Applied Physics B (2018) 124:10
https://doi.org/10.1007/s00340-017-6879-4

Applied Physics B
Lasers and Optics

Two-dimensional electroacoustic waves in silicene

Alexander V. Zhukov[1,2] **· Roland Bouffanais**[1] **· Natalia N. Konobeeva**[3] **· Mikhail B. Belonenko**[2,3,4]

Received: 5 November 2017 / Accepted: 6 December 2017

Abstract

In this letter, we investigate the propagation of two-dimensional electromagnetic waves in a piezoelectric medium built upon silicene. Ultrashort optical pulses of Gaussian form are considered to probe this medium. On the basis of Maxwell's equations supplemented with the wave equation for the medium's displacement vector, we obtain the effective governing equation for the vector potential associated with the electromagnetic field, as well as the component of the displacement vector. The dependence of the pulse shape on the bandgap in silicene and the piezoelectric coefficient of the medium was analyzed, thereby revealing a nontrivial triadic interplay between the characteristics of the pulse dynamics, the electronic properties of silicene, and the electrically induced mechanical vibrations of the medium. In particular, we uncovered the possibility for an amplification of the pulse amplitude through the tuning of the piezoelectric coefficient. This property could potentially offer promising prospects for the development of amplification devices for the optoelectronics industry.

1 Introduction

With the rapid development of laser technology, a growing interest is observed in studying the propagation of extremely short optical pulses in different environments [1–4]. Among a host of newly discovered media, graphene-like materials take a special place because of the wide range of related practical applications to modern optoelectronics stemming from peculiar nonlinear phenomena. The occurrence of the so-called "light bullets" is one such example. Light bullets are wave packets that are localized in space and that can travel through a medium while retaining their spatiotemporal shape—in spite of diffraction and dispersion effects. Over the past decade, the dynamics of light bullets in these structures has been the subject of a significant number of studies [5–14]. In particular, the effective governing equations were established and the dynamics of the pulse with the influence of impurities and the Coulomb interaction between electrons was comprehensively studied. Furthermore, the processes and mechanisms of collision between light bullets, as well as the influence of external fields have been thoroughly investigated.

Among the affected range of issues, however, there are a number of challenges remaining that are not addressed in the papers cited above. First of all, there is the question of the influence of the physical properties of the medium into which the " target material" is placed. In this regard, Refs. [15, 16] can be noted as they study the impact from the medium dispersion on the propagation of light bullets. Meanwhile, as we know, the medium can have other properties (e.g., piezoelectric, magnetic, ferroelectric, and so forth), which may have a significant influence on the propagation of light bullets. In this study, we investigate the consequences of piezoelectricity in a medium with silicene, which has a structure consisting of a single layer of silicon atoms in a hexagonal lattice [17–19]. Relatively recently, such a structure has been experimentally fabricated [20, 21]. Placed in a particular environment, the silicene structure will contribute to the propagation of light bullets, thereby generating intense electric fields. The latter contributes to the emergence of a nonlinear response of the medium.

It is important stressing that we consider here a free-standing silicene [17] immersed in a piezoelectric medium. Our primary concern is to investigate the influence of a strong spin–orbit interaction on the ultrashort pulse propagation. However, it is worth noting recent *ab initio* investigations [22],

✉ Alexander V. Zhukov
alex.zhukov@outlook.sg

1 Singapore University of Technology and Design, 8 Somapah Road, Singapore 487372, Singapore

2 Entropique Group Ltd, 3 Spylaw Street, Maori Hill, Dunedin 0910, New Zealand

3 Volgograd State University, Volgograd 400062, Russia

4 Laboratory of Nanotechnology, Volgograd Institute of Business, Volgograd 400048, Russia

Published online: 20 December 2017

showing that silicene itself can get a piezoelectric behavior under certain conditions. The choice of silicene as the central object of our study originates in the fact that silicene has a particular gap in the energy spectrum, which makes silicene-based devices very promising in modern micro- and nano-electronics. This gap arises for two reasons. First, it is a direct consequence of its atomic arrangement—silicon atoms are not strictly arranged in the same plane, unlike graphene for instance. When an electric field is applied perpendicular to that plane, the electronic degeneracy disappears, thereby leading to the appearance of an electronic bandgap. It is worth noting that this effect makes it impossible to control the size of the band-gap by applying a constant external field. The second reason is that there is a strong spin–orbit interaction in silicene. The latter induces a lifting of the electronic degeneracy between the sublattices. Finally, it is worth highlighting that the study of materials with a strong spin–orbit interaction has recently gained significant traction owing to their increasing potential of applications in electronics and spintronics.

