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LATTICE PARAMETERS OF THE $Hg_{1-X}Fe_XSe$ AND $Cd_{1-X}Fe_XTe$ SEMIMAGNETIC SEMICONDUCTORS

Dr. Ammar Sarem[*]
Dr. Soulayman Soulayman[+]
Dr. Elzbieta Dynowska[♣]

ABSTRACT

The results of lattice parameter measurements on the ternary semiconductor alloys $Hg_{1-x}Fe_xSe$ over the range ($0 \le x \le 0.15$) and $Cd_{1-x}Fe_xTe$ in the range ($0 \le x \le 0.01$), grown using modified Bridgman method, are reported. The polycrystalline samples of $Hg_{1-x}Fe_xSe$ and $Cd_{1-x}Fe_xTe$ with different nominal compositions were studied by X-ray diffraction method. The crystal structure of these compounds was determined as a cubic one of the zincblede type. The structural homogeneity of the samples was ascertained. We find that the lattice constants decreases linearly with iron concentration x according to Vegard's law in the case of $Hg_{1-x}Fe_xSe$ while this law could not be applied in the case of $Cd_{1-x}Fe_xTe$. The limit of solubility of iron in HgSe and CdTe was not observed in the range of the investigated compositions.

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[*] **Professor At Department Of Physics, Faculty Of Science, Lattakia- Syria**
[+] **Professor At Higher Institute Of Applied Sciences And Technology, Damascus-Syria**
[♣] **Professor At Institute Of Physics, Polish Academy Of Sciences Warszawa-Poland**

ثوابت الشبكة البلورية في مركبات أنصاف النواقل شبه المغناطيسية

$Hg_{1-x}Fe_xSe$ و $Cd_{1-x}Fe_xTe$

الدكتور عمار صارم[*]

الدكتور سليمان سليمان[+]

الدكتورة اليزابيت دينوفسكا[♣]

ملخص

إن نتائج قياسات ثوابت الشبكة البلورية على خلائط من أنصاف النواقل ثلاثية التركيب من $Hg_{1-x}Fe_xSe$ في المجال($0\le x\le 0.15$) و $Cd_{1-x}Fe_xTe$ في المجال ($0\le x\le 0.01$)، والمنماة باستخدام طريقة بريدجمان المعدلة مبينة في هذا البحث. إن العينات $Hg_{1-x}Fe_xSe$ و $Cd_{1-x}Fe_xTe$ بتراكيب أسمية مختلفة درست بطريقة انعراج الأشعة السينية. وان البنية البلورية لهذه المركبات حددت كبنية مكعبة تتبلور في بنية كبريت التوتياء. تم التأكد من البينة المتجانسة للعينات. وجدنا أن ثوابت الشبكة البلورية في حالة $Hg_{1-x}Fe_xSe$ تتناقص بشكل خطي بازدياد تركيز الحديد x وفقاً لقانون فيجارد، بينما هذا القانون لا يمكن أن يطبق في $Cd_{1-x}Fe_xTe$. لم يلاحظ حد انحلالية الحديد في HgSe و CdTe في مجال التراكيب المختبرة.

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[*] أستاذ في قسم الفيزياء من كلية العلوم بجامعة تشرين، اللاذقية- سوريا.

[+] أستاذ في المعهد العالي للعلوم التطبيقية والتكنولوجيا، دمشق- سوريا.

[♣] أستاذة في معهد الفيزياء من أكاديمية العلوم البولونية، وارسو- بولونيا.

1. INTRODUCTION

Bulk diluted magnetic semicondutors (DMCs) or semi-magnetic semiconductors (SMSCs) denote to semiconductor based solid solutions where some of the cations are replaced by transition metals or rare earth elements (i.e. II-VI, II-V or IV-VI materials with magnetic ions). These materials have recently received attention due to their potential use in magnetic applications including spitronics, magnetic switching and magnetic recording [1, 2]. In DMS materials, the spin exchange interaction can induce paramagnetic (PM), spin-glass (SG), antiferromagnetic (AFM) or ferromagnetic (FM) behaviour depending on the magnitude of d-d(J) and sp-d exchange integrals between the paramagnetic ions and the spin exchange interaction between magnetic ion with charge carriers [1,3]. In II-VI materials, magnetic coupling for Fe, Mn and Co SMSC materials has been observed. Moreover, in II-VI nanomaterials, Mn^{2+} -doped nanocrystals have shown evidence for size-dependent magnetism [6].

