Strain–displacement relations for strain engineering in single-layer 2d materials

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Abstract

We investigate the electromechanical coupling in single-layer 2d materials. For non-Bravais lattices, we find important corrections to the standard macroscopic strain–microscopic atomic-displacement theory. We put forward a general and systematic approach to calculate strain–displacement relations for several classes of 2d materials. We apply our findings to graphene as a study case, by combining a tight binding and a valence force-field model to calculate electronic and mechanical properties of graphene nanoribbons under strain. The results show good agreement with the predictions of the Dirac equation coupled to continuum mechanics. For this long wave-limit effective theory, we find that the strain–displacement relations lead to a renormalization correction to the strain-induced pseudo-magnetic fields. A similar renormalization is found for the strain-induced band-gap of black phosphorous. Implications for nanomechanical properties and electromechanical coupling in 2d materials are discussed.

1. Introduction

Linear continuum elasticity provides a valuable basis for the investigation of the mechanical properties of atomic monolayer materials [1, 2]. Elasticity theory is also a key element for understanding the relation between the material deformations and the corresponding modifications of its electronic structure [2–5]. Roughly speaking, strain changes the interatomic distances, thereby modulating the overlap of electronic orbitals of neighboring atoms and modifying the electronic properties of the material. To model and engineer this electromechanical coupling it is necessary to correctly relate experimentally controllable macroscopic deformations, parametrized by the strain tensor \(\varepsilon\), to microscopic atomic displacements.

The standard strain–displacement relations break down for materials characterized by a lattice with a basis [6–8]. In this Letter we show how to correct this problem for any kind of strained 2d monolayer material. First we show that, for these systems, the nearest-neighbor vectors connecting the atoms transform as \( \mathbf{r}_{ij} \rightarrow (\mathbf{J} + \varepsilon) \cdot \mathbf{r}_{ij} + \Delta \), where \( \mathbf{J} \) is the \( n \times n \) identity matrix and \( \Delta \) is a vector that depends on the material deformation energy. (For a Bravais lattice \( \varepsilon = 0 \).) Next, we introduce a systematic approach to calculate the corresponding corrected strain–deformation relations, provided that the deformation energy can be parametrized in terms of the bond vectors. We show the significance of our findings by contrasting the elastic bulk properties of graphene and black phosphorous calculated with and without the proposed corrections.

Strain–displacement relations are key for band structure calculations that use tight-binding or \( \mathbf{k} \cdot \mathbf{p} \) models, which are particularly useful for inhomogeneous strain, where other methods become computationally prohibitive. We study the effect of the strain–displacement corrections on electronic degrees of freedom in three applications. In the first one we incorporate the modified strain–displacement relations in the \( \mathbf{k} \cdot \mathbf{p} \) model for graphene, where strain can be represented by an effective gauge-field [9–11]. We show that a correct assessment of \( \Delta \) renormalizes...
the strength of the gauge vector-potential by a factor $3/5$, which means a factor $(3/5)^2$ for scattering rates relevant to transport properties[12, 13]. A similar correction has previously been identified in the study of the elastic properties of carbon nanotubes, where the strain–deformation relations were inferred from the analysis of the acoustic phonon modes [9, 14]. In the second application we study the effect of our findings on the gap engineering of graphene nanoibbons using strain. Finally, we apply our approach to single-layer black phosphorous and calculate the elastic properties and the strain-induced electronic band-gap.

In summary, our study shows that quantitative estimates of the electromechanical coupling in 2D materials—as is often required in strain-engineering applications—requires careful consideration of the lattice deformation on a microscopic level.