2 Formulation of the problem and general equations

Let us consider the propagation of two-dimensional (2D) extremely short electromagnetic pulses in silicene. The electric field of the pulse is assumed to be parallel to the (x, y)-plane of silicene. The geometry of the problem is presented schematically in Fig. 1.

The dispersion law for silicene reads [23]:

$$\epsilon_{\sigma\xi} = \pm\left\{ v^2k^2 + \frac{1}{4}\left(\Delta_z - \sigma\xi\Delta_{SO}\right)\right\}^{1/2}, \qquad (1)$$

where $\xi = \pm 1$ is the valley sign for the two Dirac points, v is the velocity of Dirac electrons, $k = (k_x, k_y)$ is the electron quasi-momentum; Δ_{SO} is the strength of the spin–orbit interaction in silicene; $\Delta_z = lE_z$ is the single-site lattice potential, where E_z is the constant electric field, and l is the distance between the two sublattice planes; σ is the electron spin. Furthermore, we only take into account the positive direction of rotation.

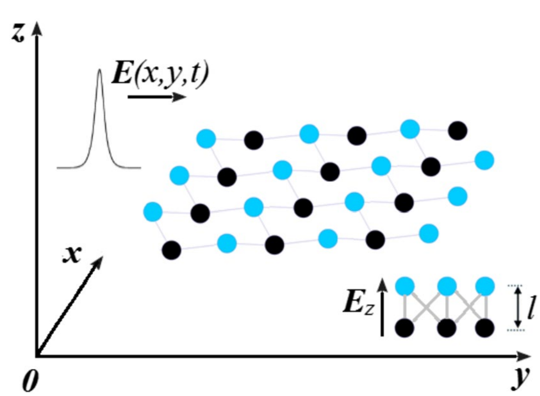

Fig. 1 Schematic diagram of the problem with associated notations

In the presence of an external electric field $\mathbf{E}$, which is considered using the particular choice of Coulomb's gauge, $\mathbf{E} = -\frac{1}{c}\partial\mathbf{A}/\partial t$, it is necessary to replace the momentum with the generalized momentum, i.e., $p \rightarrow p - eA/c$ (e being the elementary charge and c the speed of light in vacuum). Maxwell's equations with the account of the gauge in a 2D case read as follows:

$$\frac{\partial^2\mathbf{A}}{\partial x^2} + \frac{\partial^2\mathbf{A}}{\partial y^2} - \frac{1}{c^2}\frac{\partial^2\mathbf{A}}{\partial t^2} + \frac{4\pi}{c}\mathbf{j} = \frac{4\pi}{c^2}\frac{\partial^2\mathbf{P}}{\partial t^2}, \qquad (2)$$

where we neglect the diffraction spreading of the laser beam in the directions perpendicular to the axis of propagation, namely the y-axis. The vector potential is assumed to take the form $\mathbf{A} = \{0, A(x, y, t), 0\}$, and the current is $\mathbf{j} = \{0, j(x, y, t), 0\}$. To account for the properties of the medium, we have added the term with the polarization vector $\mathbf{P}$, directed along the silicene plane.

Let the electric field of the ultrashort optical pulse to be directed along y axis, namely $\mathbf{E} = \{0, E(x, z, t), 0\}$. Thus, the electron velocity is given by $v_y(\mathbf{k}) = \partial\epsilon(k_x, k_y)/\partial k_y$. Following the analytical scheme used in Ref. [24], we can rewrite Eq. (2) as follows:

$$\frac{\partial^2 A}{\partial x^2} + \frac{\partial^2 A}{\partial y^2} - \frac{1}{c^2}\frac{\partial^2 A}{\partial t^2} + \frac{4\pi}{c}j(A + \eta) = \frac{4\pi}{c^2}\frac{\partial^2 P}{\partial t^2}, \qquad (3)$$

where the electron current density $j(A)$ is now determined from

$$j(A) = \int_{-\Theta}^{\Theta} \mathrm{d}k_x \int_{-\Theta}^{\Theta} \mathrm{d}k_y v_y\left(k - \frac{e}{c}A(x, y, t)\right). \qquad (4)$$

