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CdSe and CdTe Mechanical Properties Revealed by COMSOL Multiphasics

Ali K. Mohammed Ali[1*]

[1] General Directorate of Education in Rusafa I, Ministry of Education, 10001 Baghdad, IRAQ.

*Contact: g66gg166@gmail.com

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ABSTRACT

Two Metal chalcogenide compounds CdTe and CdSe have been studied in depth because they are used in many optoelectronic and electronic devices. High pressure causes structural phase transitions in semiconductor materials, which have been the subject of much research. CdTe is a direct band-gap IIeVI semiconductor. Cadmium-tellurium crystalline compound has been used in more and more industries. High dislocation density is one of the problems with bulk-grown CdTe. Comsol Multiphysics was used to evaluate mechanical stress on a material. COMSOL Multiphysics 5.5 allows you to access a database of physics simulations. (CdSe and CdTe) were simulated to show the effects of mechanical stress. We use a physical model called Solid Mechanics to model the effect of mechanical stress. The results show that when pressure was applied at different levels (50pa, 100pa, 200pa, 300pa, 400pa), the strain values of (CdSe or CdTe) were similar, but (CdSe) was more resistant to deformation than (CdTe).

KEYWORDS: High pressure; mechanical stress; simulation; strain; semiconductor.

الخلاصة

تمت دراسة مركبي معدن الكالكوجينيد CdTe و CdSe بعمق نظرًا لاستخدامهما في العديد من الأجهزة الإلكترونية الضوئية والإلكترونية. يتسبب الضغط العالي في انتقالات طور هيكلية في مواد أشباه الموصلات ، والتي كانت موضوع الكثير من الأبحاث. CdTe هو أشباه الموصلات IIeVI ذات فجوة النطاق المباشرة. تم استخدام المركب البلوري للكادميوم والتيلوريوم في المزيد والمزيد من الصناعات. تعد الكثافة العالية للخلع واحدة من مشاكل CdTe المزروعة بكميات كبيرة. تم استخدام Comsol Multiphysics لتقييم الضغط الميكانيكي على مادة ما. يتيح لك Comsol Multiphysics ٥,٥ الوصول إلى قاعدة بيانات لمحاكاة الفيزياء. تمت محاكاة المواد (CdSe و CdTe) لإظهار تأثيرات الإجهاد الميكانيكي. إنه ينشئ نموذجًا هندسيًا ثلاثي الأبعاد للمادة لسبب بسيط وهو أن اللبنات الأساسية متماثلة بطبيعتها. نستخدم نموذجًا فيزيائيًا يسمى الميكانيكا الصلبة لنمذجة تأثير الإجهاد الميكانيكي. أظهرت النتائج أنه عند تطبيق الضغط على مستويات مختلفة (، 200 pa ، 100 pa ، 50 pa ، 300 pa) ، كانت قيم الانفعال (CdSe أو CdTe) متشابهة ، ولكن (CdSe) كانت أكثر مقاومة للتشوه من (CdTe).

INTRODUCTION

Metal chalcogenide compounds like CdTe and CdSe have been studied in depth because they are used in many optoelectronic and electronic devices, CdTe and CdSe also have interesting electronic properties that can be improved. For example, they have a direct and wide band gap, a high absorption coefficient. Because of its optimal bandgap (19 eV), high absorption coefficient, and n-type conductivity, CdSe has become highly intriguing and significant because of its key uses in solar cells and other optoelectronic devices. These materials crystallize into a variety of different crystal forms, and their degrees of covalent, ionic, and metallic bonding are distinct characteristics of each of these types of bonds [1]. High pressure causes structural phase transitions in semiconductor materials, which have been the subject of much research. Since the invention of the high-pressure method, high pressure x-ray diffraction investigations have been able to attain pressures greater than 200 GPa. The ultra-high-pressure range has yielded several novel phase structures [2]. CdSe, together with some additives that are included in it, comprises an important family of semiconductor materials. These materials find uses in devices that are very

