Structural, electronic, elastic, power, and transport properties of $\beta$-Ga$_2$O$_3$ from first principles

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We investigate the structural, electronic, vibrational, power, and transport properties of the $\beta$ allotrope of Ga$_2$O$_3$ from first principles. We find phonon frequencies and elastic constants that reproduce the correct band ordering, in agreement with experiment. We use the Boltzmann transport equation to compute the intrinsic electron and hole drift mobility and obtain room-temperature values of 258 and 1.2 cm$^2$/Vs, respectively, as well as 6300 and 13 cm$^2$/Vs at 100 K. Through a spectral decomposition of the scattering contribution to the inverse mobility, we find that multiple longitudinal-optical modes of $B_6$ symmetry are responsible for the electron mobility of $\beta$-Ga$_2$O$_3$ but that many acoustic modes also contribute, making it essential to include all scattering processes in the calculations. Using the von Hippel low-energy criterion, we computed the breakdown field to be 5.8 MV/cm at room temperature, yielding a Baliga figure of merit of 1250 with respect to silicon, ideal for high-power electronics. This work presents a general framework to predictively investigate novel high-power electronic materials.

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I. INTRODUCTION

The $\beta$ allotrope of Ga$_2$O$_3$ has attracted some attention as an ultrawide-band-gap transparent semiconducting oxide [1]. As a consequence of its large band gap, $\beta$-Ga$_2$O$_3$ possesses a very high breakdown electric field of 8 MV/cm [2] and a large Baliga figure of merit (BFOM) [3], which makes it a promising alternative to GaN and SiC for high-power electronics [4,5]. In addition, it can be synthesized by the melt-growth method, which allows for low-cost and large-scale production [6,7]. Its electronic and optical properties also make it a good candidate for UV transparent conducting oxide (TCO) [8,9].

One property of $\beta$-Ga$_2$O$_3$ that makes it so attractive is its high carrier mobility for a material with such a wide band gap. The electron mobility of $\beta$-Ga$_2$O$_3$ has been studied more extensively than the hole mobility due to experimental interest and the fact the hole mobility is two orders of magnitude smaller. Given the promise offered by $\beta$-Ga$_2$O$_3$, it is surprising that many basic properties have not been investigated in detail. From a theoretical perspective, this might be due to the fact that $\beta$-Ga$_2$O$_3$ has a 10-atom primitive cell, which makes first-principles calculations in this material more challenging than for standard tetrahedral semiconductors. In particular, the shape of the conduction band was not well understood until recently. Indeed, Ueda et al. [10] measured a strong anisotropy of the conduction-band effective mass. However, since then many experiments and theoretical studies indicated that the conduction band is nearly isotropic [6,11–17]. Another question relates to the relative importance of nonpolar optical-phonon, polar optical-phonon, and ionized-impurity scattering at room temperature. Initially it was thought that the dominant scattering mechanism in $\beta$-Ga$_2$O$_3$ was due to nonpolar optical phonons with a large deformation potential of $4 \times 10^9$ eV/cm [18]. However, Ghosh and Singisetti [19] identified a longitudinal-optical phonon mode with energy around 21 meV as the dominant mechanism in the mobility of $\beta$-Ga$_2$O$_3$, and this finding was later confirmed by multiple authors [20–22]. Finally, there is some debate about the ordering of the zone-centered phonons, namely, the Raman-active $A_x$ mode and the infrared-active $B_6$ TO mode [22–25].

One crucial material property for high-power electronics is the breakdown field, i.e., the magnitude of the external electric field that a material can sustain before incurring permanent damage. The breakdown field can be computed from first principles using the von Hippel low-energy criterion [26–28] and was recently computed ab initio by Mengle and Kioupakis [22] to be 5.4 MV/cm in $\beta$-Ga$_2$O$_3$, considering only the dominant longitudinal optic (LO) phonon mode. They further estimated that considering all modes would increase the theoretical intrinsic breakdown field by 20% to 6.8 MV/cm. Such calculation assumes total impact ionization for all electrons with energies above the band gap and should therefore be seen as a lower bound; it can also be improved by computing the impact ionization coefficient from first principles [29].

The BFOM [3] describes the current handling capability of a material and is often given relative to silicon. In addition to

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the breakdown field, the second material’s parameter entering into the BFORM is the intrinsic carrier mobility. The electron room-temperature mobility of \( \beta \)-Ga2O3 was computed to be 115 cm²/Vs at a carrier concentration of \( 10^{17} \) cm⁻³, with a temperature dependence in good agreement with experiment [19], by using Wannier interpolation of the electron-phonon matrix elements [30] and Rode’s method [31]. The mobility was also estimated to be below 200 cm²/Vs using \( k \cdot p \) perturbation theory [20].

In this context, a careful and detailed analysis of the crystal structure, electronic, optical, vibrational, elastic, and transport properties of \( \beta \)-Ga2O3 is warranted. The manuscript is organized as follows. In Sec. II we discuss the relaxed crystal structure of the monoclinic \( \beta \)-Ga2O3 and the importance of spin-orbit coupling. Section III is dedicated to the study of the electronic properties, including bandgaps, electronic band structure, and effective masses. In Sec. IV we analyze the phonon dispersion, infrared and Raman spectra, dielectric constant and Born charges, and elastic properties. Section V presents the computed electron and hole carrier mobility with temperature as well as a mode-resolved analysis of the scattering contribution to the mobility. Finally, in Sec. VI we discuss and compute Baliga’s figure of merit of \( \beta \)-Ga2O3 and compare it with silicon.

II. CRYSTAL STRUCTURE

The crystal structure of \( \beta \)-Ga2O3 was originally investigated by Geller to be monoclinic with the \( C_{2h} (2/m) \) point group [32] and later refined by Åhman et al. [33] using single-crystal diffraction. The measured lattice parameters of the conventional unit cell are \( a = 12.214 \) Å, \( b = 3.037 \) Å, \( c = 5.798 \) Å, and \( \beta = 103.83° \) [33]. The conventional cell vectors are \( (a, 0, 0), (0, b, 0) \), and \( (c \cos \beta, 0, c \sin \beta) \), while the primitive cell vectors are \( \left( \frac{a}{2}, -\frac{b}{2}, 0 \right) \), \( \left( \frac{a}{2}, \frac{b}{2}, 0 \right) \), and \( (c \cos \beta, 0, c \sin \beta) \). Any atomic coordinate expressed in the conventional cell \( (c_x, c_y, c_z) \) can be expressed in the primitive cell by using the transformation \( (c_x - c_y, c_y + c_z, c_z) \). The primitive and conventional cell are made of 10 and 20 atoms, respectively.

