Charge transport in BAs and the role of two-phonon scattering

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(Received 9 May 2023; revised 11 August 2023; accepted 12 September 2023; published 17 October 2023)

The semiconductor BAs has drawn significant interest due to experimental reports of simultaneous high thermal conductivity and ambipolar charge mobility. The *ab initio* prediction of high electron and hole mobility assumed the dominance of charge carrier scattering by one phonon. Recently, higher-order electron-phonon scattering processes in polar and nonpolar semiconductors have been reported to have a non-negligible impact on charge transport properties, suggesting they may play a role in BAs as well. Here, we report an *ab initio* study of two-phonon electron and hole scattering processes in BAs. We find that inclusion of these higher-order processes reduces the computed room-temperature electron and hole mobility in BAs by around 40% from the one-phonon value, resulting in an underestimate of experimental values by a similar percentage. We suggest an experimental approach to test these predictions using luminescence spectroscopy that is applicable to the defective samples which are presently available.

DOI: 10.1103/PhysRevB.108.165202

I. INTRODUCTION

BAs is a semiconductor of substantial recent interest beginning from the *ab initio* prediction of high thermal conductivity comparable to that of diamond [1] owing in part to the high optical phonon energy (∼80 meV) which inhibits phonon scattering. The prediction of high optical phonon energy was initially confirmed by inelastic x-ray scattering [2], but reports of the thermal conductivity values were significantly lower than the predictions due to scattering by As vacancies [3]. Theoretically, four-phonon processes were found to make a non-negligible contribution to phonon scattering, yielding a lower thermal conductivity compared with the original predictions [4]. After improvements in synthesis resulting in higher-quality samples, the high thermal conductivity was confirmed experimentally [5–7] and was found to be in quantitative agreement with predictions including four-phonon scattering.

BAs has also been predicted to exhibit simultaneous high electron and hole mobilities, with computed room-temperature values of 1400 and 2110 $\mathrm{cm^2\,V^{-1}\,s^{-1}}$, respectively [8,9]. However, initial experiments that estimated the mobility from conductivity and thermoelectric measurements and a single parabolic band model yielded a lower hole mobility of 400 $\mathrm{cm^2\,V^{-1}\,s^{-1}}$ [10]; recent direct Hall measurements yielded ∼500 $\mathrm{cm^2\,V^{-1}\,s^{-1}}$ on bulk samples [11]. The lower values obtained experimentally have been attributed to scattering by charged impurities in the defective samples which could be synthesized. Recent experiments have circumvented the need for high-quality macroscopic samples by measuring the ambipolar diffusivity of photoexcited carriers in a local region of the sample using transient grating experiments [11] or transient reflectivity microscopy [12]. Using the Einstein relation to convert the measured diffusivity into a mobility, these experiments obtained ambipolar mobilities of 1500−1600 $\mathrm{cm^2\,V^{-1}\,s^{-1}}$ at some locations on the sample. These values are in good agreement with those calculated from first principles [8].

Most first-principles studies of the electron-phonon interactions employ the lowest level of perturbation theory involving one electron and one phonon (1ph) [13,14], and this level of theory was also used for BAs [8,9]. Given the contribution of higher-order phonon processes to thermal transport in BAs [4–7], it is of interest to consider the role of higher-order processes in charge transport. Although evidence for the contribution of multiphonon processes to electron-phonon scattering has been previously reported [15–17], only recently have first-principles studies included the contribution of higher-order scattering processes, such as that of an electron with two phonons (2ph) in the electron-phonon interaction [18–20]. In GaAs at room temperature, the 2ph scattering rates were predicted to be on the order of the 1ph rates [18], resulting in an ∼40% reduction in the computed mobility at 300 K. Good quantitative agreement with experimental mobility was obtained only considering this correction. Corrections to the high-field transport properties of GaAs of a similar magnitude were also found [19]. For nonpolar semiconductors, Hatanpää *et al.* reported improved agreement of the warm electron coefficient in Si over temperatures from 190 to 310 K with the inclusion of 2ph processes [20]. These studies suggest that inclusion of 2ph processes for electron-phonon scattering may be necessary to accurately predict the charge transport properties of semiconductors.

