Ultrathin-Layer Strain-Based Electronic Devices: From-First-Principles Derivation of the Corresponding Equation

Julio C. Urenda and Vladik Kreinovich

Abstract Most information about the world comes from sensors – and from the results of processing sensor data. In many practical situations – e.g., in biomedical applications – it is desirable to make sure that the sensors are as "invisible" as possible, in particular, that they are as small as possible. One way to achieve such small size is to use ultrathin-layer materials such as graphene. It is known that for such materials, strain causes electromagnetic effects – which can be used to detect small strains. Interestingly, it turned out that the same equation describes the relation between strain and electric effects and between strain and magnetic effects – although in these two cases, physics is somewhat different. The fact that we get the same equation in two different physical situations leads to a natural conjecture that this equation should follow from first principles, without the need to use specific physical equations. In this paper, we show that this is indeed the case: one of the main equations of straintronics can be derived from first principles, without using specific equations of physics.

1 Straintronics: Use of Ultrathin-Layer Strain-Based Electronic Devices

What is straintronics. One of the main objectives of engineering is to control different systems: mechanical systems, biomedical systems – e.g., that help the heart, etc. In many such cases – e.g., in many biomedical applications – it is desirable to make the sensors as "invisible" and convenient as possible. For this purpose, they

Julio C. Urenda
Department of Mathematical Sciences, University of Texas at El Paso, 500 W. University
El Paso, Texas 79968, USA, e-mail: jcurenda@utep.edu

Vladik Kreinovich
Department of Computer Science, University of Texas at El Paso, 500 W. University
El Paso, Texas 79968, USA, e-mail: vladik@utep.edu

should be made as small as possible. One way to decrease the sensor size is to use ultrathin-layer materials such as graphene. One of the important properties of such layers is that for them, strain changes their electromagnetic properties. This can be used to design sensitive and compact strain sensors. The use of strain-related eletromagnetic effects in ultrathin-layer electronic devices is known as *straintronics*; see, e.g., [1, 2, 3, 4, 5].

The energy equation of straintronics. One of the main equations of straintronics describes the free energy of the layer as

$$E = \gamma \cdot \mathbf{P} \cdot [\mathbf{n} \cdot \operatorname{div} \mathbf{n} - (\mathbf{n}\nabla)\,\mathbf{n}], \tag{1}$$

i.e., in coordinate terms,

$$E = \gamma \cdot \sum_i P_i \cdot \left[n_i \cdot \sum_j n_{j,j} - \sum_j n_j \cdot n_{i,j} \right], \tag{2}$$

where γ is the interaction constant, $\mathbf{P}$ is the electric polarization vector (or a similar vector describing the magnetic field), $\mathbf{n}$ is unit vector describing the layer's orientation, and $n_{i,j}$ stands for the partial derivative

$$n_{i,j} \stackrel{\text{def}}{=} \frac{\partial n_i}{\partial x_j}.$$

The formula (2) can be rewritten in a simpler form if we use Einstein notations, where in a product repeated indices mean summation over this index. In terms of these notations, the formula (2) takes the following form:

$$E = \gamma P_i [n_i n_{j,j} - n_j n_{i,j}]. \tag{3}$$

Natural question. The equation (1)-(3) is usually derived from the corresponding physical equations. It was first derived for the relation between strain and electric effects. It then turned out that the same equation is applicable to the relation between strain and magnetic effects, although in this case, physical equations are somewhat different. The fact that the same equation appears in two somewhat different physical situations leads to a natural conjecture that this equation can be derived from basic first principles, without the need for specifics physical equations.

What we do in this paper. In this paper, we confirm this natural conjecture by showing that the above equation can be derived without the need to use specific physical equations.

2 Our derivation

Assumptions that are already implicity used in this equation. Since the material is ultrathin, even a minor change in the outside environment or in the geometry of the layer can cause large changes in the layer – it can also easily destroy this layer. This sensitivity is one of the features that makes these materials appropriate for sensitive sensors.

Due to the same sensitivity, the vector **P** describing electromagnetic effect has to be relatively small – otherwise, if the effect is large, the fragile ultrathin layer will simply break. Similarly, the derivatives $n_{i,j}$ that describe the non-homogeneity of the layer's state should be small: if there is a big difference between the states at the neighboring parts of the layer, the layer will break.

Since both P_i and $n_{i,j}$ are small, terms which are quadratic (or of higher order) in terms of these quantities can be safely ignored. So, we can safely assume that the energy E depends linearly on both P_i and $n_{i,j}$. In general, such a bilinear dependence takes the following form:

$$E = E_0 + E_i P_i + E_{i,j} n_{i,j} + E_{ijk} P_i n_{j,k}, \tag{4}$$

for some coefficients E_i, E_{ij}, and E_{ijk}.

When energy is 0. When there is no electromagnetic effect, i.e., when $P_i = 0$, there is no corresponding energy accumulated, so E should be 0. For $P_i = 0$ and $E = 0$, the formula (4) has the form

$$0 = E_0 + E_{i,j} n_{i,j}. \tag{5}$$

This equality should be true for all possible values of $n_{i,j}$. In particular:

- for $n_{i,j} = 0$, we conclude that $E_0 = 0$, and
- for $n_{i,j} \neq 0$, the fact that the linear function (5) is always equal to 0 means that all the coefficients are equal to 0, i.e., that $E_{i,j} = 0$.