The gallium atom sits in two inequivalent positions with octahedral and tetrahedral coordination, respectively. There are three inequivalent oxygen atoms occupying a distorted cubic lattice, with two oxygen atoms being threefold coordinated and one oxygen atom fourfold coordinated. All the five inequivalent atoms have 4\( i \) Wyckoff position which corresponds to symmetry \((x, 0, z)\) and \((-x, 0, -z)\). The system has four crystal symmetries: the identity, a \( \pi \) rotation around the Cartesian \( y \) axis, and their inversions.

To determine the atom positions, we relaxed the lattice parameters and atomic coordinates, starting from the experimental data. We used the QUANTUM ESPRESSO software suite [34] with relativistic local-density approximation (LDA) pseudopotentials from Pseudo Dojo [35], including the \( 3s^2\ 3p^6\ 3d^{10}\ 4s^2\ 4p^1 \) semicore states for gallium and the \( 2s^2\ 2p^4 \) electrons for oxygen. The wave functions were expanded in a plane-wave basis set with energy cutoff of 120 Ry (160 Ry for the elastic response) and a homogeneous \( \Gamma \)-centered Brillouin-zone sampling of \( 8 \times 8 \times 8 \) points. We converged the structure such that the maximum force was smaller than \( 2 \times 10^{-7} \) Ry/Å and the maximum stress component was lower than \( 0.07 \) Ry/Å³. The relaxation yielded the lattice parameters \( a = 12.128 \) Å, \( b = 3.016 \) Å, \( c = 5.752 \) Å, and \( \beta = 103.75° \), which slightly underestimates the experimental one as expected from LDA. The relaxed primitive cell crystal structure is shown in Fig. 1 and is formed by two distorted octahedra and two distorted tetrahedra. The gallium and oxygen atoms occupy two and three inequivalent sites at the 4\( i \) Wyckoff position, respectively, whose coordinates are provided in Table I and are in close agreement with the experimental assignment [33]. The inequivalent gallium-oxygen bond lengths are also reported in Table I, with the tetrahedra having smaller bond lengths than the octahedra. Interestingly, due to their distorted nature, there are two inequivalent \( Ga_{II}-O_{III} \) bond lengths in the octahedral configuration, despite having only one inequivalent oxygen position.

We also report in Table I the volume, density, atomic coordinates, and bond lengths and compare them with experimental data. The calculations were made without spin-orbit coupling (SOC), but we tested that including this effect modifies the crystal data shown in Table I by less than 0.005%. Hence, this effect is neglected for the rest of this work. We finally note that the primitive cell vectors can equivalently be rotated such that \( a = b = 11.809 \) Å, \( c = 10.869 \) Å, \( \alpha = \beta = 103.335° \), and \( \gamma = 27.933° \).

III. ELECTRONIC PROPERTIES

The room-temperature optical band gap of \( \beta \)-Ga2O3 obtained through absorption measurements is estimated to be between 4.54 and 4.90 eV [37–39]. Our calculated direct band gap at the zone center is 2.55 eV, strongly underestimating experiments as expected from density functional theory (DFT). In agreement with prior work [15], we find that the valence band maximum (VBM) is located on the \( L \rightarrow \Gamma \) high-symmetry lines in the Brillouin zone and yields a slightly smaller indirect band gap of 2.53 eV. A comparison with an earlier work is given in Table II. Our values are consistent with calculations at an equivalent level of theory; hybrid functionals slightly overestimate room-temperature experimental band gaps.

There has been some confusion in the literature about the shape of the Brillouin zone of \( \beta \)-Ga2O3 [11,40–43]. The first band structure using the correct monoclinic variation was reported in 2015 [15]. It is therefore important to pay close attention when constructing the Brillouin zone of \( \beta \)-Ga2O3.
We note that as the definition of two of the primitive cell vectors in the QUANTUM ESPRESSO software are inverted with respect to prior studies, we had to adapt the definition of the high-symmetry points of the Brillouin zone. We give the conversion for clarity in the Table III as well as the value of the high-symmetry points of the Brillouin zone. We give the level of agreement gives us confidence that our calculations of electronic transport properties will be reliable.

In contrast, the hole effective mass at the zone center is highly anisotropic, with very heavy masses along the Γ-X and Γ-Y direction, and a small hole mass of 0.35 m_e along the Γ-Z direction. As a result, this should be an ideal hole transport direction. However, the VBM is not located at the zone centered but 26 meV higher in energy on the I-L line. The transverse and perpendicular hole effective mass at that point is 3.0 m_e and 3.6 m_e, respectively, in agreement with previous studies.

We computed the electron effective mass using finite differences, and found 0.267, 0.254, and 0.244 along the Γ-X, Γ-Y, and Γ-Z direction, respectively. The electron effective mass is quite isotropic, with an average value of 0.255 as reported in Table II, which compares well with prior theoretical work and is also close to the experimental value of 0.28 [40,42]. This level of agreement gives us confidence that our calculations of electronic transport properties will be reliable.

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Cs hole mobility than the electron mobility. The effective mass, we expect at least an order of magnitude lower as transport properties scale inversely with the phonon operations: the identity operation \( \epsilon \) (point group), and the blue line are lines with inversion symmetry \( C_m(m) \) point group.

**IV. VIBRATIONAL PROPERTIES**

**A. Phonon dispersions**

We now study the vibrational properties of \( \beta\)-Ga\(_2\)O\(_3\) using density functional perturbation theory (DFPT) \[45,46\]. The calculated phonon band structure along the monoclinic Brillouin zone is presented in Fig. 2(b).

The point groups along high-symmetry lines are either \( C_\text{m}(m) \) or \( C_\text{2} \). The \( C_\text{m}(m) \) point group contains two symmetry operations: the identity \( \epsilon \) and a mirror plane \( \sigma \). This point group possess two irreducible representations: the phonon branches belonging to the \( A' \) irreducible representation are symmetric with respect to both the identity operation and reflection through the mirror plane, while the branches belonging to the \( A'' \) representation are symmetric with respect to the identity but antisymmetric with respect to reflection [colored in Fig. 2(b) in gray and blue, respectively]. The other point group is the \( C_\text{2} \) point group, which contains the identity (gray) and a \( \pi \) rotation around the [0,1,0] Cartesian axis [displayed with red lines in Fig. 2(b)]. Note that some directions in the Brillouin zone are less symmetric and only possess the identity (gray). In addition, specific high-symmetry points have higher symmetries: (i) the point group at the \( N \) and \( M \) points is \( C_\text{2h}(5) \) with \( A_g \) and \( A_u \) symmetry operation; (ii) the point group at the \( X \), \( M \) points is \( C_\text{2v}(4) \) with identity \( E \) and \( C_\text{2} \) with \( \pi \) rotation around the [0,1,0] Cartesian axis; (iii) the point group at the \( \Gamma \), \( L \), \( Y \), \( Z \) point is \( C_\text{2}(2/m) \) with \( A_g \), \( B_g \), \( A_u \), \( B_u \) symmetries.

