Total Negative Refraction in Real Crystals for Ballistic Electrons and Light

Yong Zhang, B. Fluegel, and A. Mascarenhas
National Renewable Energy Laboratory, 1617 Cole Boulevard, Golden, Colorado 80401, USA
(Received 17 April 2003; published 9 October 2003)

It is found that there exists a category of material interfaces, readily available, that not only can provide *total refraction* (i.e., zero reflection) but can also give rise to *amphoteric refraction* (i.e., both *positive* and *negative refraction*) for electromagnetic waves in any frequency domain as well as for ballistic electron waves. These two unusual phenomena are demonstrated experimentally for the propagation of light through such an interface.

DOI: 10.1103/PhysRevLett.91.157404 PACS numbers: 78.20.Ci, 42.25.Gy, 73.40.–c, 73.50.–h

The phenomenon of *refraction* of light at the interface of two transparent media A and B is the underlying mechanism for steering light in many optical devices [1]. However, the necessity of a refractive index mismatch ($n_A \neq n_B$) for achieving this effect inevitably results in a finite *reflection* loss. In the propagation of an electron wave through discontinuous media, one encounters a situation quite analogous to that for light. Perhaps the closest analogy to the refraction of light would be that of a ballistic electron beam propagating through a heterojunction of semiconductors A and B which differ only in their effective masses ($m_A \neq m_B$). Here again, refraction inevitably is associated with a finite reflection, because of the effective mass mismatch [2]. Furthermore, for most of the commonly encountered situations, there will always be an energy discontinuity between A and B [2–4], causing an additional intensity loss for the transmission across such an interface. The first intriguing finding to be presented in this Letter is a unique type of interface that enables refraction without any reflection, i.e., *total refraction*, for either an electron or a light beam.

Recently, the phenomenon of *negative refraction* [5] has attracted a great deal of attention, because of its implications for realizing a "superlense" with a resolution smaller than the wavelength of light, as well as for observing a reversal of the Doppler shift and Vavilov-Cerenkov radiation [6–14]. It was first suggested by Veselago [5] that negative refraction can occur at the interface of a normal medium, with both permittivity ε and permeability μ being positive, and an abnormal medium, with both ε and μ being negative. It has been pointed out lately that if the abnormal side is a uniaxial medium, negative refraction can arise with just one of the four components of ε and μ being negative [15]. There has so far been only one experimental demonstration of negative refraction, which occurs in a small window of microwave frequencies with a low transmission typically below -24 dB [7,16], and the validity of the interpretation is still under debate [11,17]. The second interesting finding presented in this Letter is that the same type of interface that can yield *total refraction* for electrons and light can in fact yield *amphoteric refraction*, i.e., the refraction can be either *positive* or *negative*, depending on the incident angle, despite all components of $\boldsymbol{\varepsilon}$ and $\boldsymbol{\mu}$ being positive. These two findings, in principle, apply to the full spectrum of electromagnetic waves as well as ballistic electron waves, and thus should simplify the study of negative refraction.

The unique interface proposed here can be viewed as a homojunction that belongs to a special category of twinning structures in uniaxial crystals. For such a twin structure, the interface is a reflection symmetry plane for the two twin components: their symmetry axes are coplanar with the normal to the interface and oriented symmetrically with respect to the interface. Figure 1 shows a real twin structure of this type frequently observed in spontaneously ordered III-V semiconductor alloys [18]. The ordering direction or the symmetry axis switches from the crystallographic direction $[\bar{1}11]$ (A side) to $[1\bar{1}1]$ (B side) across the twin plane whose normal is in the $[\bar{1}10]$ direction. This type of domain twin structure can be found in many naturally or synthetically formed crystals that are classified as ferroelastic materials [19]. With the advances in semiconductor growth techniques, they can now be obtained during epitaxial

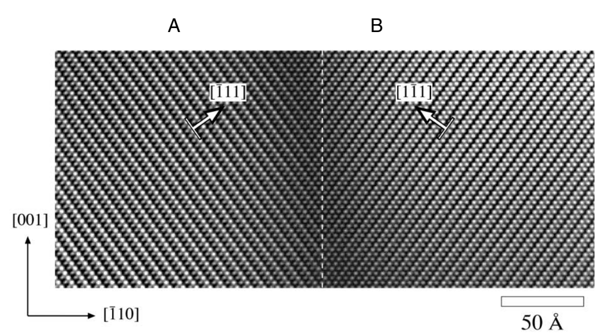

FIG. 1. Electron microscopy of a domain twin. A typical high-resolution cross-sectional TEM picture of domain twin structures frequently observed in CuPt ordered III-V semiconductor alloys. The ordering directions are $[\bar{1}11]$ (left) and $[1\bar{1}1]$ (right). The vertical dashed line indicates the twin boundary.

growth in a controllable manner with domain sizes ranging from nm to μm [20].