2. Results

The atomic lattices of 2D materials are characterized by primitive unit cells (PUCs) with a set of basis atoms and two primitive lattice vectors $\mathbf{a}_1$ and $\mathbf{a}_2$. In a homogeneously strained sample it is sufficient to consider the deformation of a single unit cell under an applied strain. The deformed primitive lattice vectors read

$$\mathbf{a}_i' = (\mathbf{J}_i + \mathbf{u}) \cdot \mathbf{a}_i,$$

where $\mathbf{u}$ is the strain tensor and $i = 1, 2$. This equation also holds for nonuniform strain, for which $\mathbf{u} = \mathbf{u}(\mathbf{r})$ varies on length scales much longer than the lattice parameter. In general, the lattice vectors can be expressed by a linear combination of the bond vectors $\mathbf{r}_{ij}$,

$$\mathbf{a}_i = \sum_{\mathbf{r}_{ij} \in \{\mathbf{r}_i\}} C_{ij} \mathbf{r}_{ij},$$

where $\{\mathbf{r}_i\}$ is the set of bond vectors contained within each unit cell and $C_{ij}$ is a tensor encoding the lattice connectivity. We address the case where the strain field deforms the lattice, but preserves its connectivity. We show that for materials with a non-Bravais lattice structure, the modifications of the bond vectors due to strain do not follow equation (1). Let us start from the most general relation

$$\mathbf{r}_{ij}' = (\mathbf{J}_i + \mathbf{u}) \cdot \mathbf{r}_{ij} + \mathbf{\Delta}_{ij},$$

where the vectors $\mathbf{\Delta}_{ij}$ contain the differences between the strain displacement relations for $\mathbf{a}_i$ and $\mathbf{r}_{ij}$. The number of independent vectors $\mathbf{\Delta}_{ij}$ is determined by the number of basis atoms and $\sum_{\mathbf{r}_{ij} \in \{\mathbf{r}_i\}} C_{ij} \mathbf{\Delta}_{ij} = 0$. For a Bravais lattice $\mathbf{\Delta}_{ij} = 0$. Each additional atom in the basis introduces three degrees of freedom, that can be expressed by an in-plane vector $\mathbf{\Delta}_i$, and an out-of-plane component $\Delta_z \hat{z}$. The number of independent displacement vectors obtained in this way can, in general, be reduced by enforcing the lattice symmetry and connectivity. In this Letter, we consider the most important 2D materials [15] under current investigation, divided in three groups, shown in figure 1.

The first class contains graphene and graphene-like materials, such as boron nitride, as well as non-planar materials, such as silicene and germanene. The PUC consists of two basis atoms and two lattice vectors $\mathbf{a}_1 = a_0 (3/2, \sqrt{3}/2, 0)$ and $\mathbf{a}_2 = a_0 (3/2, -\sqrt{3}/2, 0)$, see figure 1(a). The three nearest neighbor vectors are given by $\mathbf{r}_i = (-a_0, 0, 0) - \mathbf{h} \hat{z}$, $\mathbf{r}_2 = \mathbf{a}_1 + \mathbf{r}_i$ and $\mathbf{r}_3 = \mathbf{a}_2 + \mathbf{r}_i$, where $\mathbf{h}$ is the PUC corrugation height. The lattice vectors are written in terms of the bond vectors as $\mathbf{a}_1 = \mathbf{r}_2 - \mathbf{r}_i$ and $\mathbf{a}_2 = \mathbf{r}_3 - \mathbf{r}_i$. The bond vectors transform as $\mathbf{r}_i' = \mathbf{r}_i + \mathbf{u} \cdot \mathbf{r}_i + \mathbf{\Delta}_i$, with the constraints $0 = \Delta_{x} - \Delta_{y}$ and $0 = \Delta_{y} - \Delta_{x}$. Hence, $\mathbf{\Delta}_i \equiv \mathbf{\Delta}_i$. The latter is conveniently expressed by in-plane deformations $\mathbf{\Delta}_i$ and the corrugation change $\Delta_z \hat{z}$. Graphene is a special case for which $\mathbf{\Delta}_i \equiv 0$.

