

## The electron density distribution and the structure of semiconductor HgCdTe

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### 반도체 HgCdTe의 전자 밀도 분포와 결정 구조

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**Abstract** A Hg(0.79)Cd(0.21)Te single crystal has been grown by the Traveling Heater Method (THM). Its zinc blende cubic structure is identified from the X-ray diffraction patterns and its lattice constant is determined to be 6.464 Å using the least-square method of Cohen. From the values of the lattice constant, the composition  $x$  is determined to be 0.21. The electron density is calculated from the relative intensities of the scattered X-ray and compared with the theoretically calculated values. From the electron density distribution, it is shown that the crystal binding of Hg(1-x)Cd(x)Te (MCT) is mainly covalent and has tetrahedron bonds between adjacent atoms.

**요 약** 단결정 Hg(1-x)Cd(x)Te (MCT,  $x = 0.21$ )가 특수 제작된 고압로에서 Traveling Heater Method(THM)으로 성장되었다. X-선 회절 실험으로 MCT는 입방 ZnS 구조임을 확인하였다. 측정된 격자상수는 6.464 Å 이었으며, J.C. Wooley가 측정한 값과 비교하여 얻은 MCT의 성분비는 0.21이었다. MCT의 결정 구조를 분석하기 위하여 X-선 회절 강도로 부터 전자 밀도를 계산하였다. 전자 분포 밀도도로 부터 MCT는 주로 공유 결합을 하고 있으며, 인접 원자들 사이에는 사면체 구조를 이루고 있음을 알 수 있다. 격자 상수가 Vegard line으로 부터 편이 되는 원인은 성분비  $x$ 가 증가될 때 원자간 거리 변화의 비선형적 증가로 판단되며, 이것은 결합 에너지와 관련될 것으로 추측된다.

### 1. Introduction

The  $Hg_{1-x}Cd_xTe$  (MCT) alloy system has been extensively studied and developed as a variable energy gap infrared detector material ( $x$  is the mole ratio) [1]. An important property of MCT is a variation in energy gap with composition  $x$ . The energy gap in MCT varies nearly linearly with composition  $x$  between the two end point values (from  $x = 0$  to 1). In this paper we have briefly described the growing procedure and the crystal structure of MCT single crystal grown by the Traveling Heater Method (THM) using Te solvent [2]. The crystal structure of MCT crystal has been investigated by the X-ray powder method, and the electron density has been calculated from the relative intensities of the scattered X-ray and compared with theoretical calculations. From the electron density distribution, the type of crystal binding has been determined. By using the formulas of J.C. Woolley and B. Ray on the relationship of composition  $x$  to lattice constant for MCT

[3], we have determined the composition  $x$ . The lattice constant vs. composition  $x$  is plotted for MCT in Fig. 1. There is a small deviation from Vegard's Law, i.e., a non-linearity in the lattice constant a versus  $x$  curve. We suggest the reason why the lattice constant deviates from the Vegard line.

### 2. Experimental

#### 2.1. Crystal growth

The binary compounds, CdTe and HgTe crystals, were synthesized by the low temperature nondetonative synthesis method and by THM, respectively, prior to MCT growth. To grow MCT from CdTe and HgTe polycrystals, CdTe and HgTe were pulverized and mixed in the proper mole ratio and the mixture moulded under a pressure of 5000 kg/cm<sup>2</sup>. Figure 2 shows an outline of the crystal growing system. MCT mould was loaded inside a fused quartz ampoule and

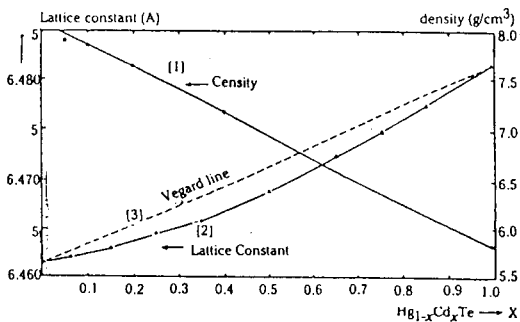


Fig. 1. Lattice constant and density of MCT as a function of composition  $x$  [3].