Thus, the formula (4) takes the following simplified form:

$$E = E_i P_i + E_{ijk} P_i n_{j,k}. \tag{6}$$

Similarly, if there is no non-homogeneity of the layer, i.e., if the layer is still in its original state $n_{i,j} = 0$, there is no energy accumulated, so E should also be 0. Substituting $n_{i,j} = 0$ and $E = 0$ into the formula (6), we get

$$0 = E_i P_i. \tag{7}$$

This formula has to be true for all P_i, so we can conclude that all the coefficients E_i of the linear form $E_i P_i$ are equal to 0. Substituting $E_i = 0$ into the formula (6), we get a simplified formula

$$E = E_{ijk} P_j n_{j,k}. \tag{8}$$

The values E_{ijk} depend only on n_i. This dependence should be rotation-invariant, so E_{ijk} should be an algebraic combination of n_i and the unit matrix δ_{ij} for which $\delta_{ii}=1$ and $\delta_{ij}=0$ for all $i \neq j$. Here, n_i is a unit vector, so $n_i n_i = \delta_{ij} n_i n_j = 1$. Thus, the only possible combinations are

$$E_{ijk} = c_1 \cdot n_i \cdot \delta_{jk} + c_2 \cdot n_j \cdot \delta_{ik} + c_3 \cdot n_k \cdot \delta_{ij} + c_4 \cdot n_i \cdot n_j \cdot n_k. \quad (9)$$

Substituting the expression (9) into the formula (8), we conclude that

$$E = P_i \cdot [c_1 n_i n_{j,j} + c_2 n_j n_{j,i} + c_3 n_j n_{i,j} + c_4 n_i n_{j,k} n_j n_k]. \quad (10)$$

The term $n_j n_{j,i}$ is equal to $(1/2)(n_j n_j)_{,i}$. Since n_i is a unit vector, $n_j n_j$ is a constant: $n_j n_j = 1$. So, the derivative of $n_j n_j$ is equal to 0. Hence, $n_j n_{j,i} = n_{j,k} n_j = 0$ and so, $c_2 n_j n_{j,i} = c_4 n_i n_{j,k} n_j n_k = 0$. Thus, the expression (10) takes the following simplified form:

$$E = P_i [c_1 n_i n_{j,j} + c_3 n_j n_{i,j}]. \quad (11)$$

This is a multi-D effect. Another idea is that this is a multi-D effect, it can be observed in 2D layers, but not in the 1D case. So, for the 1D case, the energy should also be equal to 0. The 1-D case means that:

- the electromagnetic effect is 1-D, i.e., $P_1 \neq 0$ while $P_2 = \ldots = 0$, and
- the vector n_i only depend on x_1, i.e., $n_{i,j} = 0$ for all $j > 1$.

In this case, $E = 0$, $P_1 \neq 0$, $n_{j,j} = n_{1,1}$ and $n_j n_{i,j} = n_1 n_{i,1}$. So, the formula (11) takes the following form:

$$0 = P_1 [c_1 n_1 n_{1,1} + c_3 n_1 n_{1,1}], \quad (12)$$

i.e.,

$$0 = P_1 (c_1 + c_3) n_1 n_{1,1}. \quad (13)$$

Since $P_1 \neq 0$, we can divide both sides by P_1 and get

$$0 = (c_1 + c_3) n_1 n_{1,1}. \quad (14)$$

This expression has to be true for all possible values of n_1 and $n_{1,1}$, so we must have $c_1 + c_3 = 0$ and $c_3 = -c_1$. Thus, if we denote $\gamma \stackrel{\text{def}}{=} c_1$, the formula (11) takes the desired form

$$E = \gamma P_i [n_i n_{j,j} - n_j n_{i,j}]. \quad (3)$$

Conclusion. So, we have indeed derived the formula (3) without using any specific physical equations.

Acknowledgments

This work was supported in part by the National Science Foundation grants 1623190 (A Model of Change for Preparing a New Generation for Professional Practice in Computer Science), HRD-1834620 and HRD-2034030 (CAHSI Includes), EAR-2225395 (Center for Collective Impact in Earthquake Science C-CIES), and by the AT&T Fellowship in Information Technology.

It was also supported by a grant from the Hungarian National Research, Development and Innovation Office (NRDI), and by the Institute for Risk and Reliability, Leibniz Universitaet Hannover, Germany.

References

1. S. Bandyopadhyay, *Magnetic Straintronics: An Energy-Efficient Hardware Paradigm for Digital and Analog Information Processing*, Springer, Cham, Switzerland, 2022.
2. S. Bandyopadhyay, “There is plenty of room for magnetic straintronics in the analog domain”, *npj Spintronics*, 2024, Vol. 2, Paper 15, https://doi.org/10.1038/s44306-024-00018-3
3. C. S. Boland, Y. Sun, and D. G. Papageorgiou, “Bandgap engineering of 2D materials toward high-performing straintronics”, *Nano Letters*, 2024, Vol 24, No. 41, pp. 12722–12732.
4. A. A. Bukharaev, A. K. Zvezdin, A. P. Pyatakov, and Yu. K. Fetisov, “Straintronics: a new trend in micro- and nanoelectronics and materials science”, *Physics-Uspekhi*, 2018, Vol. 61, No. 12, pp. 1175–1212, arXiv:1101.5243, doi:10.3367/ufne.2018.01.038279
5. F. Mesple, A. Missaoui, T. Cea, L. Huder, F. Guinea, G. Trambly de Laissardiére, Guy, C. Chapelier, and V. T. Renard, “Heterostrain determines flat nands in magic-angle twisted graphene layers”. *Physical Review Letters*, 2021, Vol. 127, No. 12, Paper 126405, arXiv:2012.02475, doi:10.1103/PhysRevLett.127.126405