The most thoroughly studied groups of SMSC are the II-VI compounds containing substitutional Mn^{2+}, Fe^{2+} and Co^{2+} [8-11]. In comparison with Mn, an iron, Fe, atom possesses one more electron on d shell. Several methods absorption, photoemission and transport were used to determine the energy position of the Fe^{2+} ($3d^6$) donor state in the band structure of the semimagnetic semiconductors $A^{II}_{1-x}Fe_xB^{VI}$. Fe $3d^6$ state is located above the Mn $3d^5$ state in a semiconductor band structure [16]. Therefore, the SMSCs containing substitutional Fe^{2+} ions have been extensively studied recently, because of their interesting magneto-optical and magnetic properties.

$Hg_{1-x}Fe_xSe$ and $Cd_{1-x}Fe_xTe$ are the members of SMSC alloys. These materials are of considerable interest because, apart from the opportunities provided by the ternary nature of these compounds (e.g., tunability of the energy gap or the lattice constant), they display interesting magnetic properties as well as exchange interaction between the localized Fe^{2+} moments and band electrons, resulting in a host of novel effects.

For many applications the use of Vegard's law is useful. This law expresses the linear interpolation of the lattice constant of alloys as a function of parameter x, defining the chemical composition of the alloy (compound). According to this law one can write for A_xB_{1-x} compounds:

$$a_{alloy} = xa_A + (1 - x)a_B$$

The Vegard's law was introduced as a phenomenological formula. Experimental findings, in most cases, did not confirm such behaviour, howewer exist alloys where Vegard law is observed.

In this paper we investigate the behavior of the crystal lattice of $Hg_{1-x}Fe_xSe$ and $Cd_{1-x}Fe_xTe$. The purpose of the study is providing precise quantitative data for the lattice parameter as a function of x, which could be used for determining the composition of the corresponding material.

2. EXPERIMENT

The X-ray measurements were made using a DRON diffractometer with filtered *Co* radiation ($\lambda_{k\alpha1}$=1.78892Å; $\lambda_{k\alpha2}$=1.79278Å). The diffraction patterns with a scan rate of 1° 2θ/min were taken. Precise measurements of the lines position diffracted and extrapolation method to determine *a* to value θ=90° were made by Least Square Method. This method allowed determining cell parameters for each sample with accuracy ±0.0005Å.

3. RESULTS AND DISCUSSION

It is well known that cadmium telluride (CdTe) has a zincblende (sphalerite) crystal structure with lattice parameter a = 6.482 Å and melting temperature T_m= 1092°C while iron telluride (FeTe) has a nickel arsenide crystal structure with lattice parameters a = 3.80 Å and c = 0.565 Å and melting temperature T_m = 914°C. On the other hand, mercury selenide (HgSe) has a zincblende crystal structure with lattice parameter a = 6.08 Å and melting temperature T_m= 583.5°C and iron selenide (FeSe), has a zincblende crystal structure with lattice parameter a = 3.64 Å.

The samples $Hg_{1-x}Fe_xSe$ containing 0, 4, 5, 12 and 15 and $Cd_{1-x}Fe_xTe$ containing 0, 0.3, 1 mole percent of iron were investigated. The single crystals were powdered and one part of the powder of each sample was subjected to chemical analysis for determining the real concentration of iron while the remaining part of it was investigated by X-ray diffraction. The chemical measurements showed the small differences between the nominal compositions and the real ones for all investigated samples.

X-ray diffraction patterns revealed that all samples were of single phase and their crystal structure was found to be zincblende for the iron composition range. The precise measurements of the high-angle peaks were the basis of the cell parameter calculations [12].

Since the zincblende structure of $Hg_{1-x}Fe_xSe$ and $Cd_{1-x}Fe_xTe$ alloys are cubic and tetrahedrally coordinated, the local environment of the tetrahedron are formed by like atoms. Therefore, it is meaningful to consider also the mean cation-cation distance d_{c-c} over the entire range of existence of $Hg_{1-x}Fe_xSe$ and $Cd_{1-x}Fe_xTe$. The quantity d_{c-c} and the lattice parameters are related for zincblende structure, therefore $d_{c-c} = a/\sqrt{2}$ [13]. The results of the measurements as well as the lattice parameters for the investigated samples are given in the Table (I and II).