inexpensive, such as LEDs, solar panels, photodetectors, lasers, gas sensors, thin film transistors [3]. CdTe is a direct band-gap II-VI semiconductor. It's a cadmium-tellurium crystalline compound that is being used in more and more industries. There have been a number of attempts to grow large, high-quality single crystals of CdTe, but the results have been mixed. High dislocation density is one of the problems with bulk-grown CdTe. People think that dislocations spread and get bigger when the stress goes above the critical resolved shear stress (CRSS) [4]. Structure-related dynamical characteristics of CdSe and CdTe have seen less calculation and experimentation than other parameters. Consequently, the main goal of the present study is to provide further first-principal findings to help determine the predicted accuracy of existing density functional theory (DFT) codes. Materials features including interatomic forces, phase transition, transport coefficients, and electron-phonon interactions are heavily influenced by elastic and vibrational properties, making it crucial to accurately describe these characteristics for the existing solids. Particular emphasis is placed in this study on the dynamical features of elastic materials (stress, strain). The results are compared to both existing theoretical calculations and experimental data [5]. In the 20th century, simulation became a popular study approach. Simulation of physical processes and devices is a mainstay of study. Many models exist. Modeling semiconductor devices uses Sentaurus TCAD, Silvaco TCAD, Crosslight TCAD, and Cogenda TCAD. COMSOL Multiphysics also models systems with external impacts. COMSOL Multiphysics was used to evaluate mechanical stress on a material [6]. Examine the mechanical properties of the material (CdSe and CdTe) in order to use it in making electronic devices such as solar cells.

MATERIALS AND METHODS

Proposed Method

Materials (CdSe and CdTe) were simulated to show the effects of mechanical stress using the COMSOL Multiphysics 5.5 software. With this software, you may access a database containing physics simulations. These include optics, fluid mechanics, plasma physics, radio frequency technology, audiology, thermodynamics, and semiconductors. There are physical models particular to each library. Multiphysics is required if we wish to simulate many processes simultaneously. There should be consistency in the ways that numbers are crunched across all procedures. There are certain processes that can't be estimated simultaneously, such as time-dependent and stationary processes [7]. In Table 1, the parameter values utilized for the simulations are listed.

Table 1. Simulation parameters.

Material	Density kg\m^3	Poisson ratio	Young modulus (pa)
CdSe	5810	0.35	5×10^{10}
CdTe	5850	0.37	37×10^{9}

The Model

In COMSOL Multiphysics, there are seven steps to making a model of a system. These include making a geometric model, setting parameters, choosing a material type, assigning physical properties, making a geometric model based on the physical properties, entering the values of the material properties, and choosing how to calculate the results. It has a 3D geometric model of the substance for the simple reason that building blocks are inherently symmetrical. In order to simulate geometry, the component module geometry was developed. For all geometry-related measurements, centimeters have been used. To make two rectangles and one sphere, choose Geometry-> Rectangle from the menu. Where the rectangle represented the material (CdSe and CdTe) and the sphere represented the pressure force (iron material). The dimensions of the first rectangle were (width 2cm, depth 0.2cm, height 0.2cm) and the dimensions of the second rectangle were (width 0.5cm, depth 0.5cm, height 0.5cm) and the coordinates of the second rectangle position (X = 0.75cm, Y = 0.75cm, Z = 0.5cm) and the dimensions of the sphere (radius 0.2) and the coordinates of the sphere position (X = 1cm, Y = 1cm, Z = 0.35cm) [8], as shown in Figure 1.

A physical model called Solid Mechanics from the group of physical properties called Structural Mechanics was chosen to model the effect of mechanical stress. If we want to make a surface stronger, we add boundary load to the physical properties from the Solid Mechanics context menu. We can add a single "boundary load" to

give value to pressure (50pa, 100pa, 200pa, 300pa, 400pa) for two or more surfaces in the same amount and direction. All we need to do to make it stronger is to add the surfaces we want. If we want to give different surfaces different pressures, we have to add one boundary load for each pressure. If there is a part of the system, we are modeling that we don't want to move, we can add a fixed constraint from the context menu and give that part this property [9].