The second class contains the transition metal dichalcogenides (TMDs). Here the PUC contains three atoms, one transition metal (Mo or W) and two chalcogens (S or Se), see figure 1(b). The transition metal has six nearest neighbors. The bond vectors are labeled $\mathbf{r}_{1, u/d}$, $\mathbf{r}_{2, u/d}$ and $\mathbf{r}_{1, u/d}$ where the subscript $u$ or $d$ indicates whether the bond connects to the upper (u) or lower (d) layer of chalcogen atoms. The lattice vectors are given by $\mathbf{a}_1 = \mathbf{r}_{2, u/d} - \mathbf{r}_{1, u/d}$ and $\mathbf{a}_2 = \mathbf{r}_{2, u/d} - \mathbf{r}_{1, u/d}$. The bond vectors transform as $\mathbf{r}_i' = \mathbf{r}_i + \mathbf{u} \cdot \mathbf{r}_i + \mathbf{\Delta}_i$, with the constraints $0 = \Delta_{x} - \Delta_{y}$ and $0 = \Delta_{y} - \Delta_{x}$. Consequently $\mathbf{\Delta}_i \equiv \mathbf{\Delta}_i$. By inversion symmetry, vectors connecting to the upper layer and the lower layer transform in the same way, but with opposite signs in the out-of-plane direction. Hence, the strain–displacement response of TMDs is also characterized by a single in-plane vector $\mathbf{\Delta}_i$, and the change in inter-chalcogen distance $\Delta_z$.

The third class consists of a single material, phosphorene, an atomically thin puckered material derived from layered black phosphorus. Its PUC contains four atoms and six unique bond vectors, see figure 1(c). Four bond vectors are situated in the puckers and are denoted by $\mathbf{r}_{1, u/d}$ with $i = 1, 2$ and subscripts u/d. The two remaining vectors connect the upper and lower puckers, and are labeled $\mathbf{r}_{c1}$ and $\mathbf{r}_{c2}$. We find that $\mathbf{a}_1 = -\mathbf{r}_{c1} + \mathbf{r}_{1, u} + \mathbf{r}_{c2} + \mathbf{r}_{1, d}$, and $\mathbf{a}_2 = -\mathbf{r}_{c1} + \mathbf{r}_{1, u}$. Alternatively, we also write $\mathbf{a}_1 = -\mathbf{r}_{c1} + \mathbf{r}_{2, u} + \mathbf{r}_{c2} + \mathbf{r}_{1, d}$ and $\mathbf{a}_2 = -\mathbf{r}_{c1} + \mathbf{r}_{2, u}$. Hence, we obtain the constraints $0 = -\Delta_{y} + \Delta_{x} + \Delta_{c1} + \Delta_{c2} + \Delta_{2, d}$, $0 = -\mathbf{r}_{c1} + \mathbf{r}_{1, u}$. This leads to four equations for the vectors $\mathbf{\Delta}_i$. Using inversion symmetry and the same arguments as for the TMDs, the strain displacement relation in phosphorene is also characterized by a single in-plane vector $\mathbf{\Delta}_i$ and a change in vertical inter-pucker distance $\Delta_z$.

We conclude that due to lattice connectivity and symmetry constrains, the strain–displacement correction in all these monolayer 2D materials is
\[ \Delta_{ij} = \Delta_i + \Delta_j, \]  

(4)

independent of \(i\) and \(j\). Both \(\Delta_i\) and \(\Delta_j\) depend on the applied strain and on the interatomic interactions. Their calculation requires a microscopic model to account for the deformation energy. For uniform strain, one can determine the strain–displacement correction using the geometric considerations of the previous paragraph and, for instance, first principles calculations. For non-uniform strain and/or finite lattices, this procedure becomes computationally prohibitive, and one has to resort to semi-empirical force-field models.