**B. Infrared and Raman spectra**

The infrared spectrum as well as polarization and temperature-dependent Raman spectra of bulk \( \beta\)-Ga\(_2\)O\(_3\) were first measured by Dohy \textit{et al.} \[44\] in 1982. The measured normal mode frequencies are reported in Table IV along with more recent measurements and previous \textit{ab-initio} values, and are compared to the calculated frequencies from this work. Our calculated phonon band structure slightly underestimates experiments but they are in better agreement than previous calculations. Overall, our calculations agree with previous theoretical work \[22,24,47\] with a notable difference: in agreement with experiments \[23,25\] we find that the \( A_\text{g}(3) \) Raman-active mode has a lower frequency than the \( B_g \)(TO1) mode. The highest phonon frequency at the zone center is a LO mode in the \( Z \) direction, with a frequency of 97 meV, very close to the experimental value of 100 meV \[25\]. However, we note that the highest phonon frequency occurs at the \( Z \) point with a value of 99.12 meV (not shown in Table IV). Our predicted Raman-active phonon frequencies are 2.5% within the experimental data \[23\], with the largest difference being attributed to the \( A_\text{g}(6) \) mode. Our predicted infrared-active LO modes are even closer, with deviation of 1.4% from experimental data \[25\], while the agreement with LO modes is not as good, with a deviation of 5.4%.

**C. Dielectric constant and Born charges**

The high-frequency dielectric tensor is fairly isotropic, with \( \varepsilon_{xx} = 3.98 \), \( \varepsilon_{yy} = 4.09 \), and \( \varepsilon_{zz} = 4.08 \), slightly overestimating the experimental value of 3.53–3.6 \[48–50\] obtained as an isotropic average in thin films. The slight overestimation of the theoretical dielectric tensor is a direct consequence of the underestimated value of the band gap by DFT as the electronic part of the dielectric function is inversely proportional to the band gap \[51\]. We note one experimental work which obtained a direction-dependent dielectric tensor \( \varepsilon_{xx} = 3.7 \), \( \varepsilon_{yy} = 3.2 \), and \( \varepsilon_{zz} = 3.7 \) \[25\] using generalized spectroscopic ellipsometry within the infrared and far-infrared spectral region. This anisotropy was not observed in another recent experiment reporting \( \varepsilon_{xx} = 3.6 \), \( \varepsilon_{yy} = 3.58 \), and \( \varepsilon_{zz} = 3.54 \) \[52\], also using generalized spectroscopic ellipsometry. Our calculations appear to support an isotropic dielectric tensor. \( \beta\)-Ga\(_2\)O\(_3\) also possesses one nonzero off-diagonal component of the dielectric tensor, but the computed value was lower than \( 10^{-4} \) and therefore is not reported.
TABLE IV. Phonon frequencies (meV) of $\beta$-Ga$_2$O$_3$ at the zone center using a 16 $\times$ 16 $\times$ 12 $k$-grid. The three zero-frequency acoustic modes are not reported. The infrared experimental values from Dohy et al. [44] are measured by transmission, and the frequency of the maxima lies between the LO and TO frequencies.

| Mode | Calculated | Experiment |
|------|------------|------------|
| symmetry Activity | This work | Mengle [22] | Liu [24] | Schubert [25] | Machon [23] | Dohy [44] |
| $A_y$ (1) Raman | 13.3007 | 12.9204 | 12.9812 | – | – | 13.6631 |
| $B_y$ (1) Raman | 13.5463 | 13.0320 | 13.8986 | – | – | 14.0846 |
| $B_y$ (2) Raman | 18.0406 | 17.9566 | 17.5190 | – | – | 17.9405 |
| $A_y$ (TO1) Infrared | 18.7039 18.7967 18.7130 18.7071 | 18.0558 18.0583 18.1005 18.0538 | 17.5562 18.1637 | 19.1928 19.3787 | – | – |
| $A_y$ (2) Raman | 20.3690 | 19.8635 | 20.2590 | – | – | 20.9781 |
| $A_y$ (3) Raman | 23.8311 | 23.1107 | 25.0820 | – | – | 24.8464 |
| $B_y$ (TO1) Infrared | 24.2779 24.2785 24.2801 31.1559 | 21.7617 22.0556 21.7617 28.5300 | 23.2470 23.6190 | 26.5078 33.3518 | – | 31.00 |
| $B_y$ (TO2) Infrared | 31.4358 31.432 33.6936 31.5417 | 30.2249 32.8459 30.2249 31.1845 | 31.1944 32.7938 | 32.5211 35.4595 | – | – |
| $B_y$ (TO3) Infrared | 34.2134 34.2175 35.5251 34.2964 | 33.6679 34.3957 33.6679 33.6853 | 32.8930 35.1619 | 34.6164 37.8152 | – | 35.95 |
| $A_y$ (TO2) Infrared | 37.6083 42.9389 37.6085 37.6087 | 37.5883 38.0446 42.5353 37.5883 | 36.7241 40.3569 | 36.7737 42.8861 | – | 38.43 |
| $A_y$ (4) Raman | 39.3235 | 38.5678 | 39.1542 | – | – | 39.5014 resized for 39.4270 |
| $A_y$ (5) Raman | 43.0355 | 42.6692 | 42.1174 | – | – | 42.9481 resized for 42.8985 |
| $B_y$ (TO4) Infrared | 43.7333 43.6516 44.0052 43.9195 | 43.0151 44.4806 43.0163 43.7515 | 42.6010 43.9028 | 44.2376 48.2299 | – | 46.49 |
| $B_y$ (3) Raman | 44.0051 | 43.4540 | 43.1837 | – | – | 43.7664 |
| $A_y$ (6) Raman | 48.9601 | 46.6404 | 52.0982 | – | – | 51.5402 resized for 51.4534 |
| $B_y$ (TO5) Infrared | 53.1958 53.1945 64.0910 58.9781 | 52.4627 55.2015 52.4627 55.5028 | 47.5479 63.3063 | 53.6356 69.7691 | – | 56.41 |
| $A_y$ (TO3) Infrared | 55.8780 68.7760 55.8787 55.8788 | 55.5648 60.3258 67.7896 55.5648 | 50.8955 60.0951 | 55.6317 73.7706 | – | 65.09 |
| $A_y$ (7) Raman | 57.8013 | 56.5566 | 56.9583 | – | – | 58.8925 |
| $B_y$ (4) Raman | 59.2209 | 58.6049 | 58.6197 | – | – | 58.7065 resized for 58.8925 |
| $B_y$ (TO6) Infrared | 71.0646 71.0662 75.5392 80.8032 | 70.3586 76.4561 70.3586 82.6541 | 71.2041 77.5273 | 70.9810 87.9048 | – | 79.35 |
| $A_y$ (8) Raman | 77.7683 | 76.8739 | 75.2708 | – | – | 77.9489 resized for 77.8621 |
| $B_y$ (5) Raman | 80.8029 | 79.8161 | 77.7505 | – | – | 80.8997 resized for 80.7137 |
| $A_y$ (9) Raman | 81.387 | 79.9487 | 81.3460 | – | – | 81.4576 |
| $A_y$ (TO4) Infrared | 82.0108 93.3977 82.0111 82.0107 | 80.9332 81.2282 91.9864 80.9332 | 80.3294 91.5623 | 82.2263 95.4678 | – | 82.82 |
| $B_y$ (TO7) Infrared | 84.8999 84.8976 90.0416 86.9860 | 83.8146 89.3579 83.8146 85.1660 | 83.3918 90.2853 | 85.8467 96.8689 | – | 89.27 |
| $B_y$ (TO8) Infrared | 91.5781 91.5770 95.1837 97.1831 | 89.9654 92.5902 89.9654 94.7562 | 91.9467 94.7983 | 92.1823 100.4272 | – | 94.23 |
| $A_y$ (10) Raman | 94.0737 | 92.3918 | 93.9428 | – | – | 94.7115 resized for 94.5999 |
The computed diagonal Born effective charges are \( \text{GaI} = (2.74, 2.88, 3.04) \), \( \text{GaII} = (3.23, 3.42, 3.12) \), \( \text{OIII} = (-1.46, 2.09, 2.47) \), \( \text{OII} = (-2.27, 2.25, 1.39) \), \( \text{OIII} = (-2.22, 1.96, 2.28) \) in units of electron charge. The off-diagonal components are lower than 0.3 and not reported.