We first consider the transmission of a ballistic electron beam at a semiconductor twin boundary, using the structure shown in Fig. 1 as a prototype system. For such a homojunction, there is obviously no band offset between the two twin components. Thus, the two regions can simultaneously be transparent for electrons (with energy above the conduction band edge) and light (with energy below the fundamental band gap). However, the effective mass and refractive index of A and B are not matched for general directions, except for the direction of the twin plane normal. Therefore, intuitively, a finite reflection would be expected at the interface for any non-normal incidence of electron or light. The results given below are in fact counterintuitive.

In a principal coordinate system, the effective mass tensor of the uniaxial semiconductor takes the form

$$m^{-1} = \begin{pmatrix} m_\perp^{-1} & 0 & 0 \\ 0 & m_\perp^{-1} & 0 \\ 0 & 0 & m_{||}^{-1} \end{pmatrix}, \quad (1)$$

where $m_\perp$ and $m_{||}$ are effective masses (in units of the free electron mass m_0) for the wave vector $\mathbf{k}$ perpendicular and parallel to the uniaxis. In a coordinate system with z along the twin plane normal $[\bar{1}10]$, x along [001], and y along [110], the electron dispersion

$$E(k) = \frac{\hbar^2}{2m_0}\left[\frac{k^2}{\bar{m}} - \gamma(k_z^2 - k_y^2) - \text{sign}2\sqrt{2}\gamma k_x k_z\right], \quad (2)$$

where $\bar{m}$ is the average effective mass defined as $1/\bar{m} = (2/\text{m}_\perp + 1/\text{m}_{||})/3$, γ is the anisotropy parameter defined as $\gamma = (1/m_\perp - 1/m_{||})/3$, sign $= +1$ for the A side, and -1 for the B side. Since the structure is uniform along the y direction, one can choose the x-z plane as the incidence plane (i.e., $k_y = 0$) without loss of generality. For an incident electron with a given energy E and wave vector k_x (these quantities are required to be conserved across the interface), there are two allowed solutions for the wave vector k_z from the dispersion Eq. (2): k_{z1}^A and k_{z2}^A for the A side, k_{z1}^B and k_{z2}^B for the B side, respectively. Note that because of the anisotropy, the simple relations $k_{z2}^A = -k_{z1}^A$ and $k_{z2}^B = -k_{z1}^B$ are not valid any more. However, it can be shown that for each side only one solution can give rise to a positive z component of the group velocity (chosen to be k_{z1}^A and k_{z1}^B); while the other yields a negative z component of the group velocity (k_{z2}^A and k_{z2}^B).

The wave functions for the two sides can be written as

$$F^A(x,z) = a\exp[i(k_x x + k_{z1}^A z)] + b\exp[i(k_x x + k_{z2}^A z], \quad (3)$$

$$F^B(x,z) = c\exp[i(k_x x + k_{z1}^B z)], \quad (4)$$

where the "a" term describes the incident wave, the "b" term the reflected wave, and the "c" term the transmitted wave. The boundary conditions for the continuity of the wave function and the current at the interface [21] lead to two equations: $a + b = c$ and $a - b = c$. The solutions for these boundary conditions are simply $c = a$ and $b = 0$. This surprising result implies that the twin boundary is indeed *reflectionless* and *transparent* to electron propagation.

This prompts the question as to whether the electron beam will still be refracted at all. It is easy to see that there is indeed a refraction for the wave front defined by the direction of $\mathbf{k}$, since with $k_{z1}^A \neq k_{z1}^B$ the incident angle $\phi_A = \text{Arctan}(k_x/k_{z1}^A)$ differs from $\phi_B = \text{Arctan}(k_x/k_{z1}^B)$. However, in an anisotropic crystal, it is more meaningful to examine the group velocity, defined as $v = \nabla_k E(k)/\hbar$, that coincides with the direction of the electron flow, described by the probability current density $\mathbf{J}$. In an anisotropic semiconductor, $\mathbf{J}$ is given as [21]

$$J_\alpha = \text{Re}\left[F * \left(\sum_{\beta=1}^{3}\frac{p_\beta}{m_{\alpha\beta}}\right)F\right], \quad (5)$$

where $m_{\alpha\beta}$ is the $\alpha\beta$ component of the effective mass tensor. In general, we find that across the interface, the current perpendicular to the interface, J_z, is continuous, but the current parallel to the interface, J_x, is not, which results in a pure *deflection* or *bending* of the incident electron beam, since the reflection is identically zero. Negative refraction is said to occur when the sign of J_x changes across the boundary. In Fig. 2, the interrelation of

