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Cubic Boron Arsenide: A Promising Semiconductor with High Mobility and Thermal Conductivity

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Abstract. Cubic boron arsenide (c-BAs) is an emerging semiconductor material which recently gain attention due to its superior electron-hole mobility and thermal conductivity that significantly surpass those of traditional material. Its hole mobility is 4.5 times higher than that of silicon (Si) and thermal conductivity 10 times higher than Si, making it a promising material for next-generation electronics. This review examines the fundamental properties of c-BAs in the field of electronics. The crystal structure of c-BAs is introduced. This article focuses on the analysis of its electron-hole mobility and thermal conductivity. Basic mechanical properties of c-BAs are also provided. The potential application of c-BAs in high-performance electronics and thermal management system are explored. Fabrication challenges, including issues with traditional chemical vapor transport (CVT) methods, and the detrimental effects of impurities on performance are discussed, along with potential approaches to synthesizing higher-quality crystals.

Keywords: Semiconductor material, Cubic boron arsenide, High thermal conductivity, High mobility

1. Introduction

As semiconductor devices continue to shrink in size, the carrier mobility and thermal conductivity of materials become increasingly critical. High mobility allows for faster transistors switching speeds with reduced heat generation, while high thermal conductivity of materials is essential for effective thermal management, preventing performance degradation, reduce efficiency, and shorten lifespan caused by elevated temperatures. These two properties obstruct the use of mainstream materials such as silicon in next-generation electronics, because better performance in components is required for the rising demand for functionality and the decrease in size of the device. This motivated the exploration of new semiconductor materials with more suitable properties to achieve technological breakthroughs.

Cubic boron arsenide (c-BAs) has recently attracted great interest due to the exceptionally high electron-hole mobility and thermal conductivity. Both the electron and hole mobility of c-BAs was calculated to be higher than 1000 $cm^2V^{-1}s^{-1}$ while the hole mobility of the common material Silicon (Si) is 450 $cm^2V^{-1}s^{-1}$. It was also believed to be a super-thermal-conductor with thermal conductivity

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of ~2000 $Wm^{-1}K^{-1}$ at room temperature which is 10 times that of Si [1]. These properties make it a promising material for future electronic devices and prompts researches on it.

In 2013, a finding which based on three-phonon scattering by Lindsay et al. predicted that c-BAs has an extremely high thermal conductivity above 2000 $Wm^{-1}s^{-1}$ at room temperature [1]. However, the production of high-quality c-BAs crystals proved challenging. No experimental results are available until 2015, an experimental study was done by Lv et al. and measured thermal conductivity ~200 $Wm^{-1}K^{-1}$ in a crystal sized ~300 μm [2]. In 2017, Feng et al. revised the predicted thermal conductivity to 1400 $Wm^{-1}K^{-1}$, attributing the difference to four-phonon scattering effects [3]. A significant breakthrough came in 2018, when Li et al. successfully grew high-quality c-BAs crystals with a thermal conductivity of 1000 $Wm^{-1}K^{-1}$ using a modified chemical vapor transport (CVT) technique [4]. In the same year, Liu et al. discovered the high electron and hole mobilities of c-BAs, reaching 2110 $cm^2V^{-1}s^{-1}$ and 1400 $cm^2V^{-1}s^{-1}$ respectively [5].

This review provides a comprehensive overview of the crystal structure and key properties of c-BAs in the context of electronics. We delve into its carrier mobility and thermal conductivity, as well as its bandgap and mechanical properties. The potential applications of c-BAs in high-performance electronics and thermal management are explored in light of its remarkable attributes. We also address the challenges in scaling up c-BAs production, particularly the difficulty in producing high-quality bulk single crystals. Finally, we discuss possible methods to enhance crystal quality, including improvements to the CVT method and alternative growth techniques.

2. Properties

Cubic boron arsenide (c-BAs) is a transparent crystal coloured in red(Fig. 1). It is a III-V compound formed by the combination of group III element boron (B) and group V element arsenic (As) with 1:1 ratio of B and As. It is in zinc-blende structure arranged in CCP(Cubic Close Packing) manner(Fig. 2). In the crystal, Boron and arsenic atoms are covalently bonded together in tetrahedral geometry, similar to that of diamond. B atom is bonded to 4 As atoms and each As atom is bonded to 4 B atoms. B are present at the corner of the cubic shape unit cell structure and center of each face with As in the alternative tetrahedral void. Its equilibrium lattice constant is 4.78Å and the space group of c-BAs is F43m [6].