In the following, we put forward a systematic approach to calculate \(\Delta_i\) and \(\Delta_j\) for any single-layer 2d material whose deformation energy is described by a force-field model parameterized by the bond vectors. Valence force models (VFs) are a convenient choice since they offer good accuracy at low computational costs. There are various VFs for the different 2d materials [16–20]. Let us focus on graphene-like materials, which can be accurately addressed using the VFM introduced by Perebeinos and Tersoff [18] to describe the interactions between sp²-bonded carbon atoms. The deformation energy is given by [18]

\[
E_{\text{def}} = \frac{\beta_1}{a_0^2} \sum_{i,j \in I} (\delta_{ij})^2 + \frac{\beta_2}{a_0^2} \sum_{i,j,k \in I} (\delta_{ij})(\delta_{jk}) \\
+ \frac{\beta_3}{a_0^2} \sum_{i,j,k \in I} (\delta_{ij,k})^2 + \frac{\beta_4}{a_0^2} \sum_{i,j,k \in I} (\delta_{ij})(\delta_{ik}) \\
+ \frac{\beta_5}{a_0^2} \sum_{i,j,k \in I} \left( \frac{3r_{ij}^2 \cdot r_{ik}^2 \times r_{jk}^2}{r_{ij}r_{ik} + r_{jk}r_{ik} + r_{ij}r_{jk}} \right)^2,
\]

(5)

where \(r_{ij} = |r_{ij}'|\) is the bond length, \(\delta_{ij} = r_{ij}' - a_0\) is the change in bond length and \(\delta_{ij,k}\) is defined as \(\delta_{ij,k} = \cos \theta_{ij,k} - \cos \theta_{ij,k}\). Here \(\theta_{ij,k}\) is the angle between atoms \(i, j\) and \(k\) with atom \(i\) as apex in equilibrium, while \(\theta_{ij,k}'\) is the angle in the deformed lattice. The summations in equation (5) follow the convention: (a) \(j \in I\) indicates that the index \(j\) runs over the three neighbors of atom \(i\) (b) for \(j < k \in I\) both \(j\) and \(k\) are neighbors of the atom \(i\), and are ordered to avoid double counting, leaving three possible terms; (c) \(j = k < l \in I\) leaves three terms for each \(i\). The first and third terms in equation (5) give the energy cost of stretching and bending bonds as in a Keating model [21]. The second and the fourth terms couple stretching of different bonds and couple stretching and bending, respectively. The last term is related to out-of-plane displacements. In [18], there is an additional term which penalizes misalignments of neighboring \(\pi\)-orbitals that we neglect here.

For a given strain, we minimize \(E_{\text{def}}\) with respect to \(\Delta_i\) and \(\Delta_j\) to obtain

\[
\Delta_i \equiv -a_0 \kappa(h) \left( \frac{u_{yy} - u_{xx}}{2u_{xy}} \right),
\]

(6a)

\[
\Delta_j \equiv \pm a_0 \kappa_L(h)(u_{xx} + u_{yy}),
\]

(6b)

where \(\kappa(h)\) and \(\kappa_L(h)\) are functions of the unit cell corrugation height \(h\) and characterize the changes in the PUC internal structure, in addition to the trivial shift of atomic positions when the PUC is strained. To lowest order in \(h/a_0\),

\[
\kappa(h) \approx \frac{-9\beta_2 - 4\beta_1 + 2\beta_3}{9\beta_2 + 4\beta_1 - 2(\beta_2 + 3\beta_3)},
\]

(7a)

\[
\kappa_L(h) \approx \frac{-\frac{h}{a_0}}{9\beta_2}. 
\]

(7b)

(Further details of this derivation are provided in the supplemental material.)