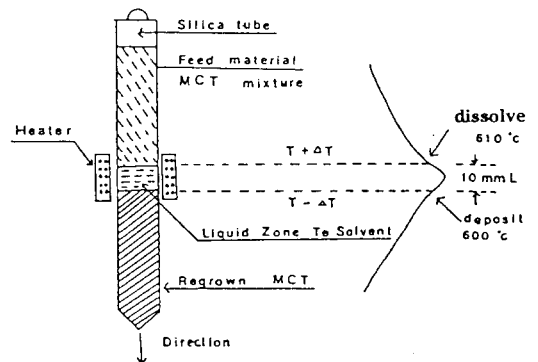


Fig. 2. Outline of the MCT crystal growth system.

maintained under argon gas pressure of 30 atm. The crystal growth was carried out over about 20 days by lowering the ampoule at the rate of 2.5 mm/day. The temperature of the THM furnace was increased by  $0.5^\circ\text{C}/\text{min}$  up to  $450^\circ\text{C}$ , and maintained at that temperature for 2 hours. It was then increased by  $0.5^\circ\text{C}/\text{min}$  again until the upper temperature in the stationary furnace reached  $610^\circ\text{C}$  and maintained there for 20 days. The obtained MCT crystal was 10 mm in diameter and 40 mm in length. The value of  $x$  for the whole ingot obtained in the present work is in the range of about 0.19 to 0.3. The midportion has a homogeneity of  $0.21 \pm 0.03$  for the axial direction. For the analysis of the crystal structure, the sample used for this study was assumed to be an alloy with atomic percent composition of Hg(0.79)Cd(0.21)Te.

### 2.2. X-ray diffraction experiment

The crystal structure of Hg(0.79)Cd(0.21)Te has been studied by X-ray diffraction. The X-ray diffraction patterns of the sample have been obtained using a Rigaku diffractometer with Cu- $K\alpha$  radiation with Ni filter. Scattered intensities are measured over  $2\theta$  angles from  $10^\circ$  to  $160^\circ$  with step intervals of  $0.01^\circ$  using filtered Cu- $K\alpha$  ( $\lambda = 1.5418 \text{ \AA}$ ) radiation. The scanning speed is 8 advances in  $2\theta$  per min.

## 3. Results

### 3.1. Diffraction patterns

Figure 3 shows X-ray diffraction pattern calculated theoretically. Figure 4 shows X-ray diffraction patterns taken at room temperature for HgTe, CdTe and Hg(0.79)Cd

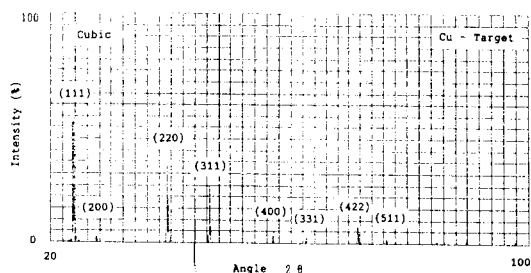


Fig. 3. X-ray pattern of MCT ( $x = 0.21$ ) calculated theoretically.

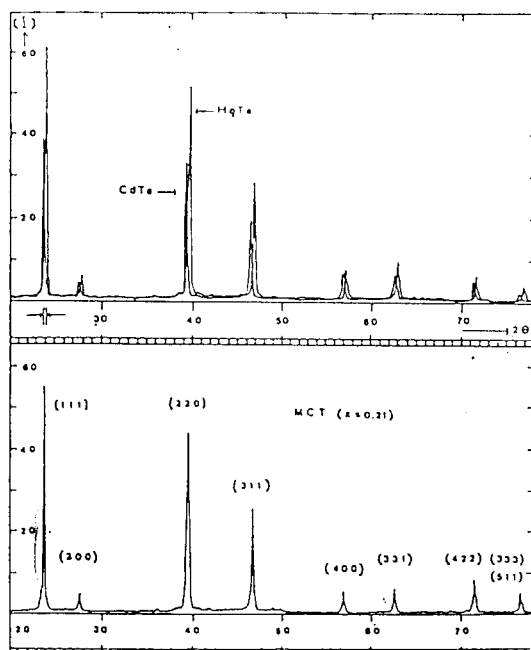


Fig. 4. X-ray patterns of HgTe, CdTe and MCT ( $x = 0.21$ ).

(0.21)Te. From the X-ray diffraction patterns, it is observed that the  $2\theta$  peak-angles and peak intensities of MCT is decreased as the composition  $x$  is increased. It is found that the shapes of the diffraction lines of MCT are similar to those of HgTe. As the angles of the diffraction lines are shifted to lower values, the lattice constant is increased. The structure factor of Hg(0.79)Cd(0.21)Te is affected by the atomic scattering factor of Cd atom which is smaller than that of Hg. Thus the diffraction intensities of Hg(1-x)Cd(x)Te are smaller than those of HgTe. The  $2\theta$  peak-angle of Hg(0.79)Cd(0.21)Te obtained for the (111) plane is  $23.806^\circ$ , shifted slightly lower from that of HgTe by about  $0.01^\circ$ . It was determined that MCT has the zinc-blende cubic structure over the whole composition range of  $x$ .