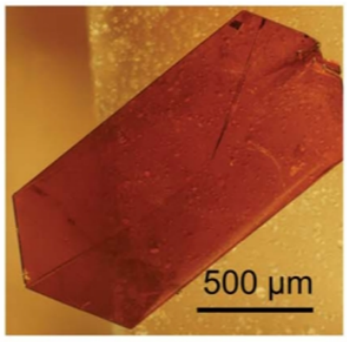


Figure 1. Optical photograph of c-Bas [9]

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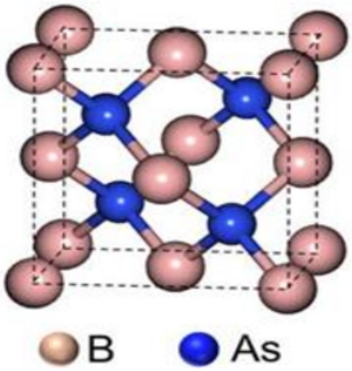


Figure 2. Unit cell structure of c-Bas [6]

2.1. Electron-hole mobility

2.1.1. Theoretical predictions of mobility

High electron mobility and hole mobility occurred simultaneously in c-BAs, which is different from other III-V group materials, which usually have high mobility for only electrons or holes. A study in 2018 performed first principles calculations using density functional theory (DFT) calculation. They discovered that c-BAs has high hole mobility and electron mobility at room temperature, 2110 cm^2V^{-1} s^{-1} and 1400 $cm^2V^{-1}s^{-1}$ respectively [5]. Compare c-BAs with other widely used semiconductors, Silicon (Si) and gallium arsenide (GaAs), electron mobility at room temperature is not exceptionally high (μ_e = 1400 $cm^2V^{-1}s^{-1}$ for Si and μ_e = 8500 $cm^2V^{-1}s^{-1}$ for GaAs), but the hole mobility of c-BAs significantly exceeds that of Si and GaAs (μ_h = 450 $cm^2V^{-1}s^{-1}$ for Si and μ_h = 400 $cm^2V^{-1}s^{-1}$ for GaAs).

Another study in 2019, also through DFT calculation, confirms the high electron-hole mobility of c-BAs. According to their calculation of mobilities in c-BAs at 300K, electron mobility of 1341 cm^2V^{-1} s^{-1} and hole mobility of 1387 $cm^2V^{-1}s^{-1}$ are obtained [7]. This result for electron mobility is in agreement with the previous study, but hole mobility obtained is only 2/3 of that. The discrepancy occurred because the study in 2019 did not include the effect of spin-orbit coupling, which affects the scattering channels of electron-phonon interactions. Thus, the commonly seen theoretical value of electron mobility in c-BAs is 1400 $cm^2V^{-1}s^{-1}$ and hole mobility 2100 $cm^2V^{-1}s^{-1}$, all rounded to the nearest hundred.

2.1.2. Experimental observations and measurements

Apart from theoretical values, experimental studies were hindered by the inability to produce high-quality c-BAs single crystal. The highest experimentally measured hole mobility of BAs is ~400 $cm^2V^{-1}s^{-1}$ measured in 1972 due to the presence of impurities [5]. A major breakthrough turned out in 2021, bulk carrier mobility of 650 $cm^2V^{-1}s^{-1}$ was obtained from a crystal grown using GaAs nucleation and local carrier mobility up to 1500 $cm^2V^{-1}s^{-1}$ was attained [8]. In 2022, researchers successfully synthesized high-quality c-BAs samples using multistep chemical vapor transport [7,9]. The mobility was measured through pump-probe transient reflectivity microscopy, where the diffusion of photoexcited carriers in c-BAs was monitored and an ambipolar mobility of 1500 $cm^2V^{-1}s^{-1}$ ± 120 $cm^2V^{-1}s^{-1}$ was obtained [7]. Although largely different from the predicted hole mobility of c-BAs, the result is considered to be close to the predicted value because the ambipolar mobility is

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dominated by the low mobility carrier, which is in this case the electron mobility of c-BAs (1400 $cm^2V^{-1}s^{-1}$) [5,7,9]. Another experiment measured the mobility using the optical transient grating technique and obtained ambipolar mobility of 1600 $cm^2V^{-1}s^{-1}$ ± 170 $cm^2V^{-1}s^{-1}$, similar to the predicted value and other experimental values [9].

2.1.3. Theory behind high mobility

The high mobilities in c-BAs was caused by its unique feature of lattice dynamics. In common semiconductors, electrons are predominantly scattered by phonons. In polar crystals, polar-optical-phonon scattering acts as one significant scattering channel to electrons [5]. This is caused by atoms in the lattice experiencing optical vibration which produce polarization effect and scatters the electrons. c-BAs is slightly polar, therefore exhibits polar-optical-phonon scattering [10]. However, the similarity of static and high frequency dielectric constant indicated that c-BAs is only weakly ionic, so scattering by them should be weaker than other III-V group materials [11]. Furthermore, compare with other semiconductors such as GaAs, polar-optical-phonon has much less effect in BAs due to the low occupation number of longitudinal-optical (LO) phonon. Low LO-phonon occupation, which leads to lower LO-phonon scattering rates, usually occurs when the optical mode possesses high vibrational frequencies. Thus, the high mobility of c-BAs was due to its high vibrational frequencies that reduce optical phonon occupation and suppress the polar scattering in the material [5].