### D. Elastic properties

The stiffness \( C_{ij} \) and compliance \( S_{ij} = C_{ij}^{-1} \) tensors link the stress tensor to the strain tensor following the generalized Hooke’s law:

\[
\sigma_{ij} = C_{ijkl} \varepsilon_{kl},
\]

\[
\varepsilon_{ij} = S_{ijkl} \sigma_{kl},
\]

where Einstein’s notation is implied.

The Young’s modulus \( E \) is the linear response of a material to a uniaxial stress where the response is measured in the direction of the applied stress and the bulk modulus \( B \) is the response to an isotropic stress. The Young’s and bulk moduli can therefore be expressed as a function of a single unit vector in Cartesian space expressed in spherical coordinates \( 0 \leq \theta \leq \pi \) and \( 0 \leq \phi \leq 2\pi \) as \( \mathbf{u} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \) [60]:

\[
E(\theta, \phi) = \frac{1}{u_i u_j u_k u_l S_{ijkl}},
\]

\[
B(\theta, \phi) = \frac{1}{u_i u_j S_{ijkl}},
\]

where in the case of the Young modulus we have transformed the head of the compliance tensor from the Cartesian basis to a new basis whose first unit vector is \( \mathbf{u} \) following the transformation

\[
S'_{1111} = a_{1i} a_{1j} a_{1k} a_{1l} S_{ijkl} = u_i u_j u_k u_l S_{ijkl},
\]

where \( a_{ij} \) indicates the direction cosine, specifying the angle between the \( \mathbf{i} \)th axis of the new basis and the \( \mathbf{j} \)th axis of the initial basis. The bulk modulus is simpler because it is obtained by applying an isotropic stress (pressure \( p \)) such that \( \varepsilon_{ij} = -p S_{ijkl} \).

Other elastic properties such as the shear modulus \( G \) or Poisson’s ratio \( \nu \) depend on the direction in which the stress is applied \( \mathbf{u} \) but also the orthogonal direction in which the response is measured \( \mathbf{v} \) and can be parametrized with three angles \( \theta, \phi, \) and \( 0 \leq \xi \leq 2\pi \):

\[
\mathbf{v} = \begin{bmatrix}
\cos \theta \cos \phi \cos \xi - \sin \phi \sin \xi \\
\cos \theta \sin \phi \cos \xi + \cos \phi \sin \xi \\
-\sin \theta \cos \xi
\end{bmatrix}.
\]

The shear modulus and Poisson’s ratio can therefore be obtained as

\[
G(\theta, \phi, \xi) = \frac{1}{4 u_i u_j u_k u_l S_{ijkl}},
\]

\[
\nu(\theta, \phi, \xi) = -\frac{u_i u_j u_k u_l S_{ijkl}}{u_i u_j u_k u_l S_{ijkl}}.
\]

We note that for the elastic properties studied here we only need up to two vectors (or three angles) in the new basis because the directions of applied stress and measured response are orthogonal, but a general elastic property where this was not the case would require three vectors (or four angles) in the transformed basis.

These elastic properties can be averaged by direct integration on the unit sphere to give the standard Young modulus, bulk modulus, shear modulus, and Poisson’s ratio. However, very popular averaging approximations have been developed, including the Voigt approximation, where the average bulk and shear moduli are given by [61]

\[
9B_V = C_{111} + C_{222} + C_{333} + 2(C_{122} + C_{133} + C_{233}),
\]

\[
15G_V = C_{111} + C_{222} + C_{333} - (C_{122} + C_{133} + C_{233}) + 3(C_{444} + C_{555} + C_{666}).
\]

In the Reuss approximation, the bulk and shear moduli are defined as [61]

\[
B_R^{-1} = S_{111} + S_{222} + S_{333} + 2(S_{122} + S_{133} + S_{233}),
\]

\[
15G_R^{-1} = 4(S_{111} + S_{222} + S_{333}) - 4(S_{122} + S_{133} + S_{233}) + 3(S_{444} + S_{555} + S_{666}).
\]

The Voigt approximation provides an upper bound for the bulk and shear moduli, while the Reuss approximation gives a lower bound. We can therefore define the arithmetic mean, referred to as the Void-Reuss-Hill approximation [61], as \( B_1 = (B_V + B_R)/2 \) and \( G_1 = (G_V + G_R)/2 \). We then express the effective Young \( E \) modulus and Poisson ratio \( \nu \) as

\[
E = 9BG/(3B + G),
\]

\[
\nu = (3B - 2G)/(6B + 2G),
\]

where the relations apply to the Voigt, Reuss, and Hill approximation of the Young, bulk, and shear moduli and the Poisson’s ratio. We can also define the universal elastic anisotropy as [55]

\[
A^U = 5(G_V/G_R) + (B_V/B_R) - 6.
\]