TABLE I. Lattice parameter (in Å) of $Hg_{1-x}Fe_xSe$ crystal as a function of Fe concentration.

sample	Iron Concentration %	Lattice parameters $a \pm 0.0001$	Cation-cation distance d_{c-c}
1	0	6.0838	4.3019
2	4	6.0681	4.2908
3	5	6.0632	4.2873
4	12	6.0382	4.2697
5	15	6.0225	4.2586

TABLE II. Lattice parameter (in Å) of $Cd_{1-x}Fe_xTe$ crystal as a function of Fe concentration.

sample	Iron Concentration %	Lattice parameters $a \pm 0.0003$	Cation - cation distance d_{c-c}
1	0	6.4798	4.58191
2	0.3	6.4799	4.58198
3	1	6.4795	4.58170

The lattice parameter *a*, for $Hg_{1-x}Fe_xSe$, was plotted as a function of nominally determined iron concentrations as shown in figure (1). The lattice parameter *a* decrease linearly with the increase of amount of iron. Sample containing 12 mole percent of iron run away from linearity relationship. This suggests that the real Fe concentration of the sample is smaller than the technological composition. Extrapolated velue of Fe corresponds to 11.2 %, the difference with nominal concentration is in the upper limit of the accuracy of chemical analyses. The decrease of the lattice parameter *a* is expected since ionic radius of Fe (+2) 0.76 Å is smaller than ionic radius of Hg – 1.10 Å. For $Cd_{1-x}Fe_xTe$ in the range of investigated Fe concentration (up to x = 0.01) the lattice constant does not change. Measured differences are in the range of experimental error. The value of lattice constant for x = 0.01 indicates probable decrease of *a* with x as expected from the difference of ionic radius of Cd – 0.97 Å and Fe – 0.76 Å. A further study in future is needed for higher concentrations.

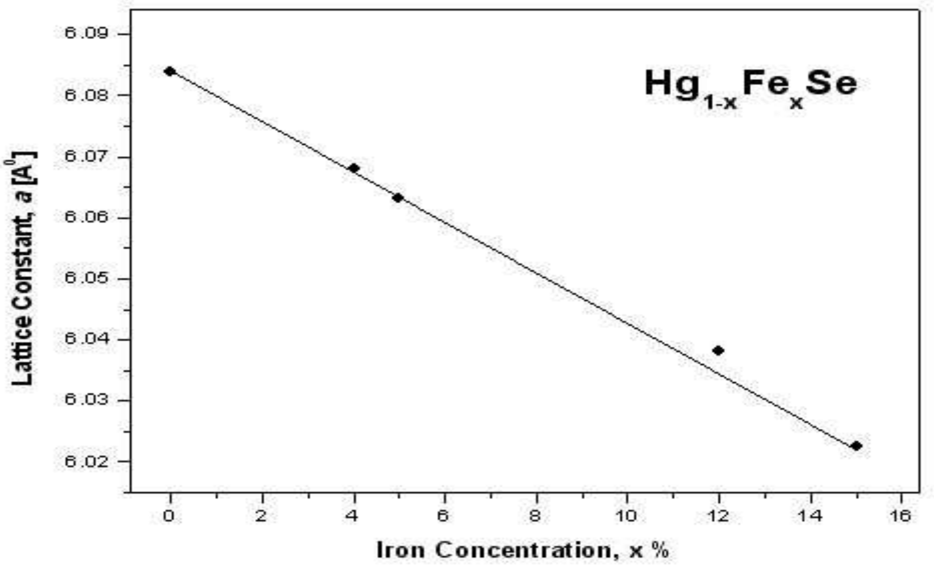

Figure 1. Variation of the lattice parameter *a* with nominal iron concentration in crystals of $Hg_{1-x}Fe_xSe$.

CONCLUSIONS:

Here one can conclude that:

- The ternary $Hg_{1-x}Fe_xSe$ and $Cd_{1-x}Fe_xTe$ crystals have the cubic structure of the zincblende type in the range of the investigated compositions.
- The Fe atoms are distributed randomly and any order or preferable position of the magnetic atoms was not observed in these crystals.
- In the case of $Hg_{1-x}Fe_xSe$ the lattice parameters *a* decrease with the increase of the iron concentration according to the Vegard's law which means that the Fe-ions substitute the Hg ions in a cubic crystal lattice. The consequence of this fact is the appearance of the local structure with the smaller nearest neighbour distance Fe-Se than Hg-Se.
- The chemical measurements showed that the nominal iron concentration is very lightly different from the real one.
- The problem of the limit of solubility of iron in HgSe and CdTe should be studied in future.

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