Here, we report an *ab initio* study of the role of two-phonon scattering of electrons and holes on the charge transport properties of BAs. We find that the two-phonon rates may be as large as ∼50% of the one-phonon rates, leading to a marked reduction in the calculated ambipolar mobility from 1420 to 810 $\mathrm{cm^2\,V^{-1}\,s^{-1}}$ at room temperature and a 35–50%

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correction to the carrier mobility over temperatures from 150 to 350 K. The experimental origin of the discrepancy could arise from the superdiffusion of hot carriers shortly after photoexcitation, an effect which has been observed using scanning ultrafast electron microscopy, leading to an overestimate of the ambipolar diffusivity. On the theory side, an underestimate of the predicted value is possible owing to cancellation between the iterated and direct contributions to 2ph scattering, the latter of which is neglected here. To test our predictions given the defective samples presently available, we suggest an experimental approach based on direct measurements of hot-carrier lifetimes using the broadening of photoluminescence spectra.

II. COMPUTATIONAL METHODS

We computed the mobility of electrons and holes in BAs using established methods based on density functional theory (DFT) and density functional perturbation theory (DFPT) [14,21–23]. Briefly, we obtained the electronic structure and electron-phonon matrix elements using QUANTUM ESPRESSO [24] with a relaxed lattice constant of 4.819 Å, a coarse $12 \times 12 \times 12$ **k** grid, and a plane-wave cutoff of 80 Ry. A fully relativistic ultrasoft potential with the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional was used. For the DFPT calculations, we employed a $6 \times 6 \times 6$ phonon **q** grid. The band structure and electron-phonon matrix elements were interpolated onto fine 160^3 and 80^3 **k** and **q** grids, respectively, using PERTURBO [25]. Increasing the grid density to 200^3 and 100^3 for the **k** and **q** grids, respectively, changed the mobility by 2%. The Fermi level was chosen so as to obtain a carrier concentration of 10^{15} cm^{-3} at all temperatures. The energy window was set to 200 meV above (below) the band extremum for electrons (holes). Increasing the energy window to 250 meV changed the mobility by 0.6%. We explicitly constructed the collision matrix and solved the Boltzmann transport equation using numerical linear algebra, from which transport properties were calculated. Details of this approach are given elsewhere [19–21]. The contributions of the next-to-leading-order electron-phonon scattering (2ph) processes originally derived in Ref. [18] were computed following the implementation used in Ref. [19]. The 2ph rates were iterated five times. Increasing the number of iterations to 6 changed the mobility by 2.7%.

III. RESULTS

The calculated scattering rates for electrons and holes are shown in Figs. 1(a) and 1(b). The trend of the 1ph scattering rates agrees with that reported previously [8]; quantitative differences are due to the differing exchange-correlation functional or pseudopotential necessitated by the use of PERTURBO in this paper. We observe the characteristic sharp increase in the scattering rate for electrons and holes near $\hbar\omega_{\mathrm{LO}} \sim 80$ meV as longitudinal optical (LO) phonon emission starts to dominate the electron-phonon interaction. The 2ph rates largely follow the same trend and are on the order of the 1ph rates, consistent with previously published 2ph calculations for GaAs [18,19] and Si [20]. At 300 K, the 2ph rates are around 50% of the 1ph rates. Prior works have examined