Finally, we can obtain the bulk sound velocity \( v_B \), the compressional velocity \( v_P \), shear velocity \( v_G \), and the average sound velocity \( v_{av} \) as

\[
v_B = \sqrt{B/\rho},
\]

\[
v_P = \sqrt{\left(B + \frac{4}{3}G\right)/\rho},
\]

\[
v_G = \sqrt{G/\rho},
\]

\[
v_{av} = \left[\frac{1}{3} \left(\frac{2}{v_G} + \frac{1}{v_P}\right)\right]^{1/2},
\]

where \( \rho \) is the average mass density. Using the average sound velocity, the Debye temperature can be estimated within the Debye model as

\[
\Theta_D = \frac{h}{k_B} \left(\frac{3N_{av}}{4\pi \rho}\right)^{1/3},
\]

where \( h, k_B \), and \( N_{av} \) are the Planck constant, Boltzmann constant, and the number of atoms in the primitive cell, respectively.
We studied the elastic properties of $\beta$-Ga$_2$O$_3$ using the thermo_pw code [62]. The stiffness tensor of Laue class $C_{2h}$ for base centered monoclinic crystals has 13 independent elastic constants written in Voigt notation as follows: $C_{11}, C_{12}, C_{13}, C_{15}, C_{22}, C_{23}, C_{25}, C_{33}, C_{35}, C_{46}, C_{56}, \text{ and } C_{66}$. The stiffness matrix $C_{ij}$ was obtained by third-order polynomial fitting using 12 deformations with strain intervals of 0.001 to remain in the linear regime. The strains were applied along the crystal lattice vector of the $\beta$-Ga$_2$O$_3$ primitive cell presented in Fig. 1 such that the resulting stiffness matrix is expressed in that basis. For each strain, the ions were relaxed to their equilibrium positions with a very tight convergence threshold of $4 \times 10^{-6}$ Ry/Å on forces. We used a 160-Ry energy cutoff on plane waves and a 12-point grid. All the elastic coefficients and elastic properties are reported in Table V. Our calculations compare well with prior theoretical work and with resonant ultrasound spectroscopy coupled with laser-Doppler interferometry [53]. We computed all coefficients independently such that we can estimate off-diagonal accuracy when symmetry constraints are not precisely fulfilled. The most sensitive coefficient is the $C_{12}$, with an accuracy of $\pm$3.4 GPa.

Using Eqs. (9)–(14), we obtained a bulk modulus of 184 GPa, a Young modulus of 207 GPa, a shear modulus of 79 GPa, and a Poisson’s ratio of 0.313. Those numbers agree well with recent experimental elastic constants of $B = 183$ GPa, $E = 210$ GPa, $G = 80$ GPa, and $\nu = 0.31$ [53]. Finally, using Eqs. (15), (17)–(19), and (20), we compute the universal elastic anisotropy $A^U$ to be 0.84, the average sound velocity to be 4.01 km/s, and the estimated Debye temperature $\Theta_D$ to be 551 K.

Using the ELATE software [59,60], we show in Fig. 3(a) the parametrized Young modulus of Eq. (3) as a parametrized three-dimensional surface and in Figs. 3(b) and 3(c) the parametrized shear modulus and Poisson’s ratio of Eqs. (7) and (8), where the maximum and minimum value of the third angle is shown in blue and green, respectively. Compared to simple semiconductors where the bulk modulus is spherical, $\beta$-Ga$_2$O$_3$ is strongly anisotropic. For example, the Young modulus has a minimum value of 134 GPa in the $xz$ plane with a unit vector (0.94, 0, 0.34), while the maximum value of the Young modulus is 293 GPa in the (0.34, 0.93, 0.13) direction. In the case of the shear modulus and the Poisson’s ratio presented in Fig. 3, they are also highly anisotropic, with values ranging from 50 to 133 GPa for the shear modulus and from 0 to 0.67 for the Poisson’s ratio, which displays a flowerlike shape along the diagonal axes.

V. CARRIER MOBILITY

We now analyze the intrinsic carrier transport properties of $\beta$-Ga$_2$O$_3$. We compute the ab initio drift carrier mobility

$$\mu_{\alpha\beta} = \frac{e}{V_{sc}n_c} \sum_n \int \frac{d^3k}{\Omega_{BZ}} v_{\beta k}^\alpha \partial_{E_{\beta k}} f_{nk} \quad (21)$$

through the linear response $\partial_{E_{\beta k}} f_{nk}$ of the electronic occupation function $f_{nk}$ to the electric field $E$, where $V_{sc}$ is the unit-cell volume, $\Omega_{BZ}$ the first Brillouin-zone volume, and $n_c = (1/V_{sc}) \sum_n \int (d^3k/\Omega_{BZ}) f_{nk}$ is the carrier concentration. We solve the linearized Boltzmann transport equation (BTE) [63,64],

$$\partial_{E_{\beta k}} f_{nk} = e v_{\beta k}^\alpha \frac{\partial f_{nk}}{\partial E_{\beta k}} \tau_{nk} + \frac{2\pi \tau_{nk}}{h} \sum_{m\nu} \int \frac{d^3q}{\Omega_{BZ}} |g_{mn\nu}(k, q)|^2 \times \left[ (n_{q\nu} + 1 - f_{nk+q}) \delta (E_{nk+q} - E_{nk+q+ h\omega_{q\nu}}) \right. \left. + (n_{q\nu} + f_{nk}) \delta (E_{nk} - E_{nk+q+ h\omega_{q\nu}}) \right] \delta_{E_{\beta k}} f_{nk+q+}. \quad (22)$$

with $\tau_{nk}$ being the total scattering lifetime,

$$\tau_{nk}^{-1} = \frac{2\pi}{h} \sum_{m\nu} \int \frac{d^3q}{\Omega_{BZ}} |g_{mn\nu}(k, q)|^2 \times \left[ (n_{q\nu} + 1 - f_{nk+q}) \delta (E_{nk+q} - E_{nk+q+ h\omega_{q\nu}}) \right. \left. + (n_{q\nu} + f_{nk+q}) \delta (E_{nk} - E_{nk+q+ h\omega_{q\nu}}) \right]. \quad (23)$$

Here $v_{nk}$ is the electronic velocity of the eigenstates $E_{nk}$, $f_{nk}$ is the Fermi-Dirac occupation, and $n_{q\nu}$ is the Bose-Einstein distribution function. The electron-phonon matrix elements $g_{mn\nu}(k, q)$ are the probability amplitude for scattering from...
an initial state \( \hbar \mathbf{k} \) to a final state \( \hbar \mathbf{k} + \mathbf{q} \) via the emission or absorption of a phonon of frequency \( \omega_{\mathbf{q}} \). A common approximation, known as the self-energy relaxation time approximation (SERTA), consists in neglecting the second term on the right-hand side of Eq. (22). The mobility then takes the simpler form:

\[
\mu_{\alpha \beta, \text{SERTA}} = \frac{1}{V_{\text{DC}}} \sum_{\mathbf{k}} \int \frac{d^3k}{\Omega_{\text{BZ}}} v_{\alpha \mathbf{k}} v_{\beta \mathbf{k}} n_{\mathbf{k}}.
\]