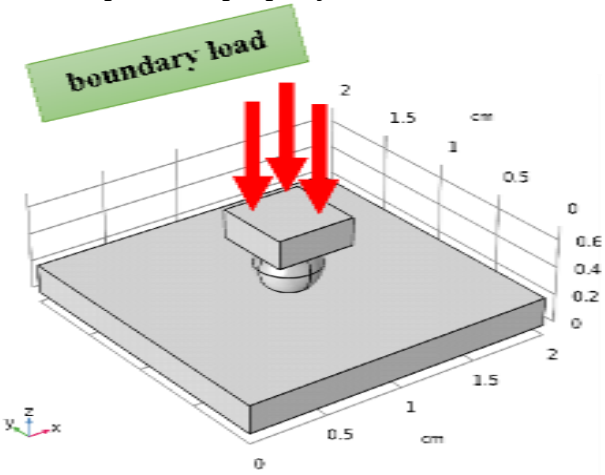

Figure 1. Geometrical model used for CdSe and CdTe.

We establish a network for the whole system based on the aforementioned physical characteristics. This is done so that we can be certain that a numerical method of computation was used. Also, by connecting the system to a network, we can easily get the values of each node. Therefore, the smaller the grid, the more precise the result. However, performance in computing tasks slows. By changing how much force or mechanical stress you put on a material (like CdSe or CdTe), you can learn about its mechanical properties under different stress conditions [10].

Model Theory

We are aware that generic processes in physics are described by equations that rely on time. All of these processes may be represented by a single set of equations called time equations. Stationary equations are derived from the assumption that all parameters and variables are constant across time. As such, time-dependent equations include the particular case of stationary equations [11]. We know that if we put force on a body, it will respond with the opposite force in the opposite direction. The name for this force is volumetric force. At a stationary state, the sum of the volumetric force gradient and the mechanical stress gradient is zero as shown in Equation 1 [12].

$$\nabla S + F_V = 0 \quad (1)$$

where, S means mechanical stress and F_v means volume force. A design tensor links overall mechanical stress and relatively elastic elongation by Equation 2 [13].

$$S = S_{ad} + C : \varepsilon_{el} \quad (2)$$

where: S_{ad} is Extra mechanical stress, ε_{el} is relative mechanical expansion, and builder (C:). ε_{el} can be computed by Equation 3.

$$\varepsilon_{el} = \varepsilon - \varepsilon_{inel} \quad (3)$$

where: ε is total mechanical expansion, ε_{inel} is inelastic mechanical expansion. This can be expressed in Equation 4.

$$\varepsilon_{inel} = \varepsilon_0 - \varepsilon_{ext} + \varepsilon_{th} + \varepsilon_{hs} + \varepsilon_{pl} + \varepsilon_{cl} + \varepsilon_{vp} \quad (4)$$

where, ε_0 is the primary mechanical expansion, ε_{ext} is the outer mechanical expansion, and ε_{th} is any other mechanical expansion. Equation (3, 4, 5, 6, and 7) was used in COMSOL to figure out the amount of inelastic relative elongation. There are other effects that are also taken into account [14].

$$S_{ad} = S_0 + S_{ext} + S_q \quad (5)$$

where: S_0 is primary mechanical stress, S_{ext} = outer mechanical stress, S_q is other mechanical stress.

$$\varepsilon = \frac{1}{2}[(\nabla u)^T + \nabla u] \quad (6)$$

$$C = C(E, V) \quad (7)$$

where: u is the field of mechanical stress, E = Yung modulus, V is poisson ratio [15]. Equations (3, 4, 5, 6, and 7) were used in COMSOL to figure out the amount of inelastic relative elongation. There are other effects that are also taken into account [14].