2.1.4. Dual high mobility of electrons and holes

c-BAs is different from common group III-V semiconductors because it possesses simultaneously high electron and hole mobilities, whereas III-V compounds tend to have only high electron mobility or hole mobility. It was caused by the relatively small difference between the effective mass of electrons and holes [5,8]. c-BAs has an effective mass ratio of about 2, where the effective mass of electrons (me) ~1.10 and effective mass of holes (mhh) ~0.56. Compare with other III-V material like GaAs, a ratio of about 5 was observed (me ~0.067 and mhh ~0.34 in GaAs) [5]. Since mobility increase as effective mass decrease, effective mass of electrons and holes in GaAs suggests that it has high electron mobility and low hole mobility. Similar in c-BAs, the effective mass of holes smaller than effective mass of electrons indicates that its hole mobility is higher than its electron mobility [8,11,12].

High electron and hole mobilities indicate that c-BAs has a low electrical resistance since both charges can be transferred easily. Less energy is wasted as heat during the process and its efficiency will be higher. It also means that a relatively high current can be achieved with a lower doping level. In addition, simultaneous high electron and hole mobilities enables c-BAs to be competent for both n-type doping and p-type doping, which further increase its potential in future devices.

2.1.5. Temperature dependence of mobility

Carrier mobility of in c-BAs is sensitive to temperature. As temperature increases, both electron and hole mobility decrease. The rate at which mobilities falls relative to temperature decreases with higher temperature (shown in Fig. 3). According to DFT calculation, the effect of temperature on hole mobility is significant. An 85% reduction in hole mobility (6360 $cm^2V^{-1}s^{-1}$ to 930 $cm^2V^{-1}s^{-1}$) was shown when temperature rises from 200K to 400K [5]. This can be attributed to the increase in phonon occupation number as temperature rises [5]. In reality, the measured ambipolar mobility in

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c-BAs crystal shows good agreement with the calculation, mobilities decrease as temperature increases(Fig. 4). The difference between measured data and theoretical values is probably due to the presence of impurities in the crystal [9].

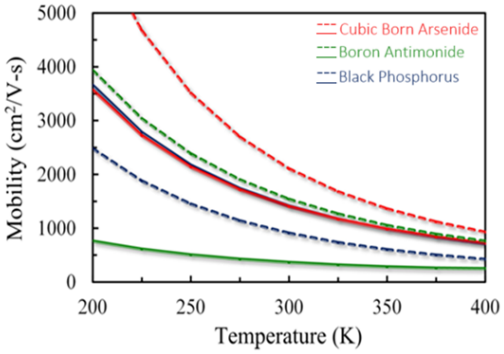


Figure 3. Carrier mobility of c-BAs(red) with varying temperature. Solid line and dashed line represent electrons and holes mobility respectively [5]

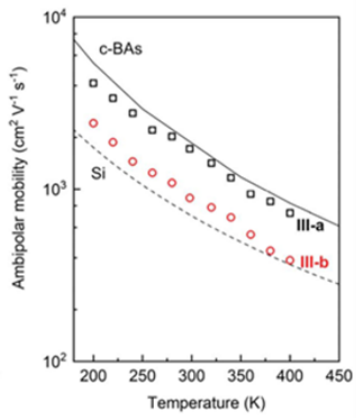


Figure 4. Measured ambipolar mobility in c-BAs crystal with varying temperature. III-a and III-b are different sports on the crystals [9]

2.2. Thermal conductivity

2.2.1. Theoretical predictions of thermal conductivity

Under room temperature, thermal conductivity of c-BAs can up to 1400 W/m·K which is greater than most semiconductors. The Boltzmann Transport Equation (BTE) and first-calculation principle commonly used to calculate thermal conductivity. BTE describes scattering and transport behaviour of phonons in lattice. The equation can be represented as

$$k = \frac{1}{3} \cdot C \cdot v^2 \cdot \tau \tag{1}$$

which is derived from the Boltzmann Transport Equation. C is thermal capacity. v is group velocity. τ is phonon lifetime. What's more, first-principle calculation is a theoretical method used in the most fundamental physics theorem to predict and explain the properties.

Jungwoo Shin with his team members predicted that c-BAs has exceptionally high room temperature thermal conductivity of ~1400 $Wm^{-1}K^{-1}$ [9]. Nowadays, Silicon and Gallium arsenide

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are the mainstream material. The thermal conductivity of Si is 140 $Wm^{-1}K^{-1}$ which has one-tenth the thermal conductivity of cubic boron arsenide. The thermal conductivity of GaAs is 45 $Wm^{-1}K^{-1}$. It is far less than the thermal conductivity of c-BAs. They stated that in addition to the diamond-like face center cubic(FCC) structure of cubic boron arsenide, the strong covalent bond between its atoms allows cubic boron arsenide to transfer heat efficiently, and the high propagation velocity of phonons and the scattering of low phonons lead to high thermal conductivity as well.

2.2.2. Experimental measurement techniques

Optical transient grating (TG) and Time domain thermal reflection method(TDTR) will be elaborated in this article.

2.2.2.1. Optical transient grating (TG) method

Optical transient grating is a sophisticated technique used in material science and physics to study various dynamic processes in materials.

