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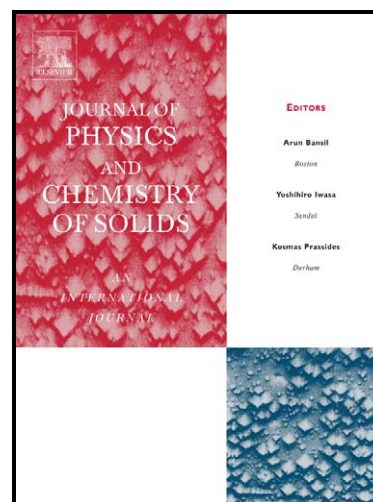
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Simulation of elastic-and-optical properties of K₂SO₄ crystals

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Abstract

The electronic optical spectra of the mechanically free and stressed crystals of potassium sulfate, K₂SO₄, in the orthorhombic phase *Pnma* have been calculated by the CASTEP (CAmbridge Serial Total Energy Package) code. On the basis of these calculations the components of the stress elastic-and-optical tensors based on the changes of refractive index $n(\pi_{im})$ and birefringence $\Delta n(\pi_{km}^*)$ ($i, k, m = 1, 2, \dots, 6$) have been obtained for the indices $i, k, m = 1, 2, 3$. Absolute magnitudes of the calculated tensor π_{im} are probably underestimated because the magnitudes of the calculated elastic stiffness tensor c_{mi} are found to be near two times overestimated. Features of the spectral dependences $n(E)$ and $k(E)$ of refractive and absorption indices of the mechanically free and stressed potassium sulfate crystal have been analyzed.

Keywords: A. Inorganic compounds; C. Ab initio calculations; D. Electronic structure;
D. Optical properties

1. Introduction

Potassium sulfate (PS) K₂SO₄ belongs at room temperature $T = 25$ °C to the orthorhombic space group $D_{2h}^{16} = Pnma$ and has four formula units per unit cell, with lattice parameters $a = 7.476$ Å, $b = 5.763$ Å, and $c = 10.071$ Å [1]. The substance transforms upon heating at $T_t \approx 587$ °C into a hexagonal structure $D_{6h}^{44} = P6_3/mmc$ with $a = 5.92$ Å and $c = 8.182$ Å (measured at 640 °C) where the oxygen positions of the SO₄²⁻ tetrahedra are only partially occupied [2]. The hexagonal high temperature phase of the crystal is known as α -K₂SO₄ and the orthorhombic phase as β -K₂SO₄. Analogous phase transformations (PT's) from α - to β -type phase are shown for the other K₂SO₄-family crystals (e.g. Na₂SO₄, LiKSO₄, K₂CrO₄, and K₂SeO₄) [3, 4]. Another PT of second order at the temperature of 56 K was detected in K₂SO₄ crystal. The crystal symmetry of this low-temperature phase (γ -K₂SO₄) is assumed to be of monoclinic [5].

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Valuable information on the structural and physical properties of a crystal can be provided by optical investigations of its refractive and birefringence characteristics. Several investigations of such type were done for PS crystal earlier in the photon energy range 1 – 5 eV of the crystal's transparency [6, 7]. It is known that PS crystal possesses two isotropic points in the spectral range 250 – 850 nm as well as demonstrates the property of *isospectrality* [7]. An influence of the uniaxial stress on these characteristics of PS crystals has been studied experimentally in [8].