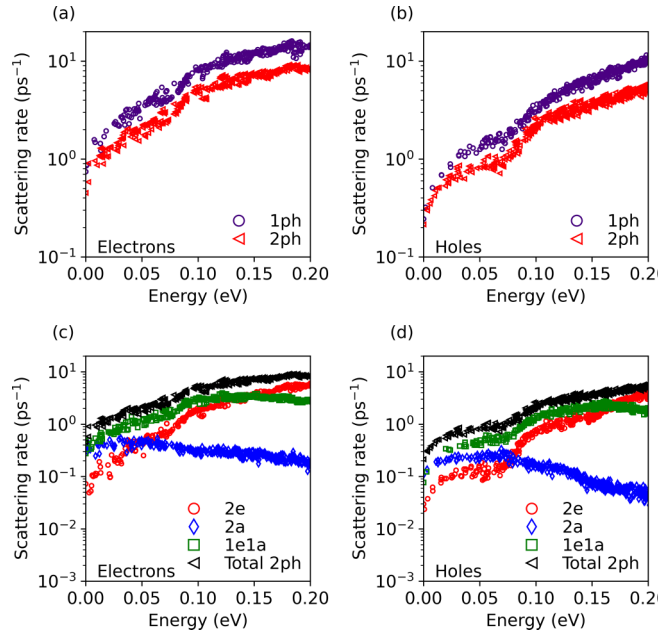

FIG. 1. Scattering rates vs energy for (a) electrons and (b) holes in BAs including 1ph (circles) and 2ph processes (triangles) at 300 K. The computed 2ph rates for electrons and holes are around 50% of the 1ph rates. Computed total 2ph (triangles), 1e1a (squares), 2a (diamonds), and 2e (circles) scattering rates vs energy for (c) electrons and (d) holes show the subprocesses that comprise the total 2ph rates. Below 150 meV, the 1e1a processes have the largest contribution to the 2ph rates at 300 K.

the influence of the exchange-correlation functional on charge carrier mobilities, finding variations on the order of ∼10–15% in Si [26] and BAs [8]. Although this uncertainty may influence the predicted absolute mobility values, we expect the relative contribution of 2ph processes compared with 1ph processes to be insensitive to the choice of functional.

The 2ph processes exhibit several different subtypes because the two phonons involved in scattering can each be emitted or absorbed. Following Ref. [18], processes where a phonon is emitted and another absorbed are denoted 1e1a, and processes where two phonons are sequentially emitted or absorbed are 2e and 2a, respectively. The individual subprocesses contributing to the total 2ph rate are shown in Figs. 1(c) and 1(d) for electrons and holes, respectively. Below $\hbar\omega_{\mathrm{LO}} \sim 80$ meV, 1e1a processes are dominant. Note that the total 1e1a rate includes processes where a phonon is first emitted and another absorbed, and processes where a phonon is first absorbed and another is subsequently emitted. Two-phonon emission (2e) processes are comparatively weak in this region since LO phonon emission is prohibited until the energy threshold of $2\hbar\omega_{\mathrm{LO}}$. Two-phonon absorption (2a) processes are generally weak throughout the energy range studied, except at sufficiently low energies where emission and therefore 1e1a events become increasingly unlikely such that 2a rates are comparable to 1e1a rates. Between $\hbar\omega_{\mathrm{LO}} \sim 80$ meV and $2\hbar\omega_{\mathrm{LO}}$, the 1e1a and 2e rates increase as LO phonon emission starts to dominate the electron-phonon scattering processes, a feature observed in polar semiconductors [27]. Beyond $2\hbar\omega_{\mathrm{LO}}$, carriers are energetic enough to emit two LO phonons,

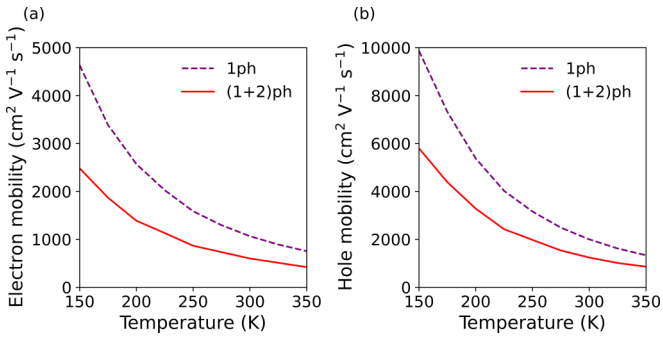

FIG. 2. (a) Electron and (b) hole mobility in BAs vs temperature at the 1ph (dashed line) and $(1+2)$ph (solid line) level of theory. For holes, the correction to the mobility at room temperature from including 2ph processes is ∼37%, while for electrons this correction is ∼43%, demonstrating the significant contribution of 2ph processes to the mobility at room temperature.

and 2e processes have the largest contribution to the total 2ph scattering rate. This energy dependence of the individual 2ph subprocesses in BAs is consistent with those reported for GaAs and Si [18–20].