The form of equation (6a) can be interpreted as follows: let us consider the atom connected to its neighbors by the vectors \(r_i\) in figure 1(a). The vector \(\Delta\) corresponds to a shift of the position of this atom with respect to its neighbors. Due to symmetry, a tensile strain (nonvanishing \(u_{xx}\) or \(u_{yy}\)) can only shift the atom in \(x\)-direction. A shift in the position in \(y\)-direction gives rise to a sheared internal structure of the PUC. Consequently, the component \(\Delta_{\phi,y}\) must be
proportional to $u_y$, Let us now recall that $\Delta$ is chosen such that $E_{\text{def}}$ of the PUC is minimized. If the latter is stretched only in the $x$-direction, all bonds become longer, but the angle between the vectors connecting one of the basis atoms and the atoms in neighboring cells becomes smaller. The associated energy cost can be reduced if the bond between the basis atoms is increased relative to the cell size, since this increases the angle. For stretching in $y$-direction, the bond has to become shorter, since the change of angle has the opposite trend. Hence, $\Delta_{xx} \sim u_{xx} - u_{yy}$. The same argument holds for silicene, where the additional $z$-component, $\Delta_z$, has the same dependence on $u_{xx}$ and $u_{yy}$ and does not depend on shear to lowest order.

Upon elimination of $\Delta_2$ and $\Delta_3$, the microscopic deformation energy per unit area, $\mathcal{E} = E_{\text{def}}/A$, becomes the standard expression for the continuum elastic energy–density of an isotropic membrane [22],

$$\mathcal{E} = \frac{1}{2} \lambda (u_{xx} + u_{yy})^2 + \mu (u_{xx}^2 + u_{yy}^2 + 2u_{xy}^2) = \frac{Y_{2d}}{2(1 - \nu^2)}(u_{xx}^2 + u_{yy}^2 + 2\nu u_{xx}u_{yy}) + (1 - \nu)u_{yy}^2,$$

reconciling our results with previous works on the long-wavelength elastic behavior of graphene [1, 23, 24]. Here, $\lambda$ and $\mu$ are the Lamé parameters of the material, and $Y_{2d}$ and $\nu$ are the 2d Young modulus and Poisson ratio, respectively. They are related via

$$Y_{2d} = (\lambda + 2\mu)(1 - \nu^2), \quad \text{and} \quad \nu = \frac{\lambda}{\lambda + 2\mu}.$$

We find that the Lamé parameters, given in terms of the microscopic parameters of equation (5), are

$$\lambda = \frac{1}{\sqrt{2}a^2} \left[ \frac{8\beta_2^2 - 18\beta_3\beta_4 + 4\beta_3\beta_2 - 3\beta_2^2}{9\beta_2 + 4\beta_3 - 2(\beta_2 + 3\beta_3) \right. + \left. \frac{9\beta_2^2 - 36\beta_3\beta_4 - 4\beta_3^2 - 12\beta_3\beta_2}{9\beta_2 + 4\beta_3 - 2(\beta_2 + 3\beta_3) \right] \right],$$

$$\mu = \frac{3\sqrt{3}}{a^2} \left[ \frac{4\beta_3\beta_4 - 2\beta_3\beta_2 - 3\beta_2^2}{9\beta_2 + 4\beta_3 - 2(\beta_2 + 3\beta_3) \right] \right].$$

For graphene, the parameter values reported in [18] together with equations (7a) and (7b) lead to $\kappa = 0.39$ and $\kappa_1 = 0$. Moreover, equations (10a) and (10b) give $\lambda = 4.4$ eV Å$^{-2}$ and $\mu = 8.5$ eV Å$^{-2}$, which implies $Y_{2d} = 329$ N m$^{-1}$ and $\nu = 0.2$.

Neglecting the bond–bond and bond–angle correlations in equation (5) (setting $\beta_2 = \beta_3 = 0$), we find that $\kappa(h)$ depends only on the Poisson ratio, $\kappa(h) \approx 2\nu/(1 + \nu)$. Consequently, $\kappa(0)$ vanishes for materials with a negligible Poisson ratio (where $\mu \gg \lambda$), and is limited from above by $\kappa(0) < 2/3$ for isotropic materials (for which [22] $\nu < 1/2$). In this simplified VFM, $\kappa(0)$ agrees with the findings of [9], and may serve as a rough estimate, since it can be readily obtained from the Poisson ratio which is a macroscopically observable quantity. For $\nu = 0.2$ this approximation gives $\kappa \approx 1/3$, which agrees reasonably well with the value obtained from the full set of parameters ($\kappa = 0.39$). Similarly, we find $\kappa_1(h) \approx -2(h/a_0)(\beta_2/(9\beta_3))$.