Because of the experimental studies of optical properties of PS crystals mentioned, it is interesting to perform theoretical first-principles calculations of the tensor of refractive index, $\mathbf{n}_p = n_p + ik_p$, in the photon energy range of electronic excitations, which determines the dispersions of refractive indices $n_p(\lambda)$ and birefringence $\Delta n_{pq}(\lambda)$ in the range of crystal's transparency. Here, $p, q = 1, 2, 3$, are principal directions of optical indicatrix of a crystal. First calculations of the band structure and optical properties of K_2SO_4 crystals were performed in the paper [9] using a norm-conserving pseudopotential method. Experimental spectra of the imaginary part of dielectric permittivity $\epsilon_2(E)$ of the crystal obtained in this paper showed some influence of the electron-phonon broadening. Because of known experimental difficulties of the investigations of absolute elastic-and-optical tensors of materials, the calculations of this tensor for K_2SO_4 crystals by the first-principles code, based on the density functional theory (DFT), presents an interest. Such type of *ab-initio* study of the pressure influence on the refractive indices of PS crystals gives possibility to obtain new respective data for the relatively big magnitudes of mechanical stresses, which are inaccessible in the experiment because of the crack of crystalline samples under the uniaxial stresses.

2. Method of calculations

Calculations of the electronic energy structure of potassium sulfate crystal have been performed within a framework of the density functional theory (DFT) using the pseudopotentials-plane-wave-basis-set CASTEP code (Cambridge Serial Total Energy Package) [10]. The calculations were performed within a framework of the generalized gradient approximation (GGA) with PW91 functional for the exchange and correlation effects [11] with the ultra-soft pseudopotentials [12]. These pseudopotentials require a quite low energy cutoff and guarantee good transferability, that is, the same potential correctly reproduces the valence electron scattering by the ionic core in different chemical

environments. The cutoff energy of 340 eV was assumed in the plane-wave basis set. Optimization (relaxation) of the atomic positions and crystal's cell parameters was performed before the main calculations of electronic characteristic: total electronic energy E , band energy dispersion $E(k)$, density of electronic states (DOS), and dielectric functions $\epsilon(E)$. Band structure of the crystal was calculated for 27 k -points of the Brillouin zone (BZ). The SCF convergence criterion of electronic energy per atom was $2 \cdot 10^{-6}$ eV and the tolerance for the electronic total energy during optimization was $1 \cdot 10^{-5}$ eV.

The CASTEP program permits to apply unlimited mechanical stress to the crystal studied, perform full structure optimization and then to calculate the respected photon energy dependences of the real and imaginary parts of dielectric permittivity, $\epsilon_1(E)$ and $\epsilon_2(E)$. These results can be presented in the form of the photon energy dependences of the refractive and absorption indices, $n(E)$ and $k(E)$, using the known relation $\epsilon = n^2$. According to the reference data [13, 14], the bulk modulus B and the Young's modulus E of PS crystal are equal to 31.9 GPa and 44.2 GPa, respectively. In the present calculation, the uniaxial stress $\sigma = 1$ GPa was applied along three Cartesian axes of the crystal matching the principal directions of optical indicatrix. Such stress still falls under the range of elastic stiffness of the crystal, if taking into account the above mentioned value of the Young's modulus E . In this range, the pressure induced change of refractive index δn is probably proportional to the stress σ .

3. Results and discussion

Spectra of the calculated refractive and absorption indices $n(E)$ and $k(E)$ of the PS are shown in figure 1 for the scissor factor of 1.0 eV. Scissor factor is often used in the DFT-based calculations of dielectrics and semiconductors to agree magnitudes of the calculated and experimental low-energy edge of fundamental absorption. However, even in this case the calculated principal refractive indices obtained for the photon energy $E = 0.01$ eV, $n_x = 1.5600$, $n_y = 1.5572$, $n_z = 1.5538$, are substantially greater than the experimental ones, $n_x = 1.5016$, $n_y = 1.4992$, $n_z = 1.4977$ [7], for the photon energy $E = 2.48$ eV. This discrepancy may be caused by the negative input from the absorption of crystal caused by atomic oscillations ($E < 0.4$ eV) into the experimental refractive index in the range of transparency 0.4 – 7.0 eV, which is not being calculated by the CASTEP code. This negative input derives from the known Kramers-Kronig's relation between the spectra of refractive (n) and absorption (k) indices of material [15, 16],

$$n(E) = 1 + \frac{2}{\pi} \int_0^{\infty} \frac{tk(t)dt}{t^2 - E^2} . \quad (1)$$

When the average difference of the calculated and experimental refractive indices at the photon energy $E = 2.48$ eV is regarded to be $\Delta n_{osc} = 0.06$, then rough calculations of the average absorption index k_{osc} in the range of atomic oscillations, $E < 0.4$ eV, by the relation (1) gives the reliable magnitude of this index, $k_{osc} \approx 6$.

