

การศึกษาไตรโนโอเบียมอาร์เซไนต์ทางผลึกวิทยาโดยรังสีเอ็กซ์



นางสาว กัดณา สาริทธาภา

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แผนกวิชา ฟิสิกส์

บัณฑิตวิทยาลัย จุฬาลงกรณ์มหาวิทยาลัย

พ.ศ. ๒๕๒๐

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AN X-RAY CRYSTALLOGRAPHIC STUDY OF  
TRINIOBIUM ARSENIDE ( $\text{Nb}_3\text{As}$ )



Miss Gannaga Satittada

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หัวข้อวิทยานิพนธ์ การศึกษาไตรโนโอเบียมอาร์เซไนต์ทางผลึกวิทยาโดยรังสีเอ็กซ์  
 ชื่อ นิสิต นางสาว กัลณกา สาธิตชากา  
 อาจารย์ที่ปรึกษา ผู้ช่วยศาสตราจารย์ ดร. พัทธนะ ภวะนันท์  
 แผนกวิชา ฟิสิกส์  
 ปีการศึกษา ๒๕๒๐



บทคัดย่อ

การศึกษาลึกลับไตรโนโอเบียมอาร์เซไนต์ ( $Nb_3As$ ) ในขั้นต้นนี้ได้จากการใช้กล้องไวซ์เซนเบิร์กแบบเอินราฟ - โนเนียส โดยใช้เปาโมลิบดีนัม  $K_\alpha$  พบว่าไตรโนโอเบียมอาร์เซไนต์อยู่ในระบบเททราโกนัล และมีหมู่สมมาตรสามมิติเป็น  $P4_2/n$  ความยาวค่านทั้งสามของหนึ่งหน่วยเซลล์ ถูกปรับให้ละเอียดแม่นยำขึ้นด้วยข้อมูลของผลึกผง และตามหลักของค่ากำลังสองน้อยที่สุด ให้ความยาวเป็นคังนี้คือ  $a = 10.294 \pm 0.001$  อังสตรอม,  $c = 5.1958 \pm 0.0007$  อังสตรอม และปริมาตร = 550.58 ลูกบาศก์อังสตรอม

ความหนาแน่นของไตรโนโอเบียมอาร์เซไนต์ที่ได้จากการทดลองที่อุณหภูมิ  $23^\circ C$  มีค่า  $7.92 \pm 0.6$  กรัม ต่อลูกบาศก์เซนติเมตร และค่าที่ได้จากการคำนวณสำหรับ 8 หน่วยสูตร ใน 1 หน่วยเซลล์มีค่า 8.29 กรัม ต่อลูกบาศก์เซนติเมตร ตำแหน่งอะตอมคำนวณหาจากแผนที่แพทเทอสัน พบว่าไม่มีอะตอมใดปรากฏ ณ ตำแหน่งพิเศษในเซลล์เลย

การปรับค่าละเอียดใช้หลักของค่ากำลังสองน้อยที่สุด โดยมีระนาบของการเลี้ยวเบนทั้งหมด 415 ระนาบ เพื่อให้ได้ค่าสตรัคเจอร์แฟคเตอร์ที่ได้จากการคำนวณ และค่าที่ได้จากการทดลองมีค่าใกล้เคียงกันที่สุดซึ่งได้  $R = 0.124$

ไตรโนโอเบียมอาร์เซไนต์มีโครงสร้างแบบโครทิเทเนียมฟอสไฟต์ มีอะตอมของไนโอเบียม และอาร์เซนิค จัดตัวแบบรูปหลายเหลี่ยม รอบอะตอมอาร์เซนิคั้นประกอบด้วยไนโอเบียม 10 อะตอม และคิตทางผลึกวิทยามีไนโอเบียมอยู่ 3 ประเภทในหนึ่งหน่วยเซลล์โดยจะมีอะตอมข้างเคียงเป็นจำนวน 14-15 อะตอมรอบไนโอเบียมแต่ละอะตอมเหล่านั้น

Thesis Title     An X-ray Crystallographic Study of Triniobium  
                       Arsenide ( $\text{Nb}_3\text{As}$ )

Name               Miss Gannaga Satittada

Thesis Advisor   Assistant Professor Phathana Phavanantha Ph.D.

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#### ABSTRACT

A preliminary X-ray investigation of triniobium arsenide,  $\text{Nb}_3\text{As}$ , was determined by using an Enraf-Nonius Weissenberg camera with MoK radiation. Triniobium arsenide is in the tetragonal system and conforms to space group  $P4_2/n$ . The unit cell dimensions as refined from powder data by the least-squares method are  $a = 10.294 \pm 0.001 \text{ \AA}$ ,  $c = 5.1958 \pm 0.0007 \text{ \AA}$  and  $V = 550.58 \text{ \AA}^3$ .

The density of  $\text{Nb}_3\text{As}$  was found to be  $7.92 \pm 0.6 \text{ gm-cm}^{-3}$  at  $23^\circ\text{C}$ , and the calculated density is  $8.29 \text{ gm-cm}^{-3}$  for eight formula units in the unit cell.

The atomic positions were determined from the Patterson map. None of the atoms were found to occupy any special positions in the cell.

The refinement by least-squares method was employed to obtain the best agreement between calculated and observed structure factors based on 415 reflections yielded the R-factor of 0.124.

$\text{Nb}_3\text{As}$  has the  $\text{Ti}_3\text{P}$ -type structure consisting of the co-ordinating

polyhedra of niobium and arsenic. The arsenic atoms have ten niobium neighbours and the three crystallographically non-equivalent niobium atoms has fourteen to fifteen nearest neighbours.

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