We next examine the effect of 2ph processes on the electron and hole mobility. The computed 1ph and $(1+2)$ph mobility versus temperature is shown in Figs. 2(a) and 2(b) for electrons and holes, respectively. With only 1ph processes, we obtain room-temperature electron mobility $\mu_e = 1066\,\mathrm{cm^2\,V^{-1}\,s^{-1}}$ and hole mobility $\mu_h = 2000\,\mathrm{cm^2\,V^{-1}\,s^{-1}}$, in quantitative agreement with previous 1ph predictions that employ the same PBE exchange-correlation functional (see Supplemental Material of Ref. [8] for calculations using the same functional as in this paper). With the inclusion of 2ph processes, μ_e and μ_h decrease to 600 and $1240\,\mathrm{cm^2\,V^{-1}\,s^{-1}}$, respectively, corresponding to a 43 and 37% reduction at room temperature. Over the temperature range from 150 to 350 K, this correction ranges from 36% at 350 K to 41% at 150 K for holes, and from 44% at 350 K to 46% at 150 K for electrons. These corrections to the electron mobility are of a comparable magnitude to those obtained for GaAs (∼45%) [18,19], but slightly higher than those for Si (∼35%) [20].

BAs exhibits several distinct features compared with other polar semiconductors such as GaAs. In GaAs and other polar materials, LO phonons make the overwhelming contribution to electron-phonon scattering [27]. In BAs, carrier scattering relevant to mobility is instead primarily due to acoustic phonons owing to the high optical phonon energy (80 versus 35 meV in GaAs) that limits scattering by LO phonon emission as well as the decreased LO phonon absorption scattering from decreased thermal population [8]. Additionally, in GaAs, intervalley processes have a negligible effect on low-field charge transport because of the Γ-L energy separation of 300 meV, but scattering processes in BAs are more similar to those in Si in that they involve intervalley transfers mediated by zone-edge wave vector phonons. Our calculations reveal that intervalley processes account for 43% of $(1+2)$ph scattering in BAs at 300 K and 20% at 150 K. The decrease with decreasing temperature occurs due to the reduced population of the zone-edge phonons required for intervalley scattering. As a comparison, intervalley processes account for 61% of $(1+2)$ph scattering in Si at 300 K and 25% at 150 K.

IV. DISCUSSION

We consider our calculated mobility values in the context of recent optical experiments on BAs that reported an ambipolar carrier mobility [11,12]. At the 1ph level of theory, we predict a high ambipolar mobility $\mu_a = 2\mu_e\mu_h/(\mu_e+\mu_h)$ of $1420\,\mathrm{cm^2\,V^{-1}\,s^{-1}}$ at 300 K using 1ph theory, consistent with a prior computed value of $1570\,\mathrm{cm^2\,V^{-1}\,s^{-1}}$ with the PBE exchange-correlation functional [8] and in agreement with recent experimental reports [11,12]. Including 2ph processes reduces μ_a to $810\,\mathrm{cm^2\,V^{-1}\,s^{-1}}$, a 43% reduction. Considering the $(1+2)$ph mobility value, the apparent agreement between theory and experiment is substantially degraded, with the experiment now overestimating the theory.

This discrepancy could arise from several factors. First, the quantity that was measured in the optical experiments of Refs. [11,12] was the ambipolar diffusion coefficient of photoexcited charge carriers, from which the mobility was obtained through the Einstein relation. In Refs. [11,12], the photoexcitation wavelength for determination of the ambipolar diffusion coefficient was chosen to be around the available estimates of the band-gap energy (∼2 eV [28–31]). If the photon energy exceeds the band-gap energy, the photoexcited carriers will have energy in excess of thermal energies, potentially causing the extracted transport properties to differ from their linear response values. This hot-carrier effect was observed in both Ref. [11] and Ref. [12] as a larger measured electronic diffusivity for pump wavelengths $\lesssim$500 nm. Evidence for the absence of the hot-carrier effect for the final reported diffusivity values was presented, for example, in Fig. 1 D of Ref. [11], as the plateau of the measured electronic decay rate with increasing wavelength. On the other hand, scanning ultrafast electron microscopy (SUEM) studies have reported observations of superdiffusion of photoexcited carriers in semiconductors persisting over hundreds of picoseconds [32–34]. This phenomenon has been attributed to the additional contribution to carrier diffusion of a pressure gradient in the nondegenerate hot-carrier gas after photoexcitation [32]. In Refs. [11,12], the diffusivity was extracted from the electronic decay curve over timescales from tens to hundreds of picoseconds, conceivably leading to an extracted diffusivity that was influenced by superdiffusion.