Jungwoo Shin [9] with his team members utilized two femtosecond laser pulses (pump) to create sinusoidal optical interference pattern on the c-BAs samples firstly. This pattern forms a transient grating. Then, the third laser pulse was introduced at a controlled delay time t after the initial pulses. This pulse will interact with the transient grating and produce a diffracted signal. Measured the intensity of the diffracted probe pulse over time. The delay of this signal provides information about the thermal and electronic dynamics in the c-BAs. The decay of the thermal grating is analysed to determine the thermal diffusivity of the material. From the thermal diffusivity and the known density and specific heat capacity of c-BAs, the thermal conductivity can be calculated using the relation:

$$k = \alpha \cdot \rho \cdot C_p \tag{2}$$

α is the thermal diffusivity. ρ is the density. C_p is the specific heat capacity. Diffusion and recombination of photoexcited carriers lead to a rapid exponential decay of the electrical signal and a slower thermal decay(Fig. 5 and Fig. 6).

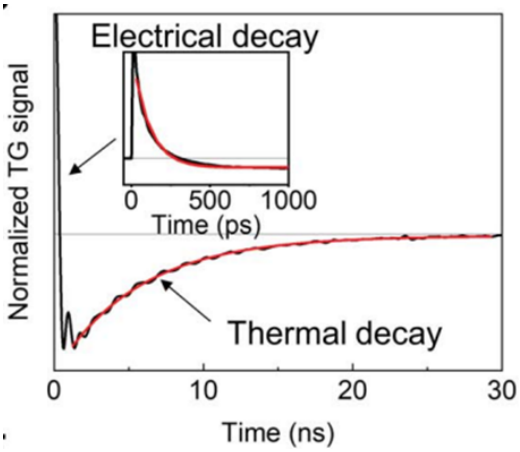


Figure 5. A TG signal for c-Bas [9]

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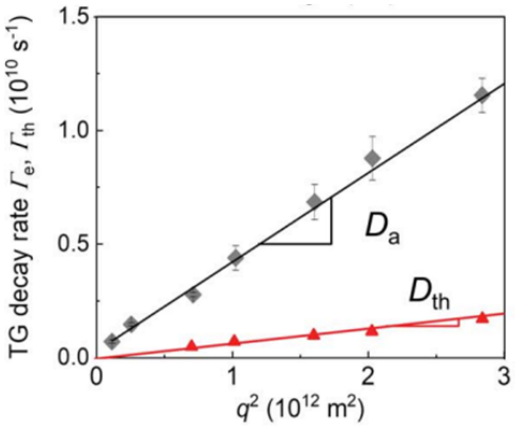


Figure 6. Electrical decay rate(black line) and thermal decay rate(red line) divided by q^2 [9]

The value of the thermal conductivity they obtained is k = 200 to 953 $Wm^{-1}K^{-1}$, which is much less than the theoretical value 1400 $Wm^{-1}K^{-1}$.

2.2.2.2. Time-domain thermoreflectance (TDTR) method

Time-domain thermoreflectance (TDTR) is a useful method used to measure the thermal properties of materials, particularly thermal conductivity. Sheng Li with his group members measured the thermal conductivity by time-domain thermoreflectance [4].

First, deposit a thin metal film such as Aluminum on the sample. This film acts as a transducer, converting thermal energy into a measurable change in reflectance. Then, they used a pulsed laser(pump) to heat the metal film. The heat will diffuse into the c-BAs sample. Meanwhile, a second laser (probe) measures the change in reflectivity of the metal film, which is related to the temperature change. The probe laser measures the reflectivity change over time and record the reflectivity data as a function of time delay between the pump and probe pulses. They analysed the reflectivity data using a thermal model to extract the thermal conductivity. This involves fitting the experimental data to the model, which accounts for heat diffusion in the metal film and the c-BAs sample.

The value of the thermal conductivity they obtained is k = 500 to 1000 $Wm^{-1}K^{-1}$, which is less than the theoretical value as well.

2.2.2.3. Conclusion

Table I. The differences between two experiments

Method	Optical transient grating (TG) Method	time-domain thermoreflectance (TDTR) Method
Group	Jungwoo Shin	Sheng Li
Result ($Wm^{-1}K^{-1}$)	920	1000
	1132	870
	163	850
	221	500

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2.2.3. Factors influencing thermal conductivity

The most important thing is the purity of the crystal. In the process of synthesizing c-BAs, crystals dope other elements, such as silicon and carbon. These defects and impurities can significantly reduce thermal conductivity. This is because defects and impurities scatter phonons which is the main carriers of heat energy, thus impeding heat flow. This is the reason why neither Li Sheng's experiment nor Jingwoo Shin's, their results have reached the ideal value.

2.3. Bandgap characteristics

Cubic boron arsenide (c-BAs) exhibits unique electronic properties that differentiate it from silicon, particularly in its excitonic spectrum and bandgap characteristics. Significant differences with silicon emerge when examining two-particle properties, which refer to interactions involving pairs of particles, typically electrons and holes. The direct bandgap of c-BAs is around 4.00 eV, but dark excitons (non-emitting) can exist at much lower energies, down to approximately 1.50 eV. This indicates that c-BAs has significant two-particle interactions that influence its electronic properties [13].