(Figure 1 here)

The calculated refractive indices of PS crystals ($n_x = 1.5600$, $n_y = 1.5572$, $n_z = 1.5538$) are a bit smaller than the corresponding values for the rubidium ammonium sulfate (RAS) crystals ($n_x = 1.5848$, $n_y = 1.5690$, $n_z = 1.5617$), which were calculated by the CASTEP code recently [17]. Thus, substitution $\text{NH}_4^+ \rightarrow \text{K}^+$ causes a decrease of refractive index by 0.008 – 0.025. This result is in good agreement with experimental data [7].

There are no crossing of the refractive index dispersions $n_i(E)$ in the range of 0.01 – 7.0 eV, this fact is in agreement with the corresponding experimental data for the temperature range $T < 617$ K [7]. In this connection, one has to remember, that PS crystal is characterized by two temperature points, 617 K and 700 K, in which the crystal becomes optically uniaxial for all photon energies in the range of crystal transparency. So, the phenomenon of the so-called “isospectrality” takes place at these temperatures: $n_x = n_y$ at 617 K, and $n_y = n_z$ at 700 K [7].

Analysis of main features of the band structure of the PS crystals reveals close similarity to the band structure of the rubidium ammonium sulfate (RAS) crystal obtained recently [17]. The main difference of the band structures of PS and RAS crystals, which can affect difference in the spectra of optical properties $n(E)$ and $k(E)$, is a presence (absence) of the electronic states of hydrogen in the bottom of conduction band [17]. Really, this difference is revealing in the low photon energy region of the spectra of absorption index $k(E)$ of PS and RAS crystals (Fig. 2). Namely, essential band of the absorption index spectrum $k(E)$ in RAS crystals observed in the region 7 - 9 eV is absent in the corresponding spectrum of PS crystal. There are no other essential differences in the absorption spectra $k(E)$ of PS and RAS crystals. This is also an evidence for the close similarity of band structures of these crystals. The magnitude of the experimental long-wavelength edge of the fundamental absorption of PS crystal, $E_{edge} = 7.2$ eV [18], is close to the theoretical one obtained in the paper with using a scissor factor of 1.0 eV. There is no possibility to compare the theoretical and experimental

dielectric functions $n(E)$ and $k(E)$ of PS crystal in the range of $E > 7$ eV because of absence of the reliable corresponding experimental data.

(Figure 2 here)

Refractive indices and birefringences of the mechanically free and uniaxially stressed PS crystals are presented in Table 1. For every direction of mechanical stress, the refractive index of stressed PS crystal is greater than the corresponding refractive index of free sample. This result agrees with the experimental data [8]. The main reason of this result is probably the pressure induced increase of the crystal density ρ and, at the same time, the relative stability of the refraction R of the crystal. This is followed from the known Lorentz-Lorenz relation [19],

$$\frac{(n^2 - 1)}{(n^2 + 2)} = \frac{R}{M} \rho, \quad (2)$$

where M is a molar weight.

(Table 1 here)

When analyzing the dispersion of birefringence $\Delta n(E)$ of PS crystals for different stresses σ (Fig. 3), one can notice that the absolute value of birefringence $|\Delta n|$ increases with increase of photon energy E in the range of transparency and therefore no “isotropic points” caused by the anisotropy of electronic excitations are expected here. Second significant feature of the results presented in figure 3 is that a birefringence Δn , corresponding to the chosen indicatrix cut, decreases when the uniaxial stress is directed along the greater refractive index of this indicatrix cut of the mechanically free crystal. At the same time, absolute refractive indices n_i ($i = x, y, z$) increase with increase of the corresponding uniaxial stresses σ_i (see Table 1).