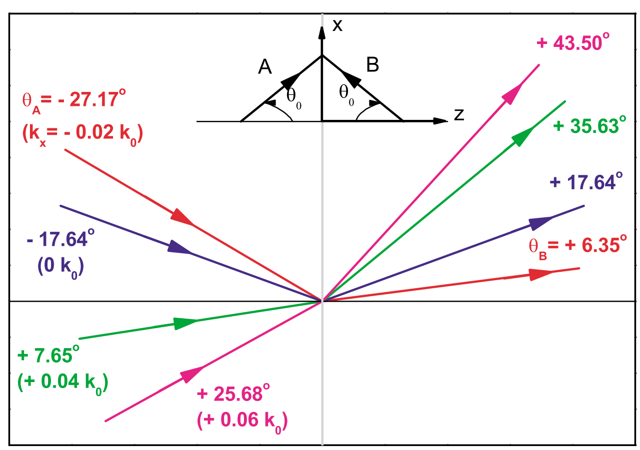

FIG. 2 (color). Refraction of a ballistic electron beam at the interface of the semiconductor twinning structure. The vertical gray line indicates the interface. Arrows A and B indicate the orientations of the uniaxis on each side with $\theta_0 = 35.3°$. The beams in the two regions (left and right) can be either on the same side (corresponding to negative refraction) or on different sides (corresponding to positive refraction) of the interface normal, depending on the value of the wave vector parallel to the interface k_x (in unit of $k_0 = 2\pi/a$, a is the lattice constant of the semiconductor). The energy of the incident electron is 0.2 eV.

the incident and refracted current **J**, described by the incident angle $\theta_A = \mathrm{Arctan}(J_x^A/J_z)$ and the refraction angle $\theta_B = \mathrm{Arctan}(J_x^B/J_z)$, is illustrated by numerical results with typical parameters achievable in III-V alloys ($\bar{m} = 0.114$ and $\gamma = 2.117$ for a fully ordered GaInP [22]). It is of particular interest to notice that it is possible to vary the incident angle from positive to negative, while keeping the refraction angle positive, i.e., the refraction can be *amphoteric*. The angle between the symmetry axis and the twin plane normal is $\theta_0 = \mathrm{Arccos}[\sqrt{2/3}] = 35.3°$ for this specific example, but the qualitative conclusions are in fact valid for any arbitrary value of θ_0, with the effect maximized at $\theta_0 = 45°$.

We next discuss the transmission of light at a twin boundary similar to that of Fig. 1, but with an arbitrary angle θ_0. Analogous to Eq. (1), the dielectric tensor of an anisotropic crystal has the following form in the principal coordinate system:

$$\varepsilon = \begin{pmatrix} \varepsilon_\perp & 0 & 0 \\ 0 & \varepsilon_\perp & 0 \\ 0 & 0 & \varepsilon_\| \end{pmatrix}. \tag{6}$$

It can be shown that for an electromagnetic wave whose electric field is polarized along the y direction (i.e., orthogonal to both the uniaxis of the A and B side and normally referred to as an ordinary wave), the twin boundary like the one shown in Fig. 1 has no effect at all on the incident wave (i.e., $\theta_A \equiv \theta_B$ with a 100% transmission). However, for a wave whose electric field is polarized in the incidence plane x-z (normally referred to as an extraordinary wave), the effects of the twin boundary are in fact very similar to the results obtained above for the electron beam. The dispersion relation can be obtained by solving Maxwell's equation for plane waves propagating within the x-z plane:

$$\frac{(k_z\cos\theta_0 + \mathrm{sign}k_x\sin\theta_0)^2}{\varepsilon_\perp} + \frac{(k_z\sin\theta_0 - \mathrm{sign}k_x\cos\theta_0)^2}{\varepsilon_\|} = \frac{\omega^2}{c^2}, \tag{7}$$