(24)

We used the EPW software [30,65] to interpolate the electron-phonon matrix element \( g_{\mathbf{mn}}(\mathbf{k}, \mathbf{q}) \) from a coarse \( 8 \times 8 \times 8 \) \( \mathbf{k} \)-point and \( 4 \times 4 \times 3 \) \( \mathbf{q} \)-point grid to dense \( 160 \times 160 \times 120 \) \( \mathbf{k} \) and \( \mathbf{q} \) grids, as required to converge the electron mobility. The interpolation uses the maximally localized Wannier function [66] and the WANNIER90 software [67]. We used 22 Wannier functions of initial \( s \) character centered on the gallium atoms and of \( p \) character centered on the oxygen atoms. The Dirac \( \delta \) functions in Eqs. (22) and (23) were computed using the adaptive smearing method of Refs. [68,69].

To reduce computational costs, we computed separately the electron and hole mobility by explicitly interpolating only the matrix elements for which their electronic eigenvalues at \( \mathbf{k} \) and \( \mathbf{k} + \mathbf{q} \) were within 0.3 eV of the band edges. We also relied on crystal symmetries to decrease the number of \( \mathbf{k} \) points. In the case of the electron mobility, we explicitly interpolated 13 516 \( \mathbf{k} \) points and 101 346 \( \mathbf{q} \) points, instead of the 3 072 000 points that would have been required by computing all the points from the \( 160 \times 160 \times 120 \) grid. In the case of the hole mobility, owing to very flat bands the majority of grid points contribute to the hole mobility, as can be seen in Fig. 2(a). Thus the computational cost is much higher and our densest interpolated grid is \( 56 \times 56 \times 42 \) points, which corresponds to 55 892 \( \mathbf{k} \) points and 131 712 \( \mathbf{q} \) points explicitly computed.

We obtained the following room-temperature electron and hole drift mobility tensor (cm$^2$/Vs) in the SERTA:

\[
\mu_{\alpha \beta, \text{SERTA}}^{\text{SERTA}} = \begin{bmatrix}
170 & 0 & 2.6 \\
0 & 165 & 0 \\
2.6 & 0 & 166
\end{bmatrix},
\]

(25)

\[
\mu_{\alpha \beta, \text{SERTA}}^{\text{SERTA}} = \begin{bmatrix}
1.1 & 0 & -0.3 \\
0 & 0.6 & 0 \\
-0.3 & 0 & 1.6
\end{bmatrix}.
\]

The results using the self-consistent BTE are

\[
\mu_{\alpha \beta, \text{BTE}}^{\mu_{\text{BTE}}} = \begin{bmatrix}
258 & 0 & 7.5 \\
0 & 277 & 0 \\
7.5 & 0 & 239
\end{bmatrix},
\]

(26)

\[
\mu_{\alpha \beta, \text{BTE}}^{\mu_{\text{BTE}}} = \begin{bmatrix}
1.2 & 0 & -0.2 \\
0 & 0.8 & 0 \\
-0.2 & 0 & 1.7
\end{bmatrix}.
\]

Interestingly, although the electron effective mass is isotropic (see Table II), we observe about 15% anisotropy for the electron mobility resulting from anisotropic electron-phonon scattering. This result is in line with the recently observed 10%–15% anisotropy in the electron mobility of \( \beta \)-Ga$_2$O$_3$ [16]. Based on our convergence study, with increasing fine grid size we estimate an accuracy of \( \pm 3 \) cm$^2$/Vs for the electron mobility and \( \pm 0.5 \) cm$^2$/Vs for the hole mobility. The anisotropy of the hole mobility is within the uncertainty of the calculations.

The temperature dependence of the BTE electron and hole mobility as a function of temperature is presented in Fig. 4, slightly overestimating experimental data. The isotropic averages of the electron and hole mobility are 258 and 1.2 cm$^2$/Vs, respectively. To our knowledge, this may be the first time that the hole mobility of \( \beta \)-Ga$_2$O$_3$ is computed from first principles.
Our room-temperature value of the electron mobility of \(\beta\)-Ga2O3 is slightly higher than prior theoretical studies: Ref. [19] gives 115 cm\(^2\)/Vs at a carrier concentration of 10\(^{17}\) cm\(^{-3}\) using Rode’s method [31] and 200 cm\(^2\)/Vs using \(k \cdot p\) perturbation theory [20]. Reference [21] obtained an electron mobility of 155 cm\(^2\)/Vs using the SERTA, in close agreement with our SERTA value of 167 cm\(^2\)/Vs.

The overestimation with respect to experimental electron mobility can be traced back to the fact that our calculated electron effective mass is 7\% smaller than in experiments and that the electron-phonon matrix elements are dominated by Fröhlich polar scattering, which in turn scales with the dielectric constant. Our calculated dielectric constant is approximately 11\% higher than in experiments. Taken together, these estimates indicate that our calculation underestimates the Fröhlich coupling by approximately 13\%. In Ref. [72] we have shown that the mobility is inversely proportional to the Fröhlich coupling and effective mass; therefore we expect that the use of DFT leads to an overestimation of the mobility by approximately 24\%. Experimental Hall electron mobilities of \(125\) cm\(^2\)/Vs [12] and \(152\) cm\(^2\)/Vs [70] were reported and are consistent with our findings.