Note that the integration range, denoted as Θ in Eq. (4), can be determined from the conservation of the number of electrons:

$$\int_{-\Theta}^{\Theta} \mathrm{d}k_x \int_{-\Theta}^{\Theta} \mathrm{d}k_y = \iint_{BZ} \mathrm{d}k_x \mathrm{d}k_y \langle a^{\dagger}_{k_x,k_y} a_{k_x,k_y}\rangle, \qquad (5)$$

where $a^{\dagger}_{k_x,k_y}$ and a_{k_x,k_y} are the electron creation and annihilation operators, respectively, and the integration of the r.h.s. term is performed over the Brillouin zone (BZ). Moreover, the quantity η in the l.h.s of Eq. (3) is associated with the nonzero component of the environment displacement vector u:

$$\eta = -cd \int_{-\infty}^{t} \frac{\partial u(z, t')}{\partial y}\mathrm{d}t'. \qquad (6)$$

Here, we consider one of the possible simplest models, such that the induced polarization in the medium admits linear variations with the applied electric field, and is directed parallel to the electric field due to the piezoelectric effect:

$$P = d\frac{\partial u}{\partial y}, \tag{7}$$

where d stands for the piezoelectric coefficient. Equation (3) in this case needs to be supplemented with the equation governing the nonzero component of the displacement vector u [24, 26, 27]:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} - \frac{1}{v_a^2}\frac{\partial^2 u}{\partial t^2} + \frac{d}{\rho}\frac{\partial P}{\partial y} = 0, \tag{8}$$

where ρ is the density of the medium and v_a is the acoustic velocity, which is taken to be $v_a = 0.001c$ in further calculations.

It is important to highlight a number of points related to the model used in this study. First, we take into consideration only one component of the displacement vector $\mathbf{u}$, which can obviously be easily generalized. More importantly, we do not take into account the possibility for nonlinear acoustic effects in the environment that would lead to a polarization vector being not collinear with the electric field.

3 Results of the numerical modeling

Equation (3) was solved numerically using the direct cross-type difference scheme [28]. The initial condition is chosen in the form of a Gaussian pulse:

$$\begin{aligned} A(x,y,t=0) &= Q\exp\left(-\frac{y^2}{\gamma_y^2}\right)\exp\left(-\frac{x^2}{\gamma_x^2}\right),\\ \frac{\mathrm{d}A}{\mathrm{d}t}(x,y,t=0) &= \frac{2yv_y}{\gamma_y^2}Q\exp\left(-\frac{y^2}{\gamma_y^2}\right),\exp\left(-\frac{x^2}{\gamma_x^2}\right), \end{aligned} \tag{9}$$

where Q and v_y are the initial pulse amplitude and velocity, respectively; γ_x and γ_y determine the pulse width in the respective directions. As for the mechanical displacement u, the initial conditions read as follows:

$$\begin{aligned} &u(x,y,t=0) = 0,\\ &\frac{\mathrm{d}u}{\mathrm{d}t}(x,y,t=0) = 0, \end{aligned} \tag{10}$$

corresponding to a medium at rest initially with a zero velocity.

For all numerical simulations, we used the following values for the involved parameters: $Q = 4\times 10^6\,\mathrm{V/m}, \gamma_y = 0.3\,\mu\mathrm{m}, \gamma_x = 0.5\,\mu\mathrm{m}, v_y = 0.95c$, where c is the speed of light in vacuum. The evolution of the electromagnetic field during its propagation through the sample is shown in Fig. 2.

It may be noted that the pulse propagates rather steadily (with regards to its amplitude and shape), experiencing only some spreading over time. One can also notice the emergence of a "tail" behind the pulse that has approximately zero area. Note that these results further reveal the fact that the dynamics of the pulse is not affected by the acoustic waves in the environment, since the speed of the pulse approaches the speed of light (~ 95% of it). Thus, it is possible to conclude that the electric field of the pulse does not "feel" acoustic vibrations in the environment induced by its passage.

The dependence of the pulse shape on the single-site lattice potential, Δ_z, is shown in Fig. 3. As can be seen from the figure, the greater the value of the potential Δ_z on the lattice site, the greater part of the energy is concentrated in the main pulse.

