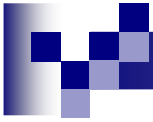


**Colloque National sur les Techniques de Modélisation
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Sidi Bel-Abbès . 23-24 Novembre 2009**

*Elastic, electronic and optical
properties of SiGe_2N_4 under
pressure : An ab initio study*

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Plan

- Introduction
- Computational method
- Résultats & discussion
- Conclusions



Introduction



Introduction

Why the compound SiGe_2N_4 ?

1. It is a stable compound
2. Favourable band gap
3. Small conduction band

Basic informations:

SiGe_2N_4 is a cubic spinel AB_2X_4

Space group $\text{Fd}\bar{3}\text{m}$ (# 227).

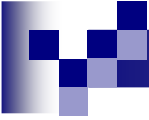
Atomic positions are: $(1/8, 1/8, 1/8)$ for A

$(1/2, 1/2, 1/2)$ for B

(u, u, u) for X $0.240 \leq u \leq 0.275$



Computational method

- 
- ❑ The performed calculations using a full-relativistic version of the full-potential with the mixed basis APW+lo method implemented in WIEN2K computer package.
 - ❑ The exchange correlation (XC) effects are treated by the generalized gradient approximation (GGA). Moreover, the (GGA-EV) is also used for band structure calculations.
 - ❑ The RMT (Si, Ge, N)=(2, 2.1, 1.4).
 - ❑ The cut-off $K_{\max}=12/R_{\text{MT}}$
 - ❑ The valence wave functions inside the spheres are expanded up to $l_{\max}=9$.
 - ❑ The charge density was Fourier expanded up to $G_{\max}=14$.
 - ❑ The integrals over the Brillouin zone are performed up to 18 k-points in the irreducible Brillouin zone (IBZ), using the Monkhorst-Pack special k-points approach .



Results and discussions



Structural and elastic properties

- Optimization of internal parameter u
- Determination of structural properties : a_0 , B_0 et B' .

In Table 1, we summarize our calculated structural and elastic properties of SiGe₂N₄ at zero pressure.

Structural and elastic properties

Table 1. Calculated lattice structural parameters

	Present work	Other theoretical works
a_0 (Å)	8.182	8.087 a; 8.142b
B (GPa)	247.09	241.7a; 277.1 b
B'	4.55	4.48 a; 3.02b
u	0.2541	0.3785a; 0.3772b
C_{11}	441.53	
C_{12}	149.8	
C_{44}	126.29	
E	340.71	
G	134.12	
ν	0.27	
μ	133.76	
λ	157.81	

Structural and elastic properties

- Pressure effect on the internal parameter $u=f(P)$

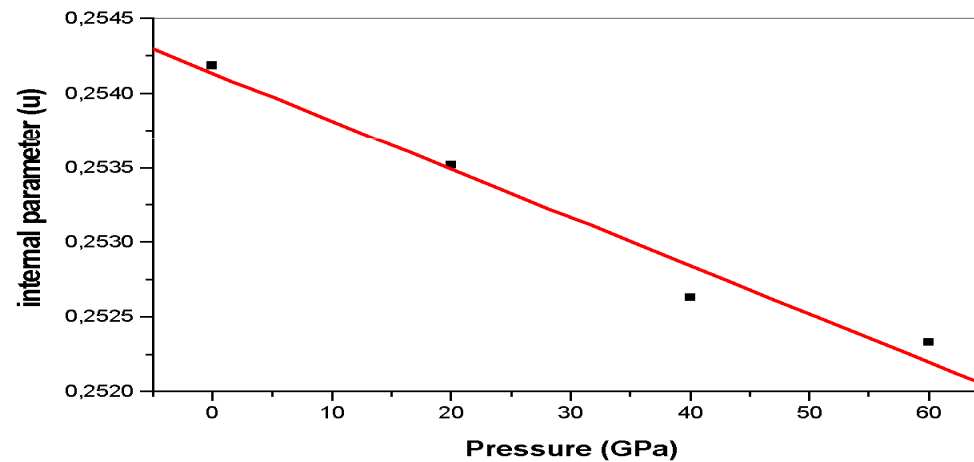


Fig.1. Pressure dependence of the internal parameter u in SiGe_2N_4 .