On the basis of the results in the figure 3 one can also suggest a receiving of the “isotropic points”, $\Delta n_{xy} = 0$ and $\Delta n_{yz} = 0$, for the corresponding uniaxial stresses σ_x and σ_y close to the magnitude of 2 GPa.

(Figure 3 here)

If taking into account the following definition of the tensor of stress elastic-and-optical coefficients π_{im} ,

$$\delta a_i = \pi_{im} \sigma_m, \quad i, m = 1, 2, \dots, 6, \quad (3)$$

where

$$\delta a_i = \delta \left(\frac{1}{n_i^2} \right) = \frac{2\delta n_i}{n_i^3}, \quad (4)$$

one can calculate several coefficients π_{im} for PS crystals using the data in Table 1. The components of the tensor of stress elastic-and-optical coefficients π_{im} , corresponding to only uniaxial stresses ($k = 1, 2, 3$) are presented in Table 2. Positive sign of π_{im} means an increase of refractive index under compression of a crystal. The characteristic feature of the elastic-and-optical tensor π_{im} of K_2SO_4 crystal obtained is that the diagonal components π_{11} , π_{22} and π_{33} are the smallest comparing with non diagonal components π_{im} ($i, m = 1, 2, 3$ and $i \neq m$).

One can estimate the validity of results on the coefficients π_{im} taking into account the experimental data on the Young's modulus E of the mineral arcanite (K_2SO_4), $E = 4.42 \cdot 10^{10}$ Pa [13, 14], and the calculated components of elastic stiffness c_{rm} of PS crystal: $c_{11} = 10.57 \cdot 10^{10}$ Pa, $c_{22} = 9.69 \cdot 10^{10}$ Pa, $c_{33} = 12.5 \cdot 10^{10}$ Pa. This comparison reveals that the calculated components of elastic stiffness c_{rm} are overestimated in our calculations approximately two times. This probably leads to the corresponding underestimation of the strain ϵ_m and the change of polarizability Δa_i of the crystal under an action of the definite stress σ_m . Then, taking into consideration the relation (3) one arrives to the conclusion of underestimation of the calculated components of the tensor of stress elastic-and-optical coefficients π_{im} .

(Table 2 here)

Using the know relation for the components of the tensor of stress elastic-and-optical coefficients regarding to birefringence π_{km}^* ,

$$\pi_{km}^* = \frac{2\delta(\Delta n_k)}{\sigma_m}, \quad (5)$$

and results presented in Table 1, the components of π_{km}^* tensor corresponding to only uniaxial stresses ($m = 1, 2, 3$) have been calculated and presented in Table 3. Here, the tensor π_{km}^* can be expressed by the following relation:

$$\pi_{km}^* = \pi_{im} n_{i0}^3 - \pi_{jm} n_{j0}^3, \quad (6)$$

where k is the direction of light propagation, m is the direction uniaxial stress, i and j are directions of light polarization and $i, j, k, m = 1, 2, 3$. Positive sign of the elastic-and-optical coefficients π_{km}^* in Table 3 corresponds to the increase of absolute value of corresponding birefringence and negative sign corresponds to the decrease of absolute birefringence. One of

the characteristic peculiarity of the results obtained is the smallest magnitudes of diagonal components π_{11}^* , π_{22}^* , and π_{33}^* . This feature however can be as a general characteristic of wide class of crystals. It is also obvious that the conclusion about underestimation of the components of tensor of stress elastic-and-optical coefficients π_{im} are also valid to the components of tensor of stress elastic-and-optical coefficients π_{km}^* based on birefringence. (Tablee 3 here)