Table 1 shows X-ray intensities and  $2\theta$  peak-angles of Hg(0.79)Cd(0.21)Te. In Table 1, there are diffraction lines of mixed indices, such as the (211), (300), (221) planes, that can not occur in the zinc-blende structure.

### 3.2. Lattice constant

The lattice constant is calculated from the  $2\theta$  peak-angles of X-ray pattern. The lattice constant of the grown sample has been determined to be  $6.464 \text{ \AA}$  using the least-square method of Cohen [4]. The composition of the MCT sample can be obtained from measurement of the lattice constant which varies with  $x$ . Comparing the value for the lattice constant with those of Woolley and Ray, the composition for this sample

Table 1

Diffraction intensities and  $2\theta$  peak-angles of Hg(0.79)Cd(0.21)Te

| Planes(hkl) | Angles( $2\theta$ ) | Intensity | Rel. Intensity<br>[(111)Stand. %] |
|-------------|---------------------|-----------|-----------------------------------|
| (111)       | 23,806              | 1,769     | 100                               |
| (200)       | 27,563              | 104       | 6                                 |
| (211)       | 35,500              | 52        | 3                                 |
| (220)       | 39,411              | 1,727     | 98                                |
| (300)       | 42,000              | 64        | 4                                 |
| (221)       |                     |           |                                   |
| (311)       | 46,581              | 1,005     | 57                                |
| (400)       | 56,967              | 245       | 14                                |
| (331)       | 62,620              | 210       | 12                                |
| (422)       | 71,463              | 199       | 24                                |
| (511)       | 76,560              | 171       | 10                                |

was determined to be  $0.21 \pm 0.03$ .

### 3.3. Electron density

In order to investigate the crystal structure of Hg(0.79)Cd(0.21)Te, the electron density is calculated from the relative intensities of scattered X-rays by the Fourier synthesis method and compared with theoretically calculated values. The electron density in the zinc blende structure [8] is

$$\rho = [8/V] \sum_0^{\infty} \sum_0^{\infty} \sum_0^{\infty} |F(hkl)| [\cos 2\pi hx \cos 2\pi ky \cos 2\pi lz \cos \alpha(hkl) - \sin 2\pi hx \sin 2\pi ky \sin 2\pi lz \sin \alpha(hkl)]$$

$$\alpha(hkl) = \tan^{-1}(B/A)$$

where A and B are  $|F(hkl)| \cos \alpha(hkl)$  and  $|F(hkl)| \sin \alpha(hkl)$ , respectively. In order to describe the electron density distribution, the structure factor  $F$  is calculated from the diffraction intensity and phase  $\alpha(hkl)$  is calculated theoretically. Figure 5 shows the electron density distribution of Hg(0.79)Cd(0.21)Te.

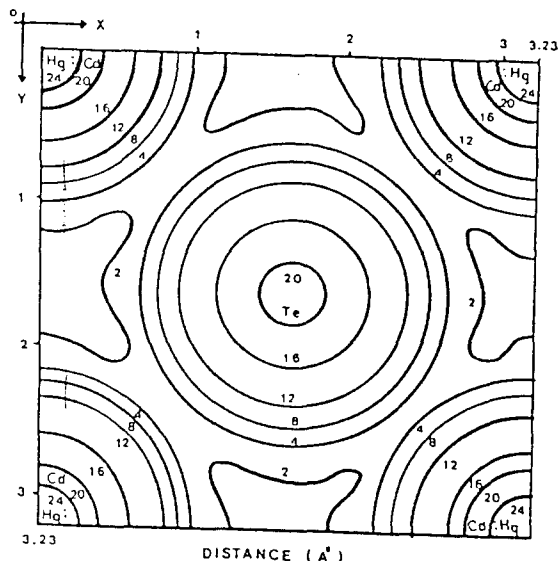


Fig. 5. Electron density distribution of Hg(0.79)Cd(0.21)Te.

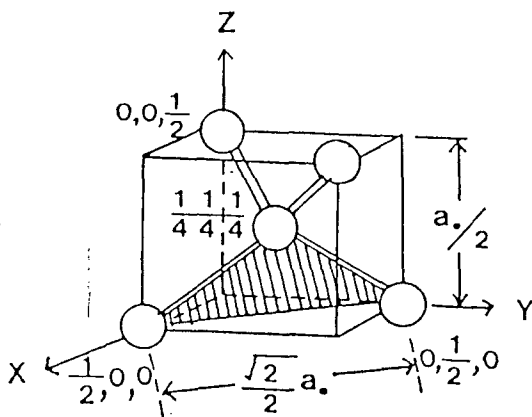


Fig. 6. Tetrahedron bond in MCT.

