) | 0.79 | 0.77 | −2.10 | 0.65 | 0.65 | −1.13 |
| (3 1 7) | 0.77 | 0.75 | −2.06 | 0.64 | 0.64 | −0.98 |
| (3 7 15) | 0.81 | 0.78 | −2.21 | 0.66 | 0.65 | −1.03 |

## V. CONCLUSION

In this work, an analytical expression has been derived for the elastic response of a material with cubic symmetry under biaxial deformations within linear continuum elasticity theory (CET) for any chosen strain plane. We determine the biaxial strain tensor in the canonic coordinates of the crystal, as well as the biaxial Poisson ratio and elastic energy. In extension to previous works we provide general, analytic expressions for arbitrary planes of biaxial strain, depending only on the elastic constants and the Miller indices of the strain plane. As a corollary, we identify subsets of strain planes (characterized by their Miller indices) that display identical elastic response. It follows from our derivation that elastic isotropy with respect to uniaxial strain implies elastic isotropy with respect to biaxial strain. Furthermore, knowledge of the strain tensor in analytical form allows us to work out an efficient scheme for numerical calculations in which one cubic unit cell is sufficient to describe biaxial strain in any plane. It should be noted that the above results only hold for cubic crystals and small magnitudes of the strain. For larger deformations, two basic assumptions break down: Linear response is no longer applicable, and further deformation of a system that is already biaxially strained would act on a noncubic system.

Motivated by our interest in InAs/GaAs heteroepitaxy, we performed DFT calculations of InAs under typical conditions of biaxial strain. The linear contributions of both, the Poisson ratio and the elastic energy for biaxial strain in selected planes, are in good agreement with the corresponding CET results. The nonlinear contributions in the DFT results are well described by a linear dependence of the Poisson ratio on the applied biaxial strain and a cubic strain dependence of the elastic energy. Performing the DFT calculations with or without atomic relaxations is found to be equivalent to the use of either $c_{44}$ or $c_{44}^0$ as shear modulus in CET.

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