Finally, we also studied the effect of the piezoelectric coefficient d on the pulse propagation through the sample (see Fig. 3). The figure shows that in stark contrast to the

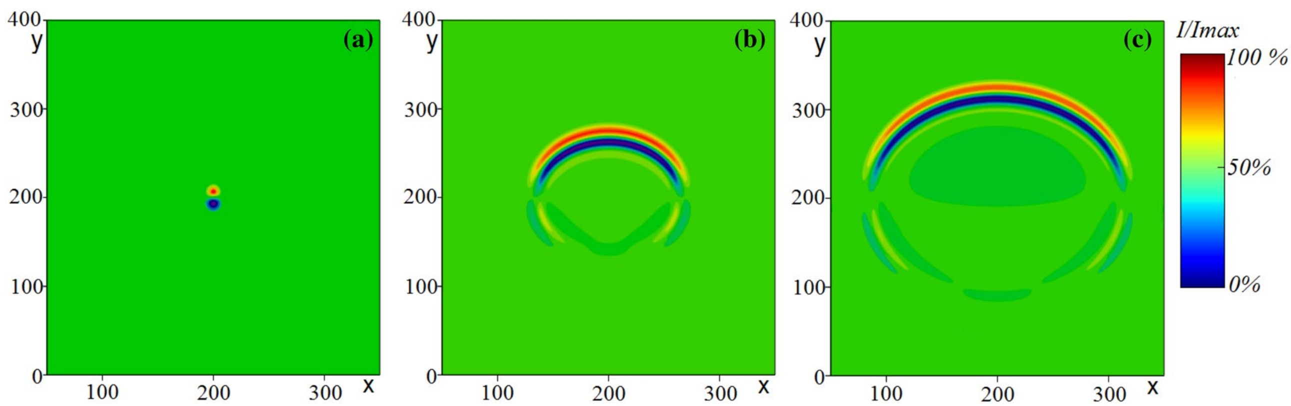

Fig. 2 Intensity of the 2D electromagnetic pulse $I(x,y,t) = E^2(x,y,t)$, with $d = 0.1$, and at different instants of time: **a** initial pulse; **b** $t = 4.0\times 10^{-13}$ s; (c) $t = 7.5\times 10^{-13}$ s. Units on x- and y-axes correspond to 30 and 20 nm, respectively