The approximation $\kappa \approx 2\nu/(1 + \nu)$ is expected to hold also for TMDCs, due to the hexagonal structure of the lattice when projected onto the monolayer plane. For example, using $\nu_{\text{MoS}_2} = 0.27$ [25], we obtain $\kappa_{\text{MoS}_2} \approx 0.43$, which is slightly larger than the estimate for graphene.

For phosphorene, the strain–displacement relation no longer obeys the simple form of equation (6a), since $\Delta$ shows a directionality reflecting the material anisotropy. Nonetheless, having a suitable VFM for the deformation energy $E_{\text{def}}$ of phosphorene, we can still estimate its elastic properties using the approach described above. Now, for a given strain, we need to minimize $E_{\text{def}}$ with respect to $\Delta_{xx}$, $\Delta_{yy}$, and $\Delta_z$ (see supplementary material). Using a VFM developed for layered black phosphorus [26], we obtain sound velocities $v_{xx} = 3508$ m s$^{-1}$, $v_{yy} = 8147$ m s$^{-1}$, and $v_{yy} = 3707$ m s$^{-1}$ in good agreement with [26] (without correction $v_{xx}$ and $v_{yy}$ are overestimated by a factor $\approx 2$). The Young moduli are $Y_x = 17$ N m$^{-1}$ and $Y_y = 94$ N m$^{-1}$ (without corrections $Y_x = 58$ N m$^{-1}$ and $Y_y = 95$ N m$^{-1}$). These values are in good agreement with DFT calculations [27–29], where $Y_x = 24–29$ N m$^{-1}$ and $Y_y = 88–102$ N m$^{-1}$. Hence, a correct treatment of the strain–displacement relations is necessary to account for the predicted anisotropy of phosphorene [30].

We illustrate our results by studying armchair graphene nanoribbons (AGNRs) stretched along the longitudinal direction. See figure 2 for a sketch of the setup. The equilibrium configuration is obtained by minimizing $E_{\text{def}}$ given by equation (5). The mechanical energy density as a function of the applied strain $u_{xx}$ is shown in figure 3(a). Numerical results are denoted by symbols, whereas full and dashed lines correspond to analytical results obtained from equation (8) for $\kappa = 0.39$ and $\kappa = 0$. By setting $\kappa = 0$, one obtains a slightly larger value of $Y_{2d}$ such that the stretching energy is overestimated. We also calculate the resulting strain $u_{yy}$ in the transversal direction. As the ribbon contracts upon stretching, $u_{yy}$ is negative for $u_{xx} > 0$ and decreases with increasing strain. This is shown in figure 3(b). The slope of the curve at $u_{xx} = 0$ gives the Poisson ratio, which agrees very well with the estimate obtained from equation (9). The standard approach, for which $\kappa = 0$, gives $\nu(\kappa = 0) \approx 0.16$, thus underestimating the Poisson ratio.

The strain–displacement relations presented above significantly modify the electronic properties of deformed 2d materials, which are crucial for strain-engineering [3, 4, 31]. Essentially, mechanical deformations have two effects on the electrons. Firstly, the change in electron-ion potential in the neighborhood
of an atom generates an on-site potential often referred to as the deformation potential. Secondly, changes in the distances between neighboring atoms modify the overlaps of the corresponding orbital wave-functions and thus the electronic structure.

