ICREN-01/2013 February 16-17, 2013 Constantine, Algeria
First International Conference on Renewable Energies and Nanotechnology impact on Medicine and Ecology

The behaviour of CdTe nuclear detector subjected under pressure conditions

Asmaa. Saim*, Abdelghani. Tebboune, Houria. Berkok, A.H.Belbachir.

Laboratoire d'Analyse et d'Application des Rayonnements, Département de Physique, Faculté des Sciences, ***USTOMB*** *: Université des Sciences et de la Technologie d'Oran Mohamed Boudiaf-BP. 1505 El Menaouer, 31000 Oran Algérie.*

Abstract

In this work, we have conducted a theoretical study on the nano-scale at the base of the simulation of phase transitions and the corresponding pressures as well as the volume discounts, the rigidity and the stability of the cadmium telluride CdTe with the Full Potential Linear Muffin Tin Orbitales FP-LMTO method. This study gave new results to verify the behavior of a solid detector in the base of semiconductor material submitted under the constraints of different pressure for change under normal operation of CdTe nuclear detector.
This study was followed by a comparable study of the rigidity between CdTe and silicon Si.

Key words: CdTe detector, transition pressure,stability, rigidity-,volume discounts,bulk modulus.

Introduction

Semiconductor nuclear radiation detectors have experienced a rather rapid development in the last few years. They are now used in a large variety of fields, including nuclear physics, X-ray and gamma ray astronomy and nuclear medicine. Their imaging capabilities, good energy resolution and the ability to fabricate compact systems are very attractive features, in comparison with other types of detectors, such as gas detectors and scintillators. In recent years, a substantial international effort has been invested in developing a range of compound semiconductors with wide band gap and high atomic number for X-ray and gamma ray detectors. Among the compound semiconductors, cadmium telluride (CdTe) and cadmium zinc telluride (CdZnTe) are the most promising materials for radiation detectors with good energy resolution, high detection efficiency and room temperature operation [1]. Cadmium telluride (CdTe) is now a well-known material for X-ray and gamma-ray applications [2]. The unique combination of high atomic number (good stopping power), good mobility lifetime product (good transport properties of the free charge carriers), large band-gap (low dark current), and the associated room temperature operation makes CdTe an attractive semiconductor detector for X-ray and gamma-ray applications [3].

In this work, we have performed a study of stability, rigidity and transitions between the four phases (NaCl, CsCl, zinc blende and wurtzite) based on the comparison and theoretical study using FP-LMTO method of ab-initio simulation.

1. Result and discussion

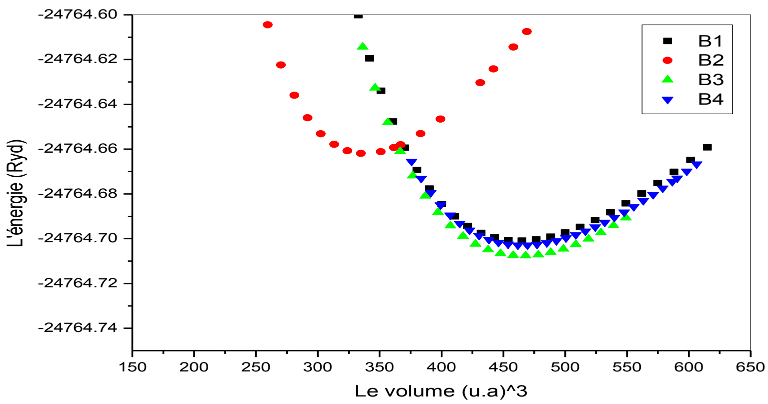

Figure 1: Represents the stability of the binary compounds CdTe using the Local Density Approximation LDA with FP-LMTO method.

Figure (1) represents the energy curves of the cadmium telluride corresponding to the volume of the four phases: NaCl (B1), CsCl (B2), zinc blend (B3) and wurtzite (B4). In new lever we have verified that CdTe stabilized in zinc blend witch corresponding to the minimum energy E=-336940.97799 eV and for a lattice parameter equal to a= 6.502 Å. The three bands corresponding to energy of (B1) and (B4) bands are very close to each other and to the stable phase (B3). This observation prompted us to calculate the phase transitions between the four bands.

Table 1. The lattice parameters (a_0, c), the volume, the density, the transition pressure and the reduction volume of CdTe for NaCl, CsCl, zinc blend and wurtzite bands.

The phase	a_0 (Å)	c (Å)	V_0 (Å^3)	ρ (g/cm^3)	P (GPa)	$V_{reduction}$ (Å^3)
NaCl	6.515	-	276.531	5.764	0.828	271.288
CsCl	3.688	-	50.162	31.775	309.084	23.572
Zinc blend	6.505	-	275.259	5.791	-	-
Wurtzite	4.604	7.518	69.004	230.986	94.756	41.171

The table (1) provides some information about the lattice parameters (a_0, c), the volume, the density, the transition pressure and the reduction volume of CdTe in NaCl, CsCl, wurtzite and zinc blend bands. An other very important result is found by FP-LMTO method which is the different possibilities of transitions of phases with the pressures: P (B1-B3) = 0.828 GPa ; P (B2-B3) = 309.084GPa et P (B4-B3) = 94.756GPa. As we found the density of this material in the four bands calculated using the lattice parameters calculated by ab-initio simulation. This study allowed us to see the behavior of the nuclear detector based CdTe semiconductor when it is subjected to pressure under normal conditions. In this case, the semiconductor changes phase so the volume changes with a reduction in the volume. This latter found inversely proportional to the transition pressure as shown in table (1).

Table 2. Represents the difference between the silicon and the cadmium telluride

The material	bande of stability	a_0 (A)	B (GPa)	B'(GPa)
Si	Diamant	5.44^o	100	-
CdTe	B_3	6.50	45.00	3.89

Knowing that we can have the silicon detectors very commercialized then the detectors based of CdTe, from where we had the idea of comparing the stiffness of the two types of semi-conductors materials resistance against different radiation and particles passing trough this material or its rigidity against changing temperature and pressure. That is why it is very important to calculate the bulk modulus and compare hardness of materials. While the bulk modulus is more important, the material used in the solid detector is more durable and hard. From table (2) we can see that the Si is almost twice as hard as CdTe.

Conclusion

Cadmium tellurium stabilizes in zinc blend (B3) and. This study show three phases transitions with a possible change of different pressures according to the volume reduction. The results gave an indication of the fragility of the CdTe detector against the change of the pressure from which we can predict the detection efficiency in nuclear powered and other applications.

Reference

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