The figure 4 illustrates that birefringence of the mechanically free PS crystal is a complicated function of the photon energy E in the range of fundamental absorption ($E > 7$ eV). The change of sign of the birefringence Δn in the range of fundamental absorption is rather a characteristic feature of every crystal. It is also seen in figure 4 that the influence of uniaxial mechanical stress also leads to the complicated changes of the dependence $\Delta n_{zx}(E)$ in the range of $E > 7$ eV. However, the uniaxial stress of 1 GPa does not change essentially characteristic structure of the dependence $\Delta n_{zx}(E)$, therefore this magnitude of pressure can be applying to similar crystals for determination of their elastic and associated properties. (Figure 4 here)

4. Conclusions

The density functional theory based CASTEP code was applied successfully to the calculation of electronic optical spectra of the potassium sulfate crystals K_2SO_4 in the orthorhombic phase $Pnma$. On the basis of these calculations the components of elastic-and-optical tensor π_{im} ($i, m = 1, 2, \dots, 6$) have been obtained for the indices $i, m = 1, 2, 3$.

Calculated principal refractive indices of K_2SO_4 crystal in the range of transparency, 0.4 – 7.3 eV, agree satisfactorily with experimental data when taking into account the input from the atomic oscillations in the range of 0 - 0.4 eV.

An increase of refractive indices of K_2SO_4 crystal under the compressive stress of 1 GPa observed agrees with the pressure induced increase of the crystal density ρ when a relative stability of the refraction R of the crystal is supposed. This conclusion is in agreement with the known Lorentz-Lorenz relation.

On the basis of present study one can suggest a receiving of the “isotropic points” in the range of transparency of K_2SO_4 crystal, $\Delta n_{xy} = 0$ and $\Delta n_{yz} = 0$, for the corresponding uniaxial compressive stresses σ_x and σ_y close to the magnitude of 2 GPa.

The calculated components of the elastic-and-optical tensor π_{im} of K_2SO_4 crystal were found to be underestimated approximately by two times. This is probably caused by the corresponding overestimation of the components of the elastic stiffness tensor c_{rm} .

The characteristic feature of the elastic-and-optical tensor π_{im} of K_2SO_4 crystal obtained is that the diagonal components π_{11} , π_{22} and π_{33} are smaller than the non diagonal components π_{im} ($i, m = 1, 2, 3$ and $i \neq m$).

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Figure captions

of the paper “Simulation of elastic-and-optical properties of K_2SO_4 crystals” by
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Figure 1. Spectra of refractive and absorption indices $n(E)$ and $k(E)$ of potassium sulfate crystal for principal directions x , y , and z of optical indicatrix.

Figure 2. Spectra of absorption index $k(E)$ of potassium sulfate (PS) and rubidium ammonium sulfate (RAS) crystals for principal directions x , y , and z of optical indicatrix.

Figure 3. Dispersion of birefringence $\Delta n(E)$ of PS crystal in the range of transparency for three principal cuts of optical indicatrix Δn_{xy} , Δn_{yz} , Δn_{zx} and different uniaxial stresses σ_x or σ_y , σ_y or σ_z , and σ_z or σ_x , in the plane of corresponding cut.

Figure 4. Dispersions of the birefringence $\Delta n_{zx}(E)$ of PS crystal in the range of transparency and fundamental absorption for the mechanically free sample ($\sigma = 0$) and for the axially stressed samples along principal axes of optical indicatrix ($\sigma_x = 1$ GPa, $\sigma_y = 1$ GPa, $\sigma_z = 1$ GPa).

Table 1. Refractive indices n_x , n_y , and n_z of potassium sulfate: experimental (at photon energy $E = 2.48$ eV) [7] and calculated (at photon energy $E = 0.01$ eV) for mechanically free ($\sigma = 0$) and uniaxially stressed crystal ($\sigma_x = \sigma_y = \sigma_z = 1$ GPa).