The bandgap of c-BAs has been extensively studied through various computational and experimental methods, resulting in a range of reported values. Past experimental studies have indicated bandgaps of around 1.50 eV [14-16], while more recent measurements report gaps of 1.82 eV and 2.02 eV from high-quality millimeter-sized crystals [6,17].There are a number of reasons of this, for instance, different experimental and computational approaches, crystal quality, environmental factors, and the intrinsic complexities of the material.

GW calculations provide bandgaps by correcting the former results more precisely, but different implementations (e.g., G0W0, QSGW) can yield slightly different values. A single-shot G0W0 calculation using BerkleyGW yielded a gap of 2.07 eV, and another work reported a gap of 1.78 eV [18]. Moreover, advanced computational techniques like quasiparticle self-consistent GW (QSGW) theory typically falls within the range of 1.85 eV to 2.00 eV [19,20]. Most other reports converge on a bandgap closer to 2.00 eV, suggesting this as a more accurate representation of the true bandgap of c-BAs when using QSGW theory [13].

These computational studies showing similarities of bandgap of c-BAs to other boron pnictides and GaAs. The conduction band minimum in c-BAs has a unique p-band character, influenced by strong covalence between boron and arsenic.

Bandgap estimates vary depending on the methodology, reflecting the complexity of accurately determining this property. Defects and impurities further affect electrical properties, and thermal properties indirectly due to changing carrier concentration, phonon interactions, and defect states. Additionally, the surface electronic properties of c-BAs remain underexplored, as surface relaxations in III-V zincblende compounds like BAs prevent intrinsic surface states from appearing in the bulk bandgap [21].

2.4. Mechanical properties

Cubic boron arsenide (c-BAs) demonstrates exceptional mechanical properties that make it highly suitable for advanced applications. It exhibits a remarkable combination of high thermal conductivity (~1300 W/m·K), with Poisson's ratio (0.22 (⟨100⟩ on (100))) and Averaged elastic modulus (326 GPa) similar to steel, and high hardness. These features could revolutionize thermal management in solid-state electronics [5].

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c-BAs is a hard material, with a Vickers hardness of 22 GPa. The bulk and Young's moduli are 142 GPa and 388 GPa [22], respectively, highlighting its robustness. The material's mechanical properties, combined with its high thermal conductivity, position it as a strong candidate for next-generation semiconductor applications.

One of the most striking mechanical properties of c-BAs is its high Vickers hardness, measured at 22 GPa [22]. Vickers hardness is a key indicator of a material's resistance to localized plastic deformation, such as indentation, scratching, or wear. This makes c-BAs highly resistant to surface damage, a critical factor for materials used in harsh environments. The average fracture toughness (KIC) is 1.18 $MPa \cdot m^{0.5}$, demonstrating its brittleness, but it is more ductile than materials like SiC, BN, and AlN [22].

The bulk modulus of c-BAs, measured at 142 GPa [22], reflects its ability to resist uniform compression. This property is crucial in applications where materials are subjected to high pressures and must maintain their volume and structural integrity. A high bulk modulus indicates that c-BAs can withstand significant compressive forces without undergoing substantial deformation.

Then, With a Young's modulus of 388 GPa [22], c-BAs is exceptionally stiff, indicating its strong resistance to elastic deformation under tensile or compressive stress. This stiffness is particularly important in applications requiring materials that maintain their shape and do not flex or bend under load. On the other hand, Poisson's ratio for c-BAs is measured at 0.22 [6], indicating that it exhibits minimal lateral expansion when subjected to axial compression. This low Poisson's ratio contributes to the material's overall dimensional stability, which is crucial in applications requiring precise geometric control.

In addition to its mechanical strength, the compatibility of c-BAs with existing semiconductor manufacturing processes, with its similar coefficient of thermal expansion to silicon, further enhances its appeal as a material that can be seamlessly integrated into advanced electronic devices. As the demand for more durable and high-performance materials continues to grow, c-BAs is poised to play a significant role in the evolution of modern technology.

3. Potential applications

3.1. 1 High-performance electronics

3.1.1. Wide bandgap advantages in power electronics and UV applications

The wide bandgap of c-BAs makes it suitable for high-power electronic devices. Materials with wide bandgaps can handle higher voltages and temperatures, making c-BAs ideal for power electronics, such as transistors and diodes, that operate under extreme conditions. The wide bandgap also allows for the efficient absorption and emission of light in the ultraviolet range, making c-BAs useful in applications requiring UV sensitivity, such as environmental monitoring, medical diagnostics, and communication systems.

This high ambipolar mobility that >1000 $cm^2V^{-1}s^{-1}$ makes c-BAs an excellent material for high-speed electronic devices, such as field-effect transistors (FETs) [9], where both n-type and p-type conduction are required. The combination of high mobility and a wide bandgap could enable faster switching speeds and lower power consumption in electronic circuits.