Structural and elastic properties

- Determination of the elastic constants C_{ii}

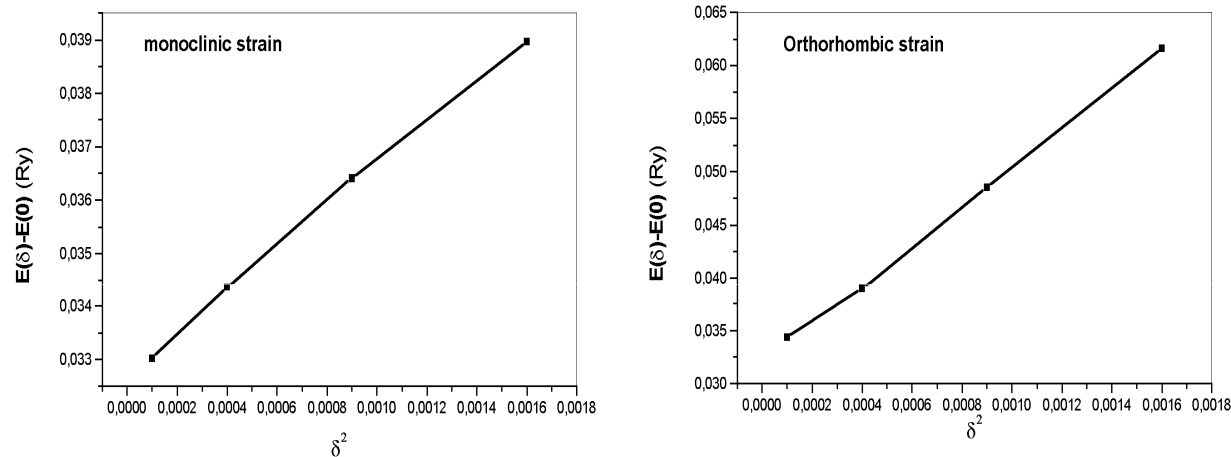


Fig. 2: Energy as function of the square orthorhombic and monoclinic strain used to determine C_{11} - C_{12} and C_{44} respectively.

- For isotropic cubic crystal, the bulk modulus is: $B=(C_{11}+2C_{12})/3$



Structural and elastic properties

- Derivation of shear modulus G , Young's modulus E , Poisson's ratios (ν) , Lamé's coefficients μ and λ from the following equations:

$$E=9BG / (3B+G) \quad (1)$$

$$G= (C11-C12+3C44)/5 \quad (2)$$

$$\nu = (3B-E) / (6B) \quad (3)$$

$$\mu = E / (2(1+\nu)) \quad (4)$$

$$\lambda= \nu E / ((1+\nu)(1- 2 \nu)) \quad (5)$$

Structural and elastic properties

We study the pressure dependence of the elastic properties. C_{ij} & $B=f(P)$

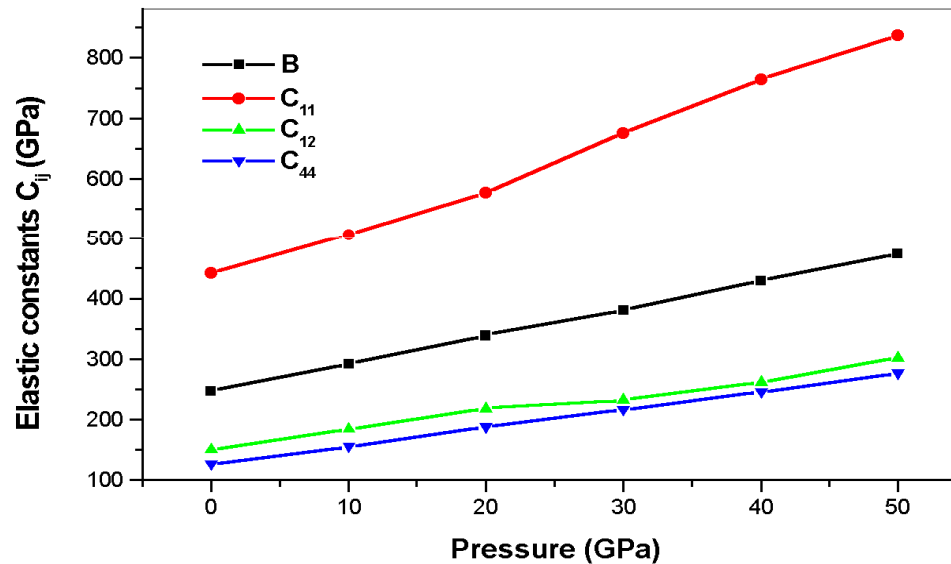


Fig. 3: Pressure dependence of C_{ij} and B for SiGe_2N_4

Structural and elastic properties

- The Debye temperature is calculated by using

with

$$\theta_D = \frac{h}{k_B} \left[\frac{3n}{4\pi V_a} \right]^{1/3} v_m$$

and

$$v_m = \left[\frac{1}{3} \left(\frac{2}{v_t^3} + \frac{1}{v_l^3} \right) \right]^{-1/3}$$

$$v_l = \left(\frac{3B + 4G}{3\rho} \right)^{1/2} \quad v_t = \left(\frac{G}{\rho} \right)^{1/2}$$



Structural and elastic properties

- Results are summarized in table2
- **Table 2:** Calculated GGA-density (ρ in g.cm^{-3}), the longitudinal, transverse and average sound velocity (ν_l , ν_t , ν_m in 10^3 m.s^{-1}) calculated from polycrystalline elastic modulus and the Debye temperature (in K) for SiGe₂N₄ compound.

ρ	ν_l	ν_t	ν_m	θ_D
34.65	3.501	1.962	2.559	356



Electronic properties

We present the (BS) of SiGe_2N_4 within GGA and EVGGA in **Fig.4**.

The valence band maximum (VBM) and the conduction band minimum (CBM) are located at Γ point, resulting in a direct band gap (Γ - Γ)

Results are summarized in **Table3**

To elucidate the nature of the electronic (BS), we have also calculated the total and the atomic DOS displayed in **Fig.5**.