## 4. Discussion

### 4.1. Electron density distribution

In Fig. 5, the electron density distribution is symmetric and distributed uniformly. The electron density distribution of Hg(0.79)Cd(0.21)Te is similar to that of HgTe with

some of the Hg (21 mol %) replaced by Cd. It is not easy to distinguish between Hg and Cd ions in Fig. 5. Figure 6 shows the hypothetical structure of Hg(0.75)Cd(0.25)Te in which the Cd ions are located only at the (0,0,0) position. Then diffraction peaks occurred only for mixed indices (hkl) planes as

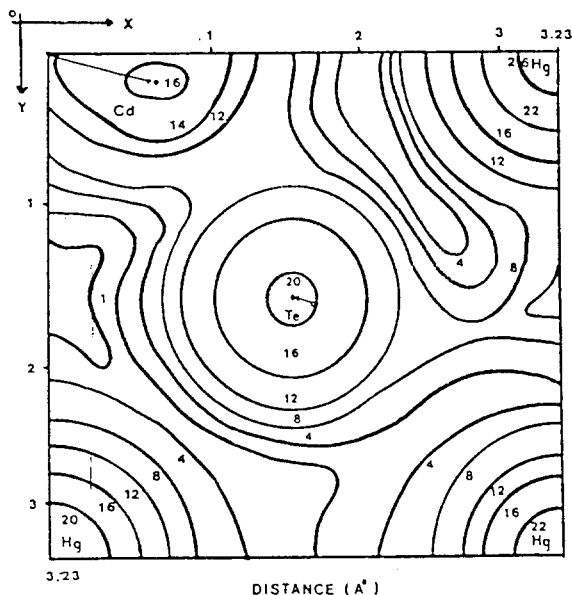


Fig. 7. Electron density distribution in Hg (0.79)Cd(0.21)Te compared with the theoretical distribution calculated assuming only mixed indices.

well as unmixed indices. The intensity for mixed indices varies with  $F = [f(\text{Cd}) - f(\text{Te})]$ , where  $f(\text{Cd})$  and  $f(\text{Te})$  are the atomic scattering factors of Cd and Hg respectively. In order to investigate the variation of electron density due to mixed indices, we have calculated the electron densities from the intensities of which the theoretical mixed indices are added as well as measured ones for comparison with the experimental electron densities when  $x$  is 0.21. This is shown in Fig. 7, and it indicates that Cd and Te ions are displaced by 0.6 Å and 0.2 Å in the  $x$ - $y$  plane, respectively. Thus the distortion of the crystal structure is inferred from the scattered intensity is due to

the mixed indices of planes. But the effect of these values is too small to be observed when the electron density is described. In fact, it is found from the electron density distribution that crystal binding of MCT is mainly covalent with tetrahedron bonds between adjacent atoms.

#### 4.2. Lattice constant and Vegard's law

Using the X-ray technique, J.C. Woolley and B. Ray determined the dependence of the lattice constant  $a$  on composition for the alloy system MCT. The resulting curve for MCT is plotted in Fig. 1. It is interesting that there is a small deviation from the Vegard line in the alloy system of MCT. The maximum deviation is about 0.002 Å. We assume two possible reasons for this deviation from the Vegard line.

- 1) Variation in lattice constant due to distortion of crystal structure.
- 2) Non-linear variation in lattice constant because the atomic distance does not vary linearly with composition as Hg ions are replaced by Cd ions.

In the first case, the deviation of lattice constant is not apparent because the electron density distribution is symmetric. Thus the first case can not be explained why the lattice constants deviate from the Vegard line. In the second case, we know that the lattice constant is related to the atomic distances in the zinc blende structure. Thus the deviation of the lattice constant from the Vegard line is inferred that non-linear variation in atomic distances are related to bind-

ing energy. It can be concluded that the non-linear variation in lattice constant is not deviated due to Cd atoms concentrated at special sites but the non-linear variation of atomic distance.

## 5. Conclusions

Hg(0.79)Cd(0.21)Te single crystals have been grown by THM and their crystal structure has investigated by the X-ray powder method. Their structure has been studied in terms of electron density distribution. The points in this paper are

1) The lattice constant is determined to be 6.464 Å. From the value of the lattice constant, the composition of this MCT is  $0.21 \pm 0.03$ .

2) The atomic bonds are mainly covalent with tetrahedron bonds between adjacent atoms based on the distribution of electron density. MCT has a structure in which Cd and Hg atoms are uniformly distributed around Te atoms in the zinc blende structure.

3) The non-linear variation in lattice constant may be related to a variation in bind-

ing energy in MCT.

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