These effects are accounted for in the nearest-neighbor hopping Hamiltonian which provides an accurate description of the low-energy $\pi$-bands in graphene \cite{2, 9, 11}, namely,

$$H = \sum_{i=1}^{N_c} \left( 3v_0(a_0) + \frac{g}{a_0} \sum_{<i,j>} \frac{r_{ij} \cdot \delta r_{ij}}{a_0} \right) c_i^\dagger c_i - t_0(a_0) \sum_{<i,j>} \left( 1 - \frac{\beta}{a_0} \frac{r_{ij} \cdot \delta r_{ij}}{a_0} \right) c_i^\dagger c_j. \quad (11)$$

Here $\beta/a_0 = -t'_0(a_0)/t_0(a_0)$, $g/a_0 = v'_0(a_0)$, where $t_0(r)$ is the (distance dependent) hopping amplitude and $v_0(r)$ is the electron-ion potential. In the following we omit the overall on-site energy $3v_0(a_0)$.

To obtain analytical insight, it is customary \cite{2, 11–13} to consider the low-energy limit of the tight-binding model above. By expressing equation (11) in reciprocal space and taking its long wavelength limit, that is, by expanding $H$ to linear order in momentum around the $K$ and $K'$-points \cite{2, 11}, one obtains an effective Dirac Hamiltonian. For $K$ we write

$$H_K = v_F\sigma \cdot (p - A) + v_D\Delta_2, \quad (12)$$

where $v_F = 3a_0 t_0/2 \approx 10^5$ m s$^{-1}$, $\sigma$ are Pauli matrices, $p$ is the momentum, $A$ is the vector potential, and $v_D$ is the scalar deformation potential. The latter are given by

$$A_x = \frac{\beta(1 - \kappa)}{a_0} u_{xy}, \quad (13a)$$

$$A_y = \frac{\beta(1 - \kappa)}{2a_0} (u_{yy} - u_{xx}), \quad (13b)$$

$$v_D = \frac{3g}{2} [1 + 2\kappa_\zeta (h\hbar)] (u_{xx} + u_{yy}). \quad (13c)$$

Considering that the elastic properties are dominated by the $\sigma$-orbitals and the electronic structure by the $\pi$-orbitals, the similarity between the dependence of $\Delta$ and $A$ on the strain tensor is remarkable. The fact that both reflect actual atomic displacements to linear order and the simplicity of the microscopic model explain why they have the same form.

Hence, we find that the strain-displacement relations renormalize $A$ by a factor $1 - \kappa$ with respect to the standard elasticity-induced gauge theory.

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**Figure 2.** Structure of an armchair nanoribbon. The highlighted area represents the system unit cell. The ribbon consists of $N_1 \times N_2$ cells, where $N_1$ counts the cells in $x$-direction and $N_2$ in $y$-direction. In the lateral direction periodic boundary conditions are imposed at the edges.

**Figure 3.** Strain $u_{xx}$ dependence of (a) the elastic energy and (b) the resulting strain $u_{xy}$ for AGNRs of different widths ($N_1 = 300$ in all cases). Symbols denote numerical results. The full (dashed) line stands for the continuum model results with $\kappa \approx 0.39$ ($\kappa = 0$). The shaded region indicates the range of Poisson ratios from $\nu (\kappa = 0) = 0.16$ to $\nu (\kappa = 0) = 1/2$. 

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The full (dashed) line stands for the continuum model results with $\kappa \approx 0.39$ ($\kappa = 0$). The shaded region indicates the range of Poisson ratios from $\nu (\kappa = 0) = 0.16$ to $\nu (\kappa = 0) = 1/2$. 

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These effects are accounted for in the nearest-neighbor hopping Hamiltonian which provides an accurate description of the low-energy $\pi$-bands in graphene \cite{2, 9, 11}, namely,
For graphene, the material parameters [11, 12, 32–35]. For graphene, the material parameters [18] give 1 − κ ≈ 3/5. (Using the approximation κ ≈ 2ν/(1 + ν) we obtain 1 − κ ≈ (1 − ν)/(1 + ν) = 2/3.) Based on a VFM that drastically overestimates the Poisson ratio, previous works [9, 14] report a reduction factor of about 1/3. Note that in the derivation above, we ignore the strain-dependent renormalization of the Fermi velocity reported previously [35], since it has a negligible effect on our results.