Since lattice scattering becomes negligible at low temperature, the mobility computed using Eq. (21) diverges when \(T\) tends to zero. At low temperature other scattering mechanisms dominate carrier transport, including defect [73] and impurity scattering [63]. The impurity scattering may be included using the semi-empirical model developed by Brooks and Herring [74–76]. The ionized-impurity limited mobility \(\mu_i\) can be evaluated analytically assuming spherical energy surfaces, negligible electron-electron interactions, and complete ionization of the impurities:

\[
\mu_i = \frac{2\gamma^2\epsilon_i^2(T)^{3/2}}{\pi^{3/2}e^3\sqrt{m^*_0G(b)}} \quad \text{[cm}^2\text{/Vs]},
\]

where \(G(b) = \ln(b + 1) - b/(b + 1)\), \(b = 24\pi m^*_0\epsilon_i(T)^2/e^3h^2n'\), and \(n' = n(2 - n_0/n_i)\). Here \(m^*_0 = 0.26m_0\) and 3.39\(n_0\) is the density-of-state effective mass for the electron and hole, respectively, \(n_i\) and \(n_0\) are the electron or hole densities and the density of ionized impurities, respectively, \(\epsilon_i = 4.05\epsilon_0\) is the average dielectric constant, \(\epsilon_0\) is the permittivity of vacuum, and \(h\) is Planck’s constant. In the above expressions, the concentrations are expressed in cm\(^{-3}\), and the temperature \(T\) is in K. The mobility including phonon (\(\mu\)) and impurity (\(\mu_i\)) scattering can be computed using the mixed-scattering formula [76] \(\mu = [1 + X(\epsilon_iX\cos(X) + \sin(X)[\sin(X) - \frac{T}{\pi}])], \) where \(X^2 = 6\mu/\mu_i\) and \(\epsilon_i\) and \(\sin(X)\) are the cosine and sine integrals. The resulting combined mobility for a concentration of 10\(^{15}\) cm\(^{-3}\) of ionized impurity is shown with a dashed line in Fig. 4, improving the agreement with experiment in the low-temperature regime.

Finally, to shed light on the microscopical mechanisms driving the electron mobility in \(\beta\)-Ga2O3 we computed the isotropic average of the momentum and mode-resolved contribution to the SERTA mobility as

\[
\mu = \sum_{qV} T_{qV}^{-1},
\]

where the mode-resolved inverse mobility \(T_{qV}\) is

\[
T_{qV} = \frac{6\pi}{h} V_{\text{av}} n_c \sum_{mn\alpha} \int \frac{d^3k}{\pi^2} \frac{w_q|g_{mn\alpha}(k, q)|^2}{\epsilon^\alpha_{nk\alpha} - \epsilon^\alpha_{nk+q} + i\hbar \omega_{qV}} \times \left[ (n_{qV} + 1 - f_{nkq})\delta(\epsilon_{nkq} - \epsilon_{nkq} + \hbar \omega_{qV}) + (n_{qV} + f_{nkq})\delta(\epsilon_{nkq} - \epsilon_{nkq} + \hbar \omega_{qV}) \right],
\]

where \(w_q\) is the weight of the \(q\) point.

We show in Fig. 5 the mode contribution to the inverse mobility as well as the density of state inverse mobility along with the cumulative integral (dashed red line). The mode contribution spans a region close to the zone center, since as discussed above, larger momenta have negligible contribution to the mobility. The spectral decomposition is separated into three defined energy regions: low-energy (\(\hbar \omega < 50\) meV), middle-energy (50 meV \(\lesssim \hbar \omega < 71\) meV), and high-energy (\(\hbar \omega \geq 71\) meV) regions. The high-energy phonons alone account for 62\% of the inverse mobility at room temperature, followed by the low-energy phonons (22\%) and middle-energy phonons (16\%). We mention the following ten modes, in relation with Table IV, that contribute significantly to reducing the mobility: the \(B_1\) (LO\(_3\) : 1–3.8) and \(B_8\) (LO\(_3\) : 2–3.5) modes. Interestingly, all the dominant modes have \(B_u\) symmetry and are longitudinal-optical modes.

As can be seen on the left side of Fig. 5, the spectral decomposition of the mode contribution to the inverse mobility is complex, with many modes contributing to the mobility.
Such complexity in the phonon spectrum of $\beta$-Ga$_2$O$_3$ with 30 crossing and intertwined phonon branches translates into many ways for the electrons to interact with the bosonic continuum, yielding increased scattering and reduced mobility. It is worth comparing such behavior of the electron scattering with a related material, wurtzite GaN, that possesses similar electron effective mass $\approx 0.2$–0.3 $m_e$. In the nitride compound, the phonon band structure is composed of 12 modes clearly separated by a 20-meV gap [77]. This translates into a reduced scattering with two dominant scatterings at around 2 and 92 meV [78] and explains why the electron mobility in wurtzite GaN is four times larger than in $\beta$-Ga$_2$O$_3$, despite similar effective masses.

VI. BALIGA’S FIGURE OF MERIT

Figures of merit have been introduced as a way to quantify the influence of materials parameters on the performance of semiconductor devices. The most common figures of merit include the Johnson figure of merit (JFOM), which assesses the quality of a semiconductor for high-frequency power transistor application [79], the Keyes figure of merit (KFOM), which quantifies the thermal limitation of transistor switching frequency [80], and the Baliga figure of merit (BFOM) [3]. In this work we focus solely on the BFOM, which is used to identify materials parameters so as to minimize losses in power field effect transistors [1]. The BFOM relies upon the assumption that power losses are solely due to power dissipation in the on state by current flow through the on resistance of the device. As a result, the BFOM is used for devices operating at low frequency, where the conduction losses are dominant.

The BFOM is given by

$$\text{BFOM} = \epsilon^0 \mu E_b^3,$$  \hspace{1cm} (30)

where $E_b$ is the computed breakdown field, $\mu$ the computed mobility from Eq. (21), and $\epsilon^0$ is the temperature-dependent experimental static dielectric function with the field perpendicular to the (100), (010), and (001) direction, respectively [81], which we reproduce in Fig. 6(c). Importantly, we stress that all the quantities entering in Eq. (30) are temperature dependent.

The temperature- and direction-dependent mobility has already been obtained in Sec. V. Therefore we only need to compute the breakdown field to obtain the BFOM. References [84,85] proposed the following model:

$$E_b = 24.442 \exp(0.315 \sqrt{E_g \omega_{\text{max}}}), \hspace{1cm} (31)$$

where $E_g$ is the band gap of the materials in eV, $\omega_{\text{max}}$ the phonon cutoff frequency in THz, and $E_b$ the breakdown field in MV/m. Although successful, the main limitation of this model is that it is independent of temperature. For this reason, we aim at computing the BFOM from first principles while retaining the temperature dependence. To do so, in addition to the intrinsic carrier mobility, we need to compute the intrinsic breakdown field.

The most common theory for a material breakdown relies on electron avalanche [86], which occurs when the electron energy reaches the threshold for impact ionization. This is the energy at which an electron generates a second conduction electron by excitation across the electronic energy gap, causing electron multiplication (avalanche) and leading to a breakdown of the material [27]. As a result, the threshold for impact ionization is usually taken as the electronic band gap. The idea behind the theory relies on accelerating the conduction
electron with a laser field and taking into account the electron scattering with the lattice during pumping. Indeed, the phonon collision reduces the acceleration of the electron by modifying their momentum.

