

## CBED Investigations of Boron Monoarsenide Crystals

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Boron monoarsenide (BAs), one III-V compound synthesized and grown since the 1960s [1-4], has been long-time ignored since its discovery. The unpopular material revokes scientists interesting recently because of its potentially high thermal conductivity [5-7], good photoelectric properties [8], and decent thermoelectric characteristic [9]. Single crystal X-ray diffraction [5] and powder X-ray diffraction [1,10] indicated that the space group of BAs should be  $F\bar{3}m$  with the zinc-blende structure at room temperature, similar as other III-V arsenides and boron compounds. Here, the space group of the compound is confirmed by convergent beam electron diffraction (CBED).

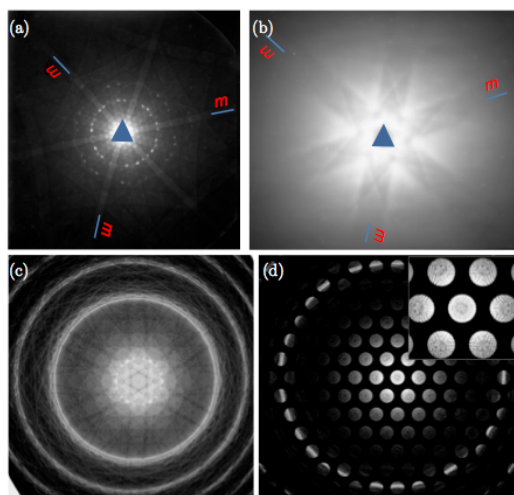
BAs single crystals were grown by a two-step procedure [5]. The grown BAs crystals with a length of 100 microns were crushed and ultrasonicated in ethanol, deposited on TEM grids. The CBED was carried out using a JEM 2000FX TEM operated at 200 kV and equipped with a LaB<sub>6</sub> emitter. All TEM work was carried out at room temperature. Whole-pattern (WP) symmetry and bright-field (BF) symmetry of CBED patterns were taken at 15 cm and 150 cm, respectively. The CBED patterns along main axes were simulated by the JEMS electron microscopy simulation software, with using the Bloch wave method at the accelerating voltage of 200 kV. The scattering factors were calculated using the Doyle and Turner atomic scattering factors for X-ray listed in International Tables for Crystallography. The electron adsorption potential was calculated by the Einstein model.

CBED patterns of BAs crystals are shown in Figures 1-3, along  $\langle 111 \rangle$ ,  $\langle 100 \rangle$  and  $\langle UWV \rangle$  zone axis respectively. Their symmetries are listed in Table 1. Potential diffraction groups and possible point groups are also listed in Table 1. Based on the symmetries of the CBED patterns and systematic extinction rules, the space group of BAs can be concluded as  $F\bar{3}m$  (No. 216). The  $F\bar{3}m$  space group was confirmed by simulations of CBED patterns. The bottom panels in Figure 1 and Figure 2 show the simulated WP and BF patterns along the  $\langle 111 \rangle$  and  $\langle 100 \rangle$  zone axes, respectively. The experimental CBED patterns are in good agreements with the simulated ones.

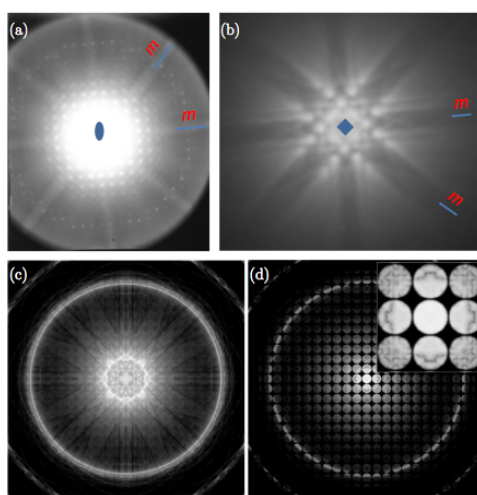
In summary, experimental and simulated CBED patterns indicated that the space group of BAs is  $F\bar{3}m$ . The CBED conclusion is in good agreements with X-ray diffraction results and Raman scattering data [11].

References:

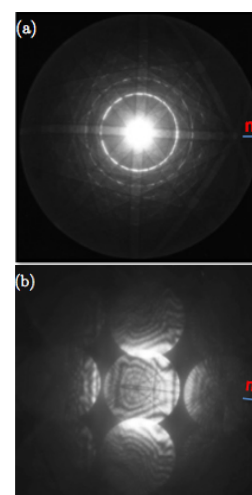
[1] J. A. Perri *et al*, *Acta Crystallogr.* **11** (1958), p. 310.  
 [2] S. M. Ku, *J. Electrochem. Soc.* **113** (1966), p. 813.  
 [3] A. F. Armington, *J. Cryst. Growth* **1** (1967), p. 47.  
 [4] T. L. Chu *et al*, *J. Appl. Phys.* **43** (1972), p. 276.  
 [5] B. Lv *et al*, *Appl. Phys. Lett.* **106** (2015), p. 074105.  
 [6] L. Lindsay *et al*, *Phys. Rev. Lett.* **111** (2013), p. 025901.  
 [7] D. A. Broido *et al*, *Phys. Rev. B* **88** (2013), p. 214303.  
 [8] S. Wang *et al*, *J. Am. Chem. Soc.* **134** (2012), p. 11056.  
 [9] J. Kim *et al*, *Appl. Phys. Lett.* **108** (2016), p. 201905.  
 [10] J. Osugi *et al*, *Rev. Phys. Chem. Jpn.* **36** (1966), p. 54.  
 [11] The work is partially supported by HDTRA122221. YCL acknowledges the support from ARL under W911NF-12-2-0022. AL is thankful to the financial support under NSF DMR 1206380 and DMR 1337916. The funding support from AFOSR (FA9550-15-1-0236) and ONR (N00014-16-1-2436) are also acknowledged.



**Figure 1.** (a,c) WP and (b,d) BF along  $\langle 111 \rangle$  zone axis. Top: experimental; Bottom: simulated.



**Figure 2.** (a,c) WP and (b,d) BF along  $\langle 100 \rangle$  zone axis. Top: experimental; Bottom: simulated.



**Figure 3.** (a) WP and (b) BF symmetry along  $\langle UVW \rangle$  zone axis.

TABLE I. Possible Diffraction Groups and Point Group

Zone axis	WP symmetry	BF symmetry	Diffraction groups	Possible point group
$\langle 111 \rangle$	$3m$	$3m$	$3m$ $6_R m m R$	$\bar{4}3m, 3m$ $m\bar{3}m, 3m$
$\langle 100 \rangle$	$2mm$	$4mm$	$4_R m m R$	$\bar{4}3m, \bar{4}2m$
$\langle UVW \rangle$	$m$	$m$	$m$	$\bar{4}3m, 6m2, 6mm, \bar{6}, 3m, \bar{4}2m, 4mm, mm2, m$
$\langle UV0 \rangle$			$2_R m m R$	$m\bar{3}m, m\bar{3}, 6/mmm, 6/m, \bar{3}m, 3, 4/m, mm2, 2/m$