Electronic properties

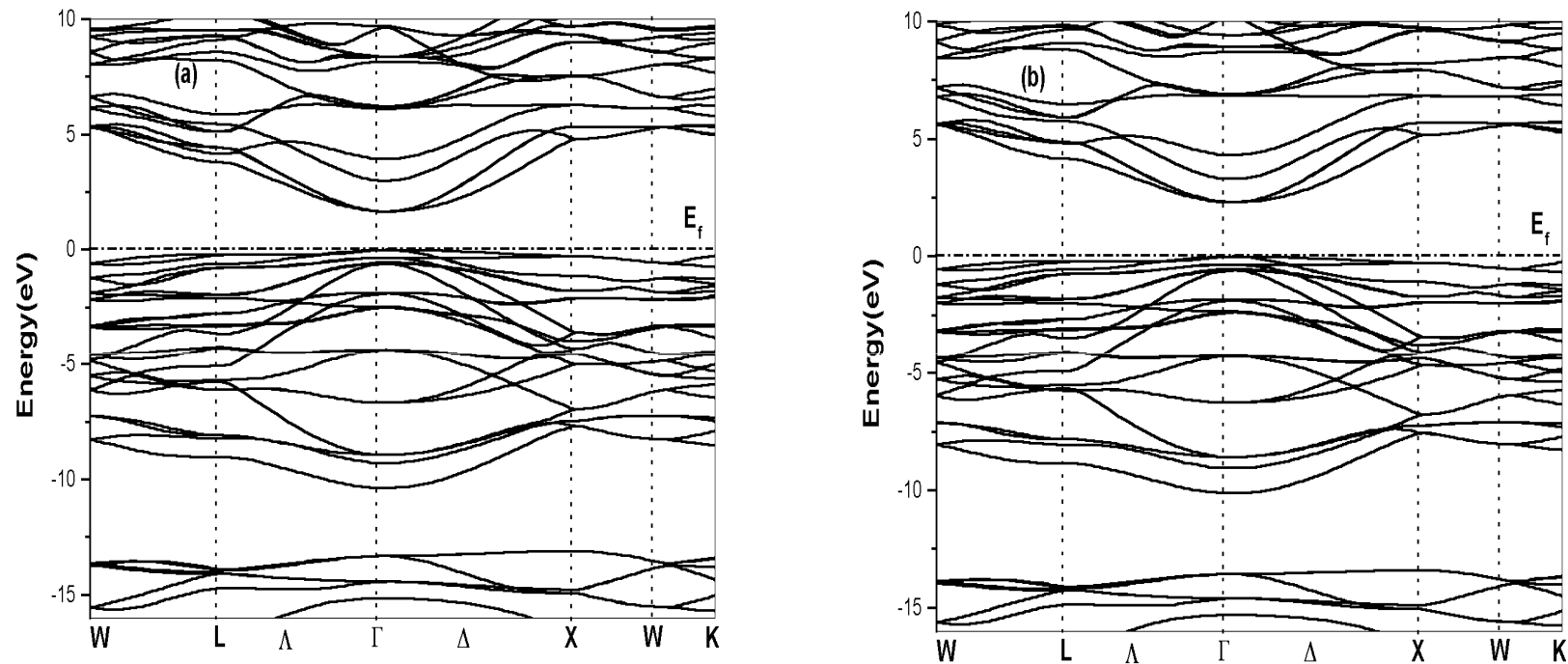


Fig. 4 : Calculated band structure of cubic spinel SiGe₂N₄ :
with GGA (a) and EVGGA (b)

Electronic properties

Table 3: Calculated first- and second-order pressure coefficients of some direct and indirect band gaps (Γ - Γ , Γ -L, and Γ -X) for spinel SiGe₂N₄. $E_g(P) = E_g(0) + \alpha P + \beta P^2$, E_g in eV, α in eV $\times 10^{-2}$ (GPa)⁻¹, β in eV $\times 10^{-4}$ (GPa)⁻².

	Γ - Γ	Γ -L	Γ -X	band-width
GGA				
$E_g(0)$	1.68	3.75	4.79	10.5
α	1.26	2.13	1.98	
β	0.80	1.29	1.44	
Other studies				
$E_g(0)$ a	1.58			
$E_g(0)$ b	1.85			
EV-GGA				
$E_g(0)$	2.35	4.1	5.14	10.2
α	0.2	1.9	1.8	
β	1.88	1.98	2.64	