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3.1.2. Precision manufacturing and optics: mechanical stability and durability

In precision manufacturing, particularly in the optics and microelectronics industries, materials with minimal deformation under stress are essential. The high Young's modulus of c-BAs (388 GPa [22]) ensures that components such as lenses, mirrors, and precision instruments retain their shape and alignment, even under mechanical load. This property is critical for maintaining the accuracy and functionality of optical systems and high-precision instruments, where even minor deformations can lead to significant performance losses.

The high bulk modulus of 142 GPa further contributes to its suitability in these environments by providing resistance to compression [22], making c-BAs an ideal material for devices that must operate reliably under varying pressure conditions, such as in MEMS (Microelectromechanical Systems) and sensors. Additionally, its Vickers hardness of 22 GPaadds to its durability, ensuring that components can withstand surface wear and damage over time [22].

Moreover, the low Poisson's ratio of 0.22 ensures that c-BAs exhibits minimal lateral expansion under compression [6], providing dimensional stability and reducing the risk of warping or distortion in critical parts. This stability, combined with its hardness, makes c-BAs ideal for use in protective coatings that shield sensitive equipment from mechanical damage, ensuring longer service life and reliability in demanding environments.

3.2. Heat dissipation system

3.2.1. Conductivity and expansion: cooling substrates for electronics

Another potential application of c-BAs is in thermal management systems. Heat dissipation is critical to modern electronics. c-BAs has great potential as cooling substrates for electronic devices because it has high thermal conductivity. As mentioned before, c-BAs was predicted to have thermal conductivity 1400 $Wm^{-1}K^{-1}$. It is 10 times that of silicon and only second to diamond. Although its thermal conductivity is lower than diamond, it has a smaller mismatch in thermal expansion coefficient. Mismatch in thermal expansion leads to problems like residual stress and thermal boundary resistance. Thermal expansion coefficient of c-BAs is 3.85 • 10^{-6} K^{-1} [6]. Compare with diamond with thermal expansion coefficient 1.6 • 10^{-6} K^{-1}, c-BAs avoids the problems caused by the mismatch in coefficient of thermal expansion [6]. Its thermal conductivity and thermal expansion coefficient give c-BAs great potential as cooling substrates for electronics.

3.2.2. Integration with GaN devices: superior interfacial thermal conductance

Furthermore, c-BAs is good cooling substrates for gallium nitride devices (GaN). According to two different studies, the interfacial thermal conductance between GaN and BAs is 250M $Wm^{-1}K^{-1}$ and 260 respectively [23-25]. It demonstrates better interfacial thermal conductance than diamond (Fig. 7) due to the phonon band structures of BAs and GaN [23]. GaN and c-BAs also has a similar thermal expansion coefficient (3.94 • 10^{-6} K^{-1} for GaN). These properties make c-BAs a potential cooling substrate material for GaN devices. According to a study in 2024 by Kang et al., the device cooling performance of c-BAs exceeds that of diamond and silicon carbide (SiC) under same device layout and operation condition, showing its potential for heat dissipation [23].

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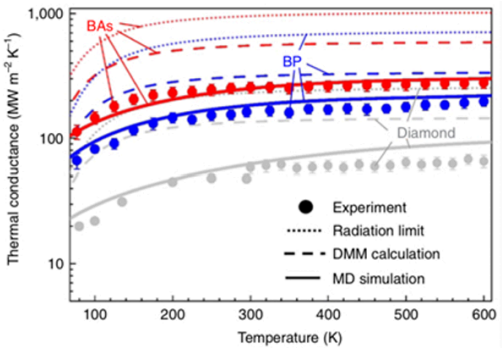


Figure 7. Thermal boundary conductance of c-BAs, BP and diamond with GaN [23]

4. Current challenges

Nowadays, c-BAs is not used in industry and has only been prepared in some laboratories. The following parts will introduce the challenges people encounter in the fabrication and the possible solutions.

4.1. Crystal quality issues

4.1.1. Limitations of Chemical Vapor Transport(CVT)

Chemical Vapor Transport (CVT) is the most common and mature method to grow high-quality single crystal material. The main principle is to place the precursor of the required growth crystal at the high temperature end of the vacuum sealed quartz tube, and use substances such as I_2 as transport agents. The transport agent reacts with the precursor in the high temperature region to form a gas that is easily transported and reaches the low temperature region. In the low temperature region, gaseous boron (B) is precipitated by the reverse reaction of the gas components, which reacts with the arsenic atmosphere (As_4), and then deposits crystals on the surface of the quartz tube or substrate, thereby synthesizing high-quality single crystal materials(Fig. 8).

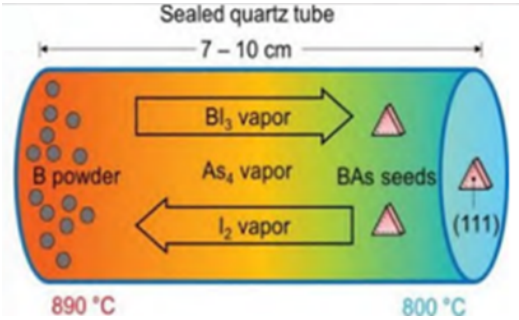


Figure 8. The schematic diagram of growing c-BAs by using CVT [26]

4.1.2. Difficulties in synthesizing high-purity single crystals

There are four difficulties in the process of synthesizing c-BAs.