The von Hippel low-energy criterion is more stringent and states that breakdown will occur when the rate of energy gain $A(E, \varepsilon, T)$ by an electron of energy $\varepsilon$ due to the external field $E$ at temperature $T$ is larger than the energy-loss rate $B(\varepsilon, T)$ to the lattice due to electron-phonon interaction [26–28]:

$$A(E, \varepsilon, T) > B(\varepsilon, T),$$  \hspace{1cm} (32)

for energies $\varepsilon$ going from the conduction-band minimum to the threshold for impact ionization, i.e., the band gap of the materials.

The steady-state solution for the average energy-gain rate from the electric field is [27]

$$A(E, \varepsilon, T) = \frac{1}{3} \frac{e^2 \tau(\varepsilon, T)}{m^*} E^2,$$  \hspace{1cm} (33)

where $e^2$ is the electron charge and $m^* = 0.3$ [87] the electron effective mass. The energy- and temperature-dependent electron-phonon lifetime is given by

$$\tau^{-1}(\varepsilon, T) = \sum_{nk} \tau_{nk}^{-1}(T) \delta(\varepsilon_{nk} - \varepsilon) / D(\varepsilon),$$  \hspace{1cm} (34)

where $D(\varepsilon)$ is the density of state and $\tau_{nk}^{-1}$ is given by Eq. (23).

The field-independent net rate of energy loss $B(\varepsilon, T)$ to the lattice is obtained by subtracting the rate of phonon absorption from phonon emission [27,28]:

$$B(\varepsilon, T) = \frac{2\pi}{\hbar D(\varepsilon)} \sum_{nm} \int \frac{d^3k d^3q}{\Omega_{BZ}^2} |g_{mn}(k, q)|^2 \delta(\varepsilon_{nk} - \varepsilon) \times \hbar \omega_{q} \left[ n_{qy} + 1/2 \right] \delta(\varepsilon_{nk} - \varepsilon_{nk+q} + \hbar \omega_{q})$$

$$- n_{qy} \delta(\varepsilon_{nk} - \varepsilon_{nk+q} - \hbar \omega_{q}),$$ \hspace{1cm} (35)

where $n_{qy}$ are the Bose-Einstein occupation factors in the absence of an electric field.

We computed the energy-gain and energy-loss rates using the EPW software by interpolation on a dense $80 \times 80 \times 60$ k-point grid and a $40 \times 40 \times 30$ q-point grid with a constant smearing of 20 meV. In Fig. 6(a) we present the change of energy-loss rate as a function of energy, starting from the conduction-band minimum (CBM). On the same figure, we compare the loss rate with the average energy-gain rate for increasing external electric field $E$ at room temperature. We define the intrinsic breakdown field $E_b$ as the smallest external electric field such that the energy-gain curve is larger than the energy-loss curve for all energies between the CBM and the CBM plus the energy of the band gap (4.5 eV). This value provides an estimate of the electric field range for which the material will not undergo dielectric breakdown. We compute that at room temperature the breakdown field is 5.8 MV/cm, including all electron-phonon scattering processes. Using the same approach for different temperatures, we can obtain the change of breakdown field with temperature shown in Fig. 6(b).

![FIG. 6. (a) Average energy-gain rate $A(\varepsilon)$ from an applied external field and average energy loss to the lattice $B(\varepsilon)$. Both quantities are for 300 K. The intrinsic breakdown occurs when the applied electric field is such that the gain rate is larger than the loss rate for all energies between the conduction-band minimum (CBM) and the CBM plus the energy of the band gap (4.5 eV). (b) Variation of computed breakdown field with temperature. (c) Experimental variation of dielectric function with direction and temperature of $\beta$-Ga$_2$O$_3$ from Ref. [81]. (d) Baliga's figure of merit (BFOM) with respect to the BFOM of silicon. The BFOM of Si was obtained using dielectric constants from Ref. [82] and a breakdown field of 0.3 MV/cm, as well as the experimental electron mobility from Norton et al. [83].]
in Fig. 6(b). We find a breakdown field of 6.64 MV/cm at 500 K.

Such calculation was performed by Mengle and Kioupakis [22] for the intrinsic electron breakdown field at 300 K. They obtained 5.4 MV/cm by considering only the dominant LO phonon mode and estimated that the contribution of other modes would lead to 6.8 MV/cm. We note that the experimental breakdown field in $\beta$-Ga$_2$O$_3$ is typically reported at around 8 MV/cm [1]. This is in line with our calculations, since the von Hippel low-energy criterion should be seen as a lower bound for the breakdown field.

Using this information and the experimental dielectric function, we can compute the temperature- and direction-dependent BFOM. The BFOM is typically given with respect to the BFOM of silicon.

In this case we computed the reference BFOM of silicon by using the temperature-dependent dielectric constant of Refs. [82,88] and a breakdown field of 0.3 MV/cm, as well as the experimental temperature-dependent electron mobility from Norton et al. [83]. The resulting change of BFOM is given in Fig. 6(d). The direction-averaged minimum and maximum values are 1130 and 2035, respectively. We see that even though the computed breakdown field underestimates the experiment, this effect is compensated by an overestimation of the mobility. As a result, our calculated BFOM is close to experimental estimates of 2000–3000 [1]. This cancellation suggests that the current level of theory could be sufficient to predict the BFOM of new materials.

VII. CONCLUSION

In this work, we performed an in-depth study of the structural, vibrational, elastic, electrical, and transport properties of $\beta$-Ga$_2$O$_3$ using state-of-the-art, first-principles simulation tools. We carefully analyzed the structural properties of the monoclinic variation of $\beta$-Ga$_2$O$_3$ and analyzed the effect of spin-orbit coupling on those properties. We studied the electronic structure and carrier effective masses. We made a careful analysis of the vibrational properties, including a symmetry analysis of $\beta$-Ga$_2$O$_3$ using first-order response function theory, including dielectric and Born effective charges study. We calculated many elastic properties by computing the elastic constants tensor, including the bulk, shear, and Young modulus tensor, using parametric three-dimensional visualization but also Poisson’s ratio, universal elastic anisotropy, sound velocities, and Debye temperature, and found a strong directional anisotropy. We used the Boltzmann transport equation to compute the intrinsic electron and hole drift mobility and obtained room-temperature values of 258 and 1.2 cm$^2$/Vs, respectively. We found that the mobility in $\beta$-Ga$_2$O$_3$ was limited by a series of longitudinal optic phonons with symmetry character $B_\alpha$ at the zone center. Finally, we used the von Hippel low-energy criterion to compute fully from first principles the breakdown field, which allowed us to compute the direction- and temperature-dependent Baliga figure of merit for high-power devices. We saw that the predicted figure of merit was in good agreement with experiment and attributed this to an overestimation of the computed mobility compensating an underestimation in the computed breakdown field.

The present analysis may serve as the basis for a general, consistent, and predictive framework to study materials for power electronics from first principles.

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