Results and Discussion

Examining a material's elastic quality is essential for understanding its chemical bonding, as well as its electrical and mechanical properties and its

stability from a mechanical perspective. To investigate a variety of important solid-state phenomena such as stability, ductility, brittleness, and anisotropy among others. It is important to show how pressure changes the mechanical properties of CdSe and CdTe nanostructures, and the only way to do this is to find the constants of elasticity. According to, the pressure experienced by a cubic lattice during a Simulation may be used to calculate stress and strain distinct elastic constants. Using COMSOL Multiphysics software, the electrical, elastic, and lattice dynamical characteristics of cadmium chalcogenides is analyzed. The aforesaid research served as the basis for our determination of the two elastic constants for the cubic CdSe and CdTe systems. Table 2 shows that both CdSe and CdTe nanostructures meet the Born stability criteria, so they are both mechanically stable. Also, it's clear that the values we got match up with what other studies have said. This proves that our calculations for different pressure values are correct.

Table 2. The effects of pressure on the elasticity of CdSe and CdTe.

	Pressure (pa)	**Stress (N/m^2)**	**Strain**
CdSe	400	7.430×10^3	1.450×10^{-7}
	300	5.590×10^3	1.090×10^{-7}
	200	3.860×10^3	0.724×10^{-7}
	100	1.930×10^3	0.362×10^{-7}
	50	0.966×10^3	0.181×10^{-7}
	Pressure (pa)	**Stress (N/m^2)**	**Strain**
CdTe	400	7.630×10^3	1.910×10^{-7}
	300	5.720×10^3	1.430×10^{-7}
	200	3.820×10^3	0.954×10^{-7}
	100	1.910×10^3	0.477×10^{-7}
	50	0.954×10^3	0.238×10^{-7}

The results shown in Table 2 indicate that the highest value of the stress and strain for materials (CdSe and CdTe) is at a pressure of (400pa) and the values decrease with the decrease in the pressure applied to the surface of the material. Figures (2 and 3) show that the value of stress and strain for (CdSe) is less than (CdTe).

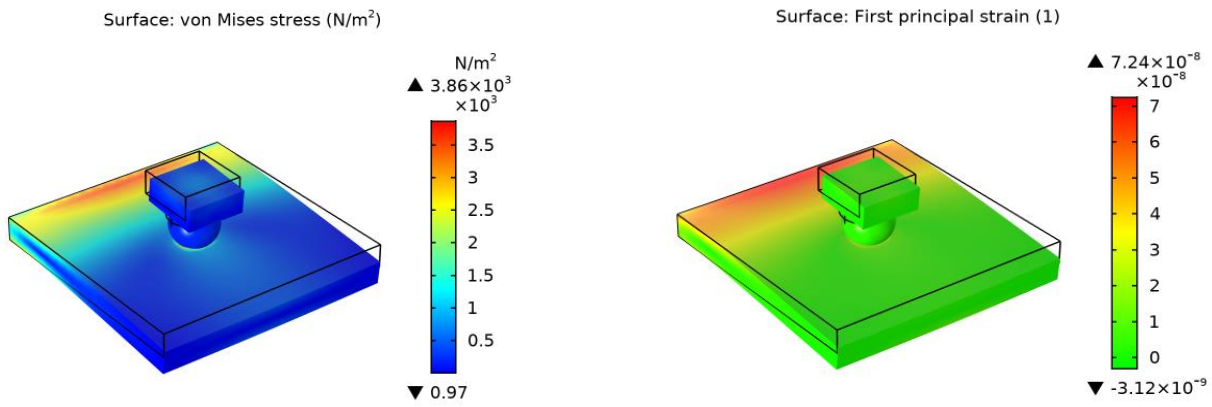

Figure 2. 3D representation of stress and strain at a pressure of CdSe.