First, the melting point of boron (2076 ℃) is much higher than the sublimation temperature of arsenic (614 ℃). Second, arsenic and related reactants are toxic, and people must have perfect protection measures. Third, boron has a strong chemistry stability and is difficult to react. Forth,

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When the temperature exceeds 920 ℃, the cubic phase BAs will decompose into hexagonal subcrystalline phase($B_{12}As_2$).

4.1.3. Impact of impurities on material performance

Today's lab-grown cubic boron arsenide is low in purity, which is why the actual thermal conductivity and electron-hole mobility are not ideal. In addition to the intrinsic defects generated during CVT growth, there are also impurities introduced from raw materials (B, As and I_2) and quartz tube pollution in BAs crystals, especially Group IV elements (C, Si and Ge). These impurities may replace atoms in lattice sites or occupy lattice gaps, leading to unwanted phonon scattering. This causes thermal conductivity and electron-hole mobility decrease(Fig. 8).

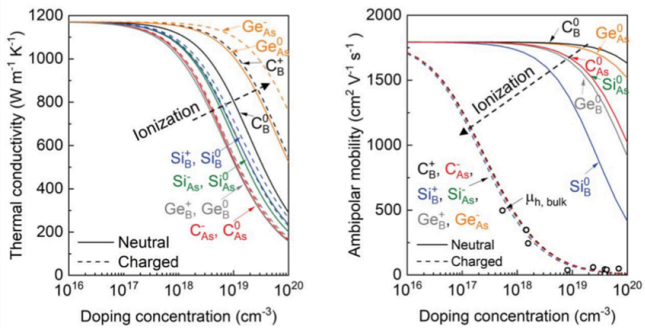


Figure 9. The relationship with thermal conductivity and ambipolar mobility and doping concentration [9]

4.2. Strategies for overcoming fabrication challenges

4.2.1. Optimizing CVT parameters for enhanced crystal growth

One way to improve the quality of c-BAs crystal produced is optimizing the conduction of the CVT process. According to a study published in 2021, c-BAs undergo irreversible decomposition at ~920°C. The hot end temperature below 820°C limits the growth of c-BAs crystals. The hot end temperature is best to be at 880°C~900°C. Experiments also show that temperature difference between hot end and cold end of the tube is best to be kept at 80°C~120°C, with tube length 10.0~12.0 cm [8]. These conditions can be combined to produce high-quality c-BAs single crystals.

4.2.2. Muti-Step CVT for improved crystal purity

Another method to improve is multistep CVT [9,22]. This method repeats the traditional CVT procedure twice. The first time using purified Boron(B) source and Arsenic (As) source to obtain c-BAs crystal. The same process was then repeated with the same conditions, but c-BAs crystal procured in the first process and purified As source was used as material. Seed materials are also placed at the cold end for better growth of the crystal [9,22].

4.2.3. Exploration of alternative growth methods: the flux method

Flux method is another widely used method for growing single-crystal materials due to its availability and accessibility. However, it is not common for c-BAs because it is hard to find a suitable flux which can dissolve Boron (B) [8]. People failed using Ni, Cu, Mg, Te, Sb and their

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mixtures as flux, but a study in 2023 claimed that they successfully produced high quality c-BAs with multi-millimeter size [8,26]. Liquid arsenic was used as a medium at high pressures and outstanding properties were observed [26].

5. Conclusion

Due to the ultra-high thermal conductivity and electron-hole mobility predicted by theory, c-BAs has attracted a lot of attention from researchers. Since then, with the development of synthesis and preparation technology, high-quality single crystal blocks have been prepared, and the ultra-high thermal conductivity and electron-hole mobility of c-BAs has been verified. On this basis, the physical properties of BAs, such as thermal properties, electrical properties, band structure and mechanical properties have also been studied and revealed. Compared with Si and GaAs semiconductors materials widely used today, c-BAs has high thermal conductivity and mobility, and also shows good substrate matching, which has broad application potential both for thermal management and as a next-generation high-performance electronics material.

At present, although the application prospect of c-BAs is good, it still needs a long time of exploration and systematic research to realize it. First of all, the preparation process of c-BAs remains in the laboratory stage after a long period of development, and the high-quality crystals prepared at this stage are only in the millimeter level. If this new material is to be used, it is necessary to break through the bottleneck of size to prepare a larger volume of single crystal materials. At the same time, due to the special physical and chemical properties of raw materials, the preparation method of c-BAs is mainly chemical vapor transfer method, which has a long preparation period and uncontrollable growth morphology, and is not suitable for commercial production. How to achieve commercial production and prepare materials with controllable morphology remains to be explored. In addition, the c-BAs prepared at present has been tested as p-type semiconductors, and how to obtain p-type and n-type BAs materials by stable doping is still a problem that needs to be solved. We hope this article can encourage other researchers to study c-BAs and find the ways to make it mass produced.