where sign $= +1$ for the A side, and -1 for the B side. We have assumed the medium is nonmagnetic (i.e., the relative permeability $\mu = 1$). Again, for each side there is one solution for k_z that can have a positive z component of the group velocity. The electric (**E**) and magnetic (**H**) waves in regions A and B can be written for both sides in a similar manner as for Eqs. (3) and (4), and on applying the boundary conditions, we arrive at the two same equations as those obtained for the electron waves: $a + b = c$ due to the continuity of the tangential component of the magnetic field in the y direction, and $a - b = c$ due to the continuity of the tangential component of the electric field in the x direction, where a, b, and c are, respectively, the amplitude of the x component of the **E** field for the incident, reflected, and transmitted waves. Thus, we again find that the amplitude of the reflected wave is identically zero, and that of the transmitted wave always equals that of the incident wave. Similar to the situation for the electron beam, the negative refraction does occur over a range of incidence angles. The largest bending or the strongest negative refraction in fact happens when $k_x = 0$, where the propagation direction of the light wave, defined by the Poynting vector $\mathbf{S} = \mathbf{E} \times \mathbf{H}$, is given as $\sin\theta_{A0} = \sin 2\theta_0(\varepsilon_\| - \varepsilon_\perp)/(2\sqrt{\varepsilon_\perp^2\sin^2\theta_0 + \varepsilon_\|^2\cos^2\theta_0})$, and $\sin\theta_{B0} = -\sin\theta_{A0}$.

To experimentally illustrate the effect, we use a YVO_4 bicrystal with $\theta_0 = -45°$ to emulate the proposed twin structure. YVO_4 is a uniaxial positive crystal with $n_0 = 2.017\,68$ and $n_e = 2.250\,81$ at 532 nm [23]. The device is formed by bonding two nominally identical crystals in optical contact. The accuracy for the optical axis orientation is $\pm 0.5°$ for each crystal. The input and output planes are antireflection coated at 532 nm. Figure 3 shows the refraction of a 532 nm laser beam at the interface of the bicrystal at two typical incident angles, which yields both positive and negative refraction. The power loss of the transmitted beam, which ideally should be zero, is measured to be in the order of 10^{-4}, due to the imperfection of the device (e.g., the relative orientation of the optical axes and the quality of the optical contact). In fact, on the images shown in Fig. 3, no reflection is visible to the naked eye at the bicrystal interface. Figure 4 shows the comparison between the measured and calculated light propagation directions, which yields a perfect agreement. Since the limitation of total internal reflection for a

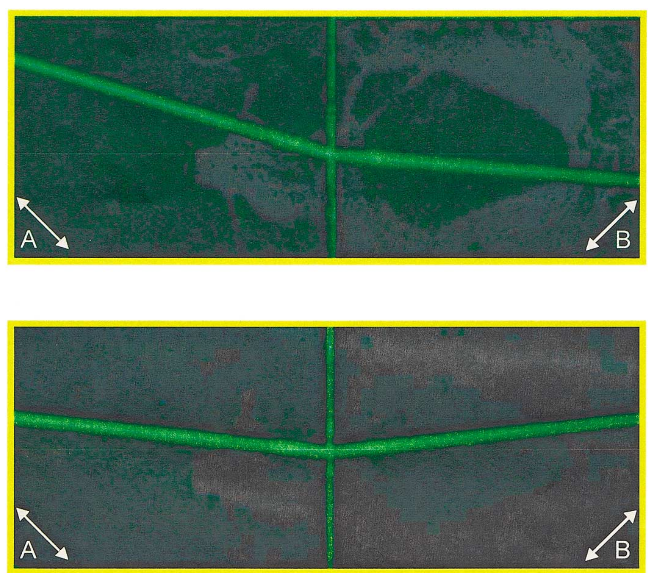

FIG. 3 (color). Images of light propagation in a YVO_4 bicrystal. The upper panel shows an example of normal (positive) refraction, the lower panel shows an example of abnormal (negative) refraction. Note that no reflection is visible at the bicrystal interface to the naked eye. The interface is illuminated by inadvertently scattered light.