	Experiment $E = 2.48$ eV	$\sigma = 0$ $E = 0.01$ eV	$\sigma_x = 1$ GPa $E = 0.01$ eV	$\sigma_y = 1$ GPa $E = 0.01$ eV	$\sigma_z = 1$ GPa $E = 0.01$ eV
n_x	1.5016	1.56004	1.56109	1.56219	1.56125
n_y	1.4992	1.55721	1.55935	1.55767	1.55852
n_z	1.4977	1.55379	1.55544	1.55626	1.55385
$\Delta n_{xy} = \Delta n_x - n_y$	0.0024	0.00283	0.00174	0.00452	0.00273
$\Delta n_{yz} = n_y - n_z$	0.0015	0.00342	0.00391	0.00141	0.00467
$\Delta n_{zx} = n_z - n_x$	-0.0039	-0.00625	-0.00565	-0.00593	-0.00740

Table 2. Components of the tensor of stress elastic-and-optical coefficients π_{im} based on refractive indices of potassium sulfate crystal (in 10^{-12} Pa^{-1}).

π_{im}	$m = 1$	$m = 2$	$m = 3$
$i = 1$	0.553	1.13	0.637
$i = 2$	1.13	0.243	0.694
$i = 3$	0.880	1.32	0.032

Table 3. Components of the tensor of stress elastic-and-optical coefficients π_{km}^* based on birefringence of potassium sulfate crystal and corresponding to the uniaxial stresses (in 10^{-12} Pa^{-1}).

π_{km}^*	$m = 1$	$m = 2$	$m = 3$
$k = 1 \text{ (yz)}$	0.98	-4.02	2.5
$k = 2 \text{ (xz)}$	-1.2	-0.64	2.3
$k = 3 \text{ (xy)}$	-2.18	3.38	-0.2