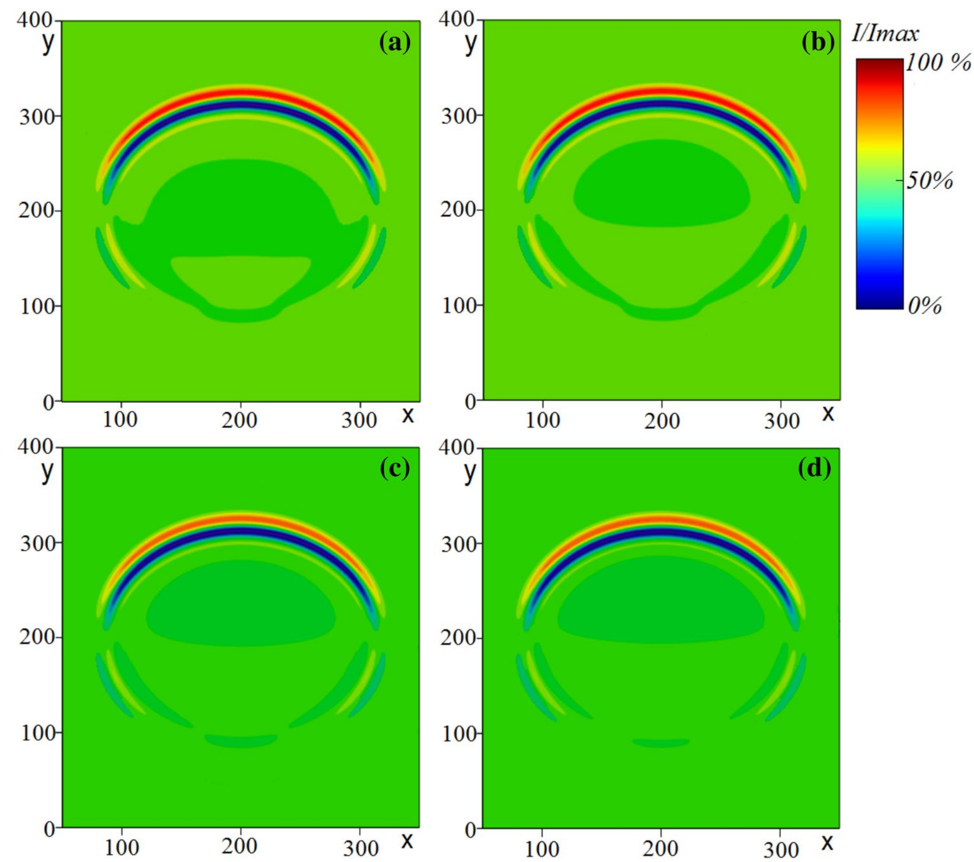

Fig. 3 Intensity of the 2D electromagnetic pulse $I(x, y, t) = E^2(x, y, t)$ with $d = 0.1$, and at time $t = 7.5 \times 10^{-13}$ s for different values of the potential Δ_z: **a** $\Delta_z = 0$ eV; **b** $\Delta_z = 0.1$ eV; **c** $\Delta_z = 0.25$ eV; **d** $\Delta_z = 0.5$ eV. Units on x- and y-axes correspond to 30 and 20 nm, respectively

case with carbon nanotubes [24], this parameter determines not only the shape of the "tail", but also has a significant impact on the main pulse propagating in a silicene-based medium. This effect manifests itself in a noticeably weaker spreading of the main pulse. The larger the value of the piezoelectric parameter d, the less energy is transferred to the "tail" due to the piezoelectric effect. It, therefore, appears that one can control the propagation regime of the pulse by selecting a particular environment with an appropriate value of the piezoelectric coefficient d (Fig. 4).

4 Conclusions

As a result of our study, the following conclusions can be made:

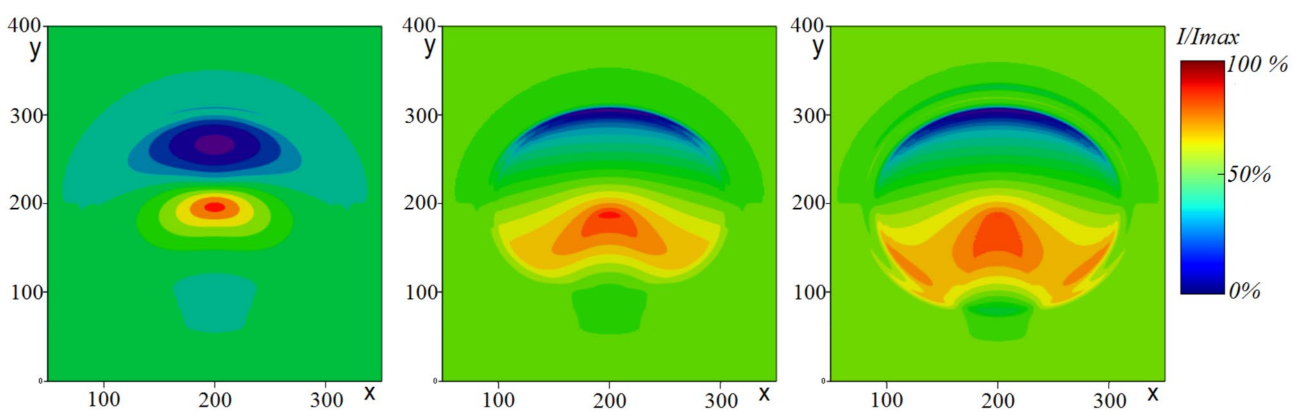

Fig. 4 Intensity of the 2D electromagnetic pulse $I(x, y, t) = E^2(x, y, t)$ at time $t = 7.5 \times 10^{-13}$ s for different values of the piezoelectric coefficient d: **a** $d = 0.1$; **b** $d = 1.0$; **c** $d = 10$. Units on x- and y-axes correspond to 30 and 20 nm, respectively

1. We demonstrate the possibility for a stable propagation of two-dimensional ultrashort optical pulses in a piezoelectric medium with silicene, which carries particular importance for practical applications in silicon-based microelectronic devices.
2. The value of the piezoelectric coefficient d determines the character of the oscillations in the "tail" following the main pulse.
3. For the first time, we observed the significant influence of the piezoelectric coefficient on the shape and amplitude of the main pulse, which is manifested by an increase of the latter. This result opens new avenues for the potential manufacturing of amplification devices for ultrashort pulses.