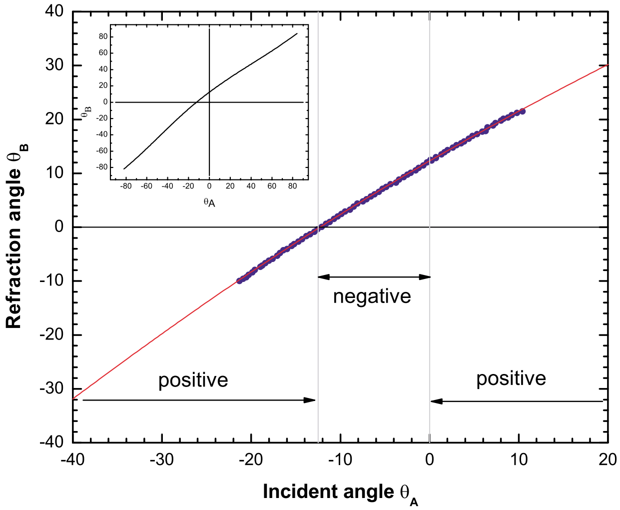

FIG. 4 (color online). Comparison of theoretical predictions with experimental data. Amphoteric refraction in a YVO_4 bicrystal is divided into three regions: one negative ($\theta_B/\theta_A < 0$) and two positive ($\theta_B/\theta_A > 0$). The data points are measured with a 532 nm laser light, the curve is calculated with the refractive index of the material (given in the text). Inset: the full operation range of the device.

conventional interface does not apply for the interface considered, a full operation range of $-90°$ to $90°$ can be obtained, as shown in the inset of Fig. 4. Note that the experiment performed here using the bicrystal also demonstrates the feasibility of obtaining similar effects for ballistic electrons.

Many potential device applications can be derived based on the unique properties of the kind of domain boundary discussed above. They can, for example, be used to provide bending, angular dispersion, energy filtering, and beam collimating for electrons in semiconductor ballistic electron devices. The ability to steer light without reflection could be extremely valuable for high power optics. Additionally, this relatively simple way to generate negative refraction may provide unique experimental opportunities for examining this unusual effect and its various physical consequences.

We thank S. P. Ahrenkiel for the electron microscopy image and M. Hanna for sample growth. The work was supported by the U.S. Department of Energy, Office of Sciences, Basic Energy Sciences under Contract No. DE-AC36-99GO10337.

[1] M. Born and E. Wolf, *Principles of Optics* (Cambridge University Press, Cambridge, 1999).
[2] V. V. Paranjape, Phys. Rev. B **52**, 10 740 (1995).
[3] G. T. Einevoll and L. J. Sham, Phys. Rev. B **49**, 10 533 (1994).
[4] J. Smoliner, R. Heer, and G. Strasser, Phys. Rev. B **60**, R5137 (1999).
[5] V. G. Veselago, Sov. Phys. Usp. **10**, 509 (1968).
[6] D. R. Smith *et al.*, Phys. Rev. Lett. **84**, 4184 (2000).
[7] R. A. Shelby, D. R. Smith, and S. Schultz, Science **292**, 77 (2001).
[8] J. B. Pendry, Phys. Rev. Lett. **85**, 3966 (2000).
[9] N. Garcia and M. Nieto-Vesperinas, Phys. Rev. Lett. **88**, 207403 (2002).
[10] C. Luo *et al.*, Phys. Rev. B **65**, 201104 (2002).
[11] P. M. Valanju, R. M. Walser, and A. P. Valanju, Phys. Rev. Lett. **88**, 187401 (2002).
[12] J. Pacheco *et al.*, Phys. Rev. Lett. **89**, 257401 (2002).
[13] D. R. Smith and D. Schurig, Phys. Rev. Lett. **90**, 077405 (2003).
[14] J. Li *et al.*, Phys. Rev. Lett. **90**, 083901 (2003).
[15] I. V. Lindell *et al.*, Microwave Opt. Technol. Lett. **31**, 129 (2001).
[16] R. A. Shelby *et al.*, Appl. Phys. Lett. **78**, 489 (2001).
[17] N. Garcia and M. Nieto-Vesperinas, Opt. Lett. **27**, 885 (2002).
[18] S. P. Ahrenkiel, in *Spontaneous Ordering in Semiconductor Alloys*, edited by A. Mascarenhas (Kluwer Academic/Plenum Publishers, New York, 2002), p. 195.
[19] K. Aizu, J. Phys. Soc. Jpn. **27**, 387 (1969).
[20] Y. Zhang *et al.*, Mater. Res. Soc. Symp. Proc. **583**, 255 (2000).
[21] R. Wessel and M. Altarelli, Phys. Rev. B **39**, 12 802 (1989).
[22] Y. Zhang, A. Mascarenhas, and L. W. Wang, Phys. Rev. B **63**, R201312 (2001).
[23] http://www.casix.com