On the theory side, a possible cause of an underestimate for the computed mobility is the cancellation of the two contributions to electron-phonon scattering at second order. Electron-2ph processes arise from the 1ph term, corresponding to the first derivative of the interatomic potential with respect to lattice displacements taken to second order in perturbation theory, or a direct 2ph term involving the simultaneous interaction of an electron with two phonons with a strength given by second-order derivative of the interatomic potential [35,36]. These two terms exhibit a nontrivial interaction owing to a cancellation in the long-wavelength acoustic phonon limit which arises from translational invariance of the crystal [37]. In this paper and other recent *ab initio* studies of 2ph scattering, only the first term is included, and thus neglect of the second term will lead to an overestimate of 2ph

scattering rate. This cancellation has long complicated the study of 2ph scattering in semiconductors [36,38]. A recent study of 2ph scattering in Si suggested that the correction could be on the order of 10–20% in that material [20]. It is possible that this effect could lead to an underestimate of the computed mobility in BAs; further study is needed to investigate this hypothesis.

Absent higher-quality samples, verifying the prediction of the role of 2ph scattering using transport measurements is challenging due to the contribution of extrinsic defect scattering. We suggest an alternative approach based on continuous-wave luminescence spectroscopy which allows the lifetimes of electronic states away from the band minimum to be determined [39]. These states are less influenced by impurity scattering compared with those near the band edge. While the contribution of these higher-energy states to carrier mobility is negligible, the contribution of 2ph processes to the total scattering rate is largely independent of energy, as shown in Fig. 1. Therefore evidence of the influence of 2ph scattering on mobility can be obtained by comparing the photoluminescence linewidths of these higher energy states with theory. In these experiments, hot electrons excited by a continuous-wave laser emit photons by recombination, and the spectrum of the emitted light exhibits a broadening that is determined by the lifetime of the state. We may predict the difference in broadening at the 1ph and $(1+2)$ph levels of theory in BAs using the same *ab initio* theory employed for transport calculations. In Fig. 3, we plot the predicted full width at half maximum (FWHM) of the luminescence peak, $2\Gamma = \tau^{-1}$, versus energy for electrons. At 0.4 eV above the conduction band minimum (CBM), we predict $2\Gamma \sim 13$ and 21 meV for 1ph and $(1+2)$ph, respectively. This 8-meV difference is almost an order of magnitude higher than the experimental uncertainty reported in Ref. [39] and thus should be discernible.

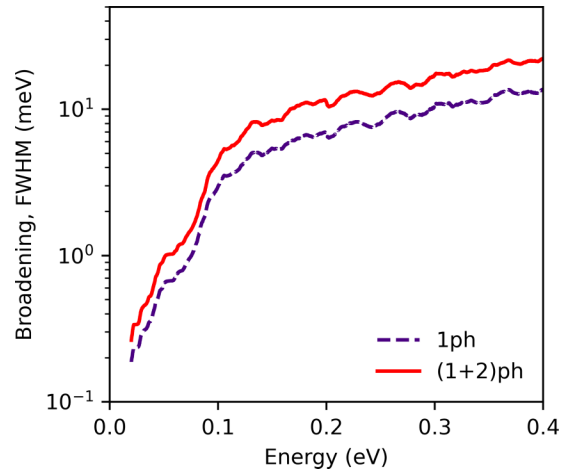

FIG. 3. Calculated broadening vs energy for electrons due to electron-phonon scattering at 77 K and carrier concentration of 10^{15} cm^{-3}. The difference in broadening between 1ph theory (dashed line) and $(1+2)$ph theory (solid line) is expected to be distinguishable considering prior reports of experimental uncertainties of $\sim$1 meV [39].

V. SUMMARY

In summary, we have reported *ab initio* calculations of ambipolar mobility in BAs considering 2ph electron-phonon processes. We find that the inclusion of these processes reduces the predicted electron and hole mobility by 43 and 37% at room temperature, respectively, lowering the ambipolar mobility by 43% and underestimating experimental reports by a similar amount. We hypothesize that the discrepancy between our results and recent optical experiments could in part arise from the superdiffusion of hot carriers, or an underestimation of the calculated mobility owing to cancellations at second order of perturbation theory. We have suggested an experimental approach based on hot-electron luminescence to test these predictions.

ACKNOWLEDGMENTS

I.E. was supported by a National Science Foundation Graduate Research Fellowship under Grant No. DGE-1745301. A.J.M. was supported by AFOSR under Grant No. FA9550-19-1-0321. The authors thank Benjamin Hatanpää for useful discussions and providing data on intervalley scattering in Si.

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