Acknowledgements A. V. Zhukov and R. Bouffanais are financially supported by the SUTD-MIT International Design Centre (IDC). Numerical modeling was carried out in the framework of the state assignment of the Ministry of Education and Science (project no. 2.852.2017/PCh).

References

1. S.A. Akhmanov, V.A. Vysloukhy, A.S. Chirikin, *Optics of femtosecond laser pulses* (AIP, New York, 1992)
2. D.K. Campbell, S. Flach, Y.S. Kivshar, Phys. Today **43**, 57 (2004)
3. H. Leblond, D. Kremer, D. Mihalache, Phys. Rev. A **053812**, 80 (2009)
4. A.V. Savin, Y.S. Kivshar, Europhys. Lett. **66002**, 82 (2008)
5. H. Leblond, D. Mihalache, Phys. Rev. A **86**, 043832 (2012)
6. A.V. Zhukov, R. Bouffanais, N.N. Konobeeva, M.B. Belonenko, Phys. Lett. A **380**, 3117 (2016)
7. N.N. Konobeeva, M.B. Belonenko, Tech. Phys. Lett. **39**, 579 (2013)
8. D. Mihalache, Rom. J. Phys. **57**, 352 (2012)
9. H. Leblond, D. Mihalache, Phys. Rep. **523**, 61 (2013)
10. A.V. Zhukov, R. Bouffanais, E.G. Fedorov, M.B. Belonenko, J. Appl. Phys. **114**, 143106 (2013)
11. D. Mihalache, Rom. J. Phys. **59**, 295 (2014)
12. A.V. Zhukov, R. Bouffanais, E.G. Fedorov, M.B. Belonenko, J. Appl. Phys. **115**, 203109 (2014)
13. A.V. Zhukov, R. Bouffanais, H. Leblond, D. Mihalache, E.G. Fedorov, M.B. Belonenko, Eur. Phys. J. D **69**, 242 (2015)
14. A.V. Zhukov, R. Bouffanais, B.A. Malomed, H. Leblond, D. Mihalache, E.G. Fedorov, N.N. Rosanov, M.B. Belonenko, Phys. Rev A **94**, 053823 (2016)
15. N.N. Yanyushkina, M.B. Belonenko, N.G. Lebedev, A.V. Zhukov, M. Paliy, Int. J. Mod. Phys. B **25**, 3401 (2011)
16. N.N. Yanyushkina, M.B. Belonenko, Tech. Phys. **58**, 621 (2013)
17. S. Cahangirov, M. Topsakal, E. Aktrk, H. ?ahin, S. Ciraci, Phys. Rev. Lett. **102**, 236804 (2009)
18. B. Aufray, A. Kara, H. Oughaddou, C. Léandri, B. Ealet, G. Lay, Appl. Phys. Lett. **96**, 183102 (2010)
19. P. Padova, C. Quaresima, C. Ottaviani, P. Sheverdyaeva, P. Moras, C. Carbone, D. Topwal, B. Olivieri, A. Kara, H. Oughaddou, B. Aufray, G. Lay, Appl. Phys. Lett. **96**, 261905 (2010)
20. P. Vogt, P. De Padova, C. Quaresima, J. Avila, E. Frantzeskakis, M. Carmen Asensio, A. Resta, B. Ealet, G. Le Lay, Phys. Rev. Lett. **108**, 155501 (2012)
21. A. Fleurence, R. Friedlein, T. Ozaki, H. Kawai, Y. Wang, Y. Yamada-Takamura, Phys. Rev. Lett. **108**, 245501 (2012)
22. M. Noor-A-Alam, H.J. Kim, Y.-H. Shin, J. Appl. Phys. **117**, 224304 (2015)
23. M. Ezawa, New J. Phys. **14**, 033003 (2012)
24. A.V. Zhukov, R. Bouffanais, N.N. Konobeeva, M.B. Belonenko, J. Appl. Phys. **120**, 134307 (2016)
25. L.D. Landau, E.M. Lifshitz, *The Classical Theory of Fields*, 4th edn. (Butterworth-Heinemann, Oxford, 2000)
26. L.D. Landau, E.M. Lifshitz, *Theory of Elasticity*, 3rd edn. (Butterworth-Heinemann, Oxford, 1986)
27. W. Känzig, *Ferroelectrics and antiferroelectrics* (Academic Press, New York, 1964)
28. J.W. Thomas, *Numerical Partial Differential Equations—Finite Difference Methods* (Springer, New York, 1995)