The reduced vector potential has an important effect on strain engineering applications [32, 34]. Let us analyze, for instance, the first (sub)band-gap of AGNRs [31]. In the long wavelength limit, the magnitude of this band gap is given by

\[ E_g \approx \sqrt{\frac{3}{2}} |t_0| \min_{n=0,1, \ldots} \left[ \frac{\pi}{N_2 + 1} (n - \varphi) \right. \]

\[ \left. - \frac{\sqrt{3} \beta_y}{2} (1 - \kappa)(1 + \nu) \mu_{xx} \right] \]

with \( \varphi = 0 \) for metallic and \( \varphi = 1/3 \) for semiconducting AGNRs and where \( N_2 \) is the number of unit cells in the transversal direction and \( n \) is the band index. The magnitude of the band-gap as a function of strain is piecewise linear and shows a characteristic zig-zag shape. We predict that the slope of the linear regions is decreased by a factor \((1 - \kappa) \approx 3/5 \) for graphene due to the strain–displacement relations, while the positions of the maxima and minima of the band gap are shifted by a factor \(1/(1 - \kappa) \approx 5/3 \) for graphene.

A similar renormalization is also found for phosphorene, which has a direct band-gap \( E_{gap} \approx 1.6 \) eV. Based on the two orbital tight-binding model put forward in [36] and the strain–displacement relations derived in the supplementary material we find an anisotropic renormalization of the strain-induced bandgap, which reduces the gap by factors 2.5 and 1.35 when straining in \( x \) and \( y \) direction, respectively. For the strain dependence of the band-gap (in eV) we find

\[ \Delta E_{gap} \approx 0.755 \mu_{xx} + 2.612 \mu_{yy}. \]

3. Conclusions

Two-dimensional materials have gained considerable interest, in particular due to the enticing prospect of engineering their electronic properties using strain. Our results show that the relationship between strain and electronic properties is less trivial than often assumed. For Bravais lattices, the relation between strain and displacements is simple, namely the bond vectors transform as \( \mathbf{r}_j \rightarrow (\mathbf{r}_j + \mathbf{u}) \). For non-Bravais lattices, the Cauchy-Born rule breaks down [6], the basis atoms introduce additional degrees of freedom, significantly modifying the relation between strain and displacement. With few exceptions [9, 14], this fact is typically neglected in the literature on electronic properties of deformed 2d materials [3, 4, 10, 11, 32–34]. We show that under an applied strain the bond vectors of 2d materials generally transform as \( \mathbf{r}_j \rightarrow (\mathbf{r}_j + \mathbf{u}) \). The vectors \( \Delta_1 \) and \( \Delta_2 \) are determined by minimizing the deformation energy. For graphene, the strain–displacement effect on the electronic properties is to renormalize the vector potential by a factor \((1 - \kappa) \approx 3/5 \) while keeping its functional form. We provide a simple estimate of this correction based on the macroscopically observable Poisson ratio \( \nu \), as \((1 - \kappa) \approx (1 - \nu)/(1 + \nu) \). The \((1 - \kappa) \) renormalization alters the dependence of the band gap in AGNRs on strain: it increases the strain required to reach a certain band gap. Having a well controlled band gap is of key importance in a variety of applications [3, 4, 37–39].

For 2d materials with a more complex crystal structure than graphene, such as the TMDCs and phosphorene, the strain–displacement relations we put forward are key to understand their fundamental material properties. For phosphorene, we show (see supplementary material) that its anisotropic mechanical properties [27, 40] can only be correctly described by considering proper strain–displacement relations. Furthermore, phosphorene is considered to be very interesting from a strain-engineering perspective as it displays a strain dependent band-gap [5, 41–43]. Our strain–displacement relations lead to an anisotropic renormalization of this gap. This Letter provides a transparent approach to estimate the electromechanical coupling in single-layer 2d materials, given that the mechanical and electrical properties are reliably parameterized.

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