Fig 1

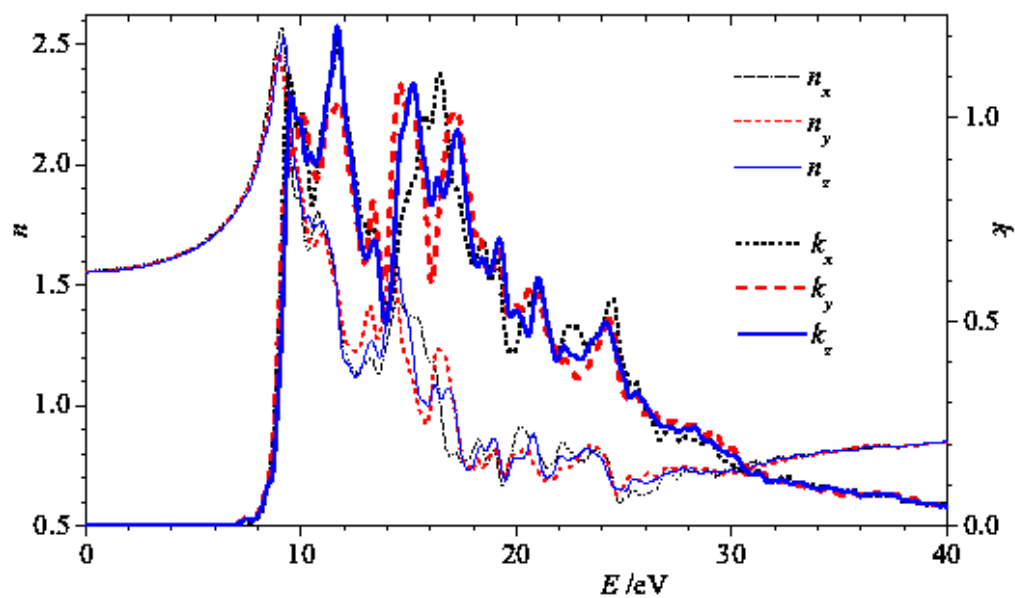


Fig 2

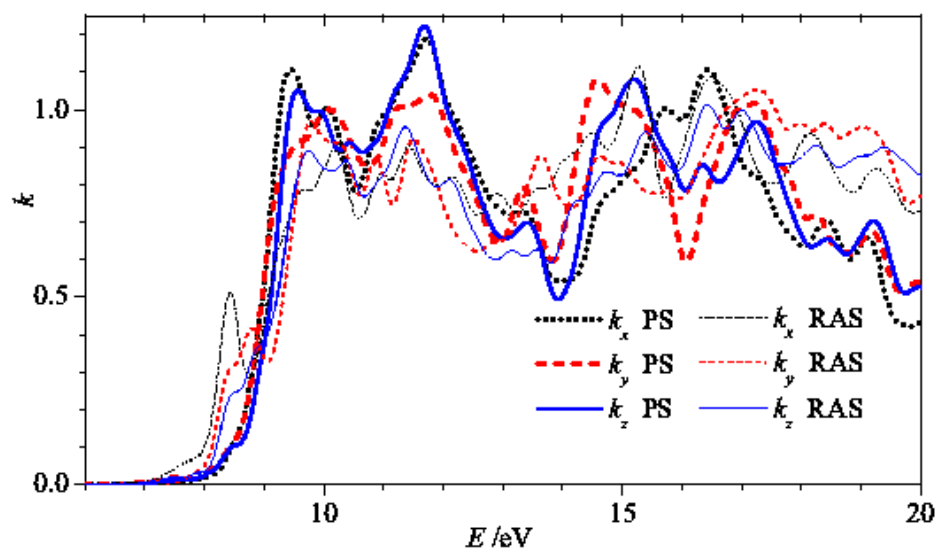


Fig 3

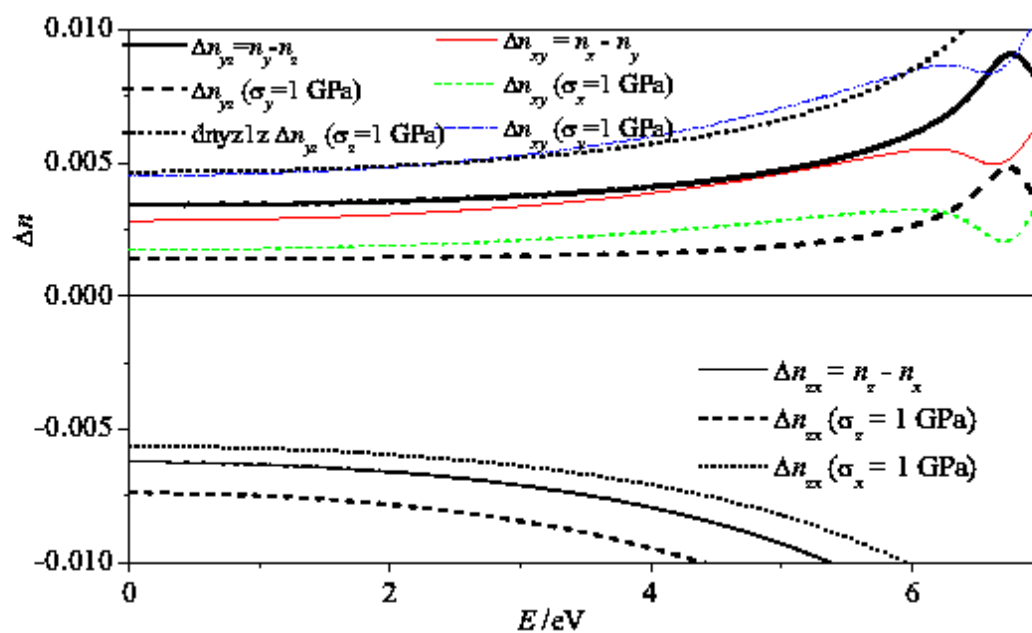


Fig 4