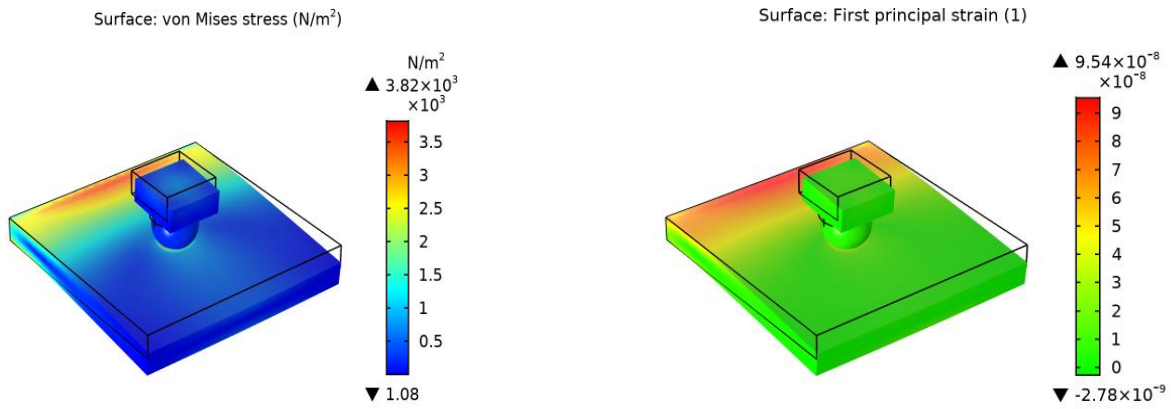

Figure 3. The values of stress and strain at a pressure of CdTe.

Figures (4 and 5) show the greatest value of stress and displacement inside the material (CdSe and CdTe) due to the compressive force is at the position (angle) of (-30), and the lowest value for the two variables is at (30). While the material (CdSe) is the value of the stress and displacement curve in the graph, it is greater than the substance (CdTe).

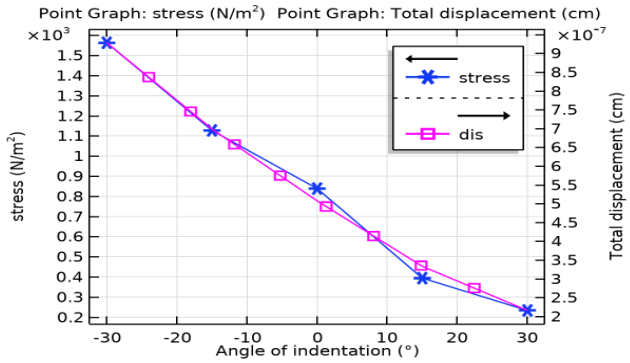

Figure 4. Stress and displacement versus position (Angle indentation) of CdSe.

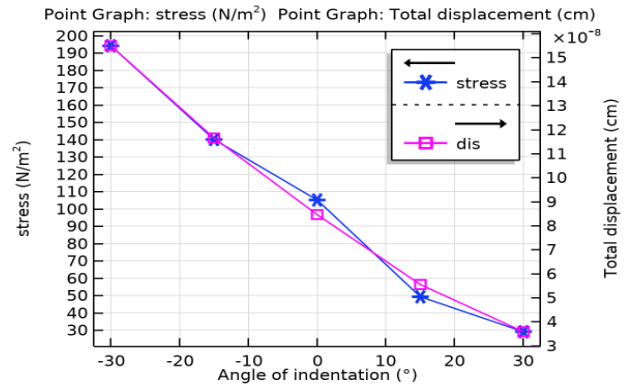

Figure 5. Stress and displacement versus position (Angle indentation) of CdTe.

CONCLUSIONS

The mechanical properties and band structure investigations of the pressure-induced CdSe and CdTe were investigated by using the simulation program COMSOL. In order to establish the various moduli, the elastic constants needed to be found. The fact that the elastic constants at (0 Pa) are found to be comparable with the previously published values is further evidence that our computations are accurate. Furthermore, it was discovered that the bulk modulus, shear modulus, and Young's modulus all increased in a consistent manner in response to an increase in pressure. Along with ductility, we also looked at the anisotropy factor and the hardness of the material. In addition, the results show that there is affinity in the mechanical properties, but the strength of resistance (CdSe) against deformation is greater than (CdTe), and therefore (CdSe) is better under pressure (from 400 pa to 50 pa). Based on the results, it is suitable for the manufacture of solar cells, electronic devices, etc.

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