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References

[1] Lindsay L, Broido D A, Reinecke T L. First-Principles Determination of Ultrahigh Thermal Conductivity of Boron Arsenide: A Competitor for Diamond? [J]. Physical review letters, 2013, 111(2): 025901.

[2] Lv B, Lan Y, Wang X, et al. Experimental study of the proposed super-thermal-conductor: BAs [J]. Applied Physics Letters, 2015, 106(7).

DOI: 10.54254/2755-2721/2025.28293

[3] Feng T, Lindsay L, Ruan X. Four-phonon scattering significantly reduces intrinsic thermal conductivity of solids [J]. Physical Review B, 2017, 96(16): 161201.
[4] Li S, Zheng Q, Lv Y, et al. High thermal conductivity in cubic boron arsenide crystals [J]. Science, 2018, 361(6402): 579-581.
[5] Liu T H, Song B, Meroueh L, et al. Simultaneously high electron and hole mobilities in cubic boron-V compounds: BP, BAs, and BSb [J]. Physical Review B, 2018, 98(8): 081203.
[6] Kang J S, Li M, Wu H, et al. Basic physical properties of cubic boron arsenide [J]. Applied Physics Letters, 2019, 115(12).
[7] Yue S, Tian F, Sui X, et al. High ambipolar mobility in cubic boron arsenide revealed by transient reflectivity microscopy [J]. Science, 2022, 377(6604): 433-436.
[8] Udalamatta Gamage G A. Achieving Ultrahigh Thermal Conductivity and Carrier Mobility in Boron Arsenide Single Crystals [D]. , 2021.
[9] Shin J, Gamage G A, Ding Z, et al. High ambipolar mobility in cubic boron arsenide [J]. Science, 2022, 377(6604): 437-440.
[10] Polar optical phonon scattering. (n.d.). Retrieved September 8, 2024, from https: //www.iue.tuwien.ac.at/phd/milovanovic/diss_htmlse12.html
[11] Bushick K, Mengle K, Sanders N, et al. Band structure and carrier effective masses of boron arsenide: Effects of quasiparticle and spin-orbit coupling corrections [J]. Applied physics letters, 2019, 114(2).
[12] Buckeridge J, Scanlon D O. Electronic band structure and optical properties of boron arsenide [J]. Physical Review Materials, 2019, 3(5): 051601.
[13] Acharya S, Pashov D, Katsnelson M I, et al. One-Particle and Excitonic Band Structure in Cubic Boron Arsenide [J]. physica status solidi (RRL)–Rapid Research Letters, 2024, 18(1): 2300156.
[14] Ku S M. Preparation and Properties of Boron Arsenides and Boron Arsenide-Gallium Arsenide Mixed Crystals [J]. Journal of The Electrochemical Society, 1966, 113(8): 813.
[15] Chu T L, Hyslop A E. Preparation and properties of boron arsenide films [J]. Journal of The Electrochemical Society, 1974, 121(3): 412.
[16] Wang S, Swingle S F, Ye H, et al. Synthesis and characterization of a p-type boron arsenide photoelectrode [J]. Journal of the American Chemical Society, 2012, 134(27): 11056-11059.
[17] Song B, Chen K, Bushick K, et al. Optical properties of cubic boron arsenide [J]. Applied Physics Letters, 2020, 116(14).
[18] Mei H, Xia Y, Zhang Y, et al. Finite-momentum excitons and the role of electron–phonon couplings in the electronic and phonon transport properties of boron arsenide [J]. Physical Chemistry Chemical Physics, 2022, 24(16): 9384-9393.
[19] van Schilfgaarde M, Kotani T, Faleev S. Quasiparticle self-consistent GW theory [J]. Physical review letters, 2006, 96(22): 226402.
[20] Pashov D, Acharya S, Lambrecht W R L, et al. Questaal: A package of electronic structure methods based on the linear muffin-tin orbital technique [J]. Computer Physics Communications, 2020, 249: 107065.
[21] Lee H, Gamage G A, Lyons J L, et al. Electronic structure of cubic boron arsenide probed by scanning tunneling spectroscopy [J]. Journal of Physics D: Applied Physics, 2021, 54(31): 31LT01.
[22] Tian F, Luo K, Xie C, et al. Mechanical properties of boron arsenide single crystal [J]. Applied physics letters, 2019, 114(13).
[23] Kang J S, Li M, Wu H, et al. Integration of boron arsenide cooling substrates into gallium nitride devices [J]. Nature Electronics, 2021, 4(6): 416-423.
[24] Wu J, Zhou E, Huang A, et al. Deep-potential enabled multiscale simulation of gallium nitride devices on boron arsenide cooling substrates [J]. Nature Communications, 2024, 15(1): 2540.
[25] Tian F, Song B, Lv B, et al. Seeded growth of boron arsenide single crystals with high thermal conductivity [J]. Applied physics letters, 2018, 112(3).
[26] Koirala P, Liu W, Wu H, et al. A flux growth technique for high quality cubic boron arsenide bulk single crystals [J]. Applied Physics Letters, 2023, 123(20).