Electronic properties

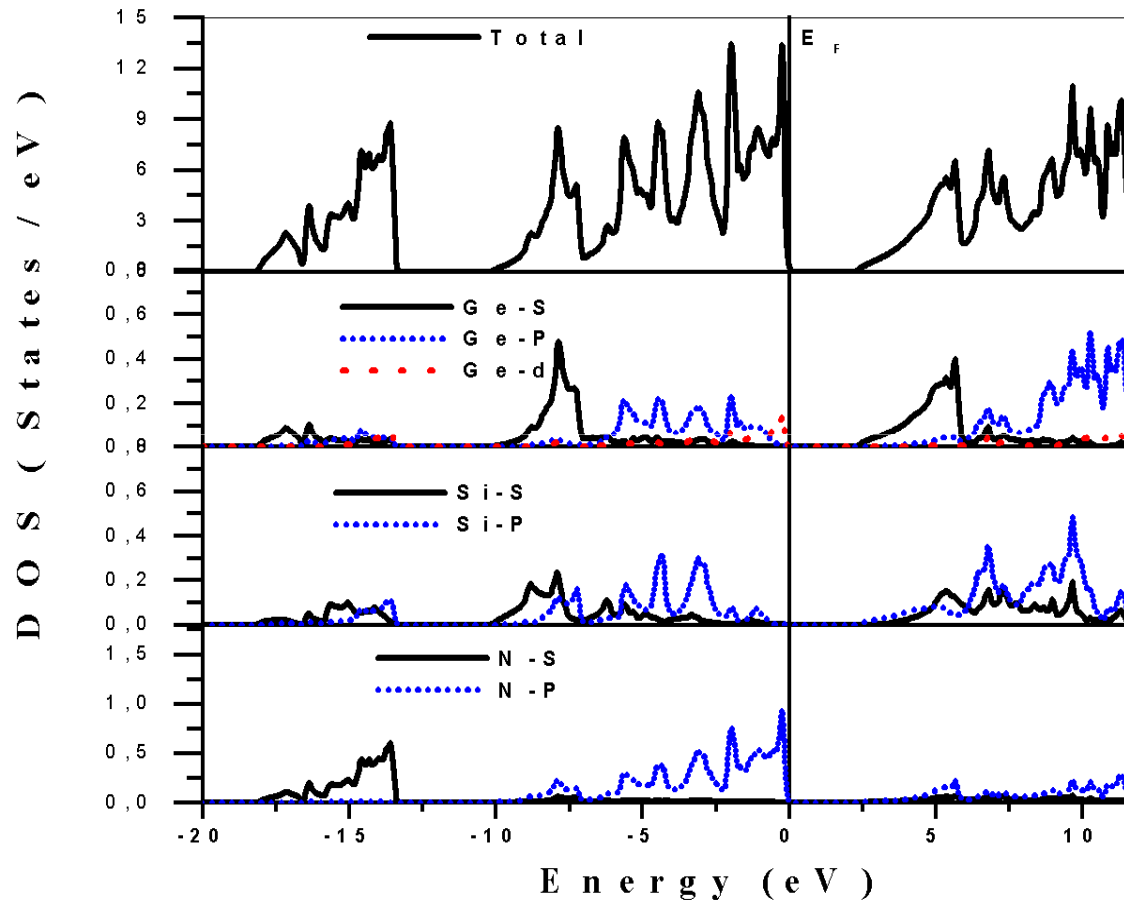


Fig. 5: Calculated Total and Partial (DOS) of SiGe₂N₄ within EVGGA

Electronic properties

- We investigate the effect of the pressure on the size of the energy gaps

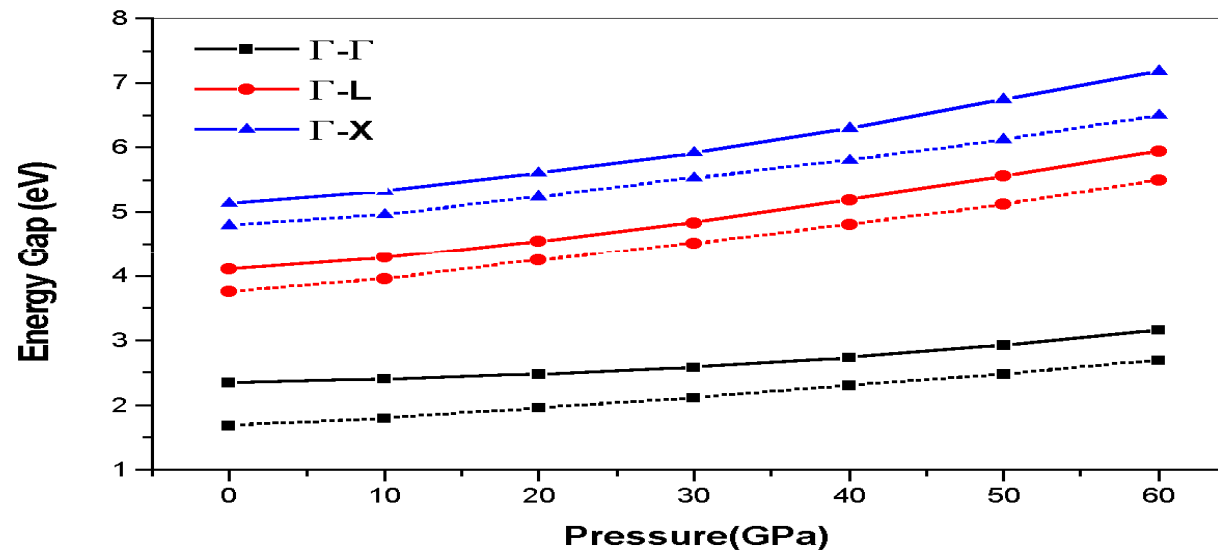


Fig. 6: The calculated energy band gap of SiGe₂N₄ versus pressure with (dotted line). GGA and, (solid line). EVGGA .

Optical properties

- Since the spinel nitride SiGe_2N_4 has cubic symmetry, we need to calculate only one dielectric tensor component to completely characterize the linear optical properties

- We note that the dielectric function is: $\boldsymbol{\varepsilon}(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$

- And the refractive index:
$$n(\omega) = \left[\frac{\varepsilon_1(\omega)}{2} + \frac{\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)}}{2} \right]^{1/2}$$

- **Fig.7.** displays the both imaginary (absorbative) and real part of the at 0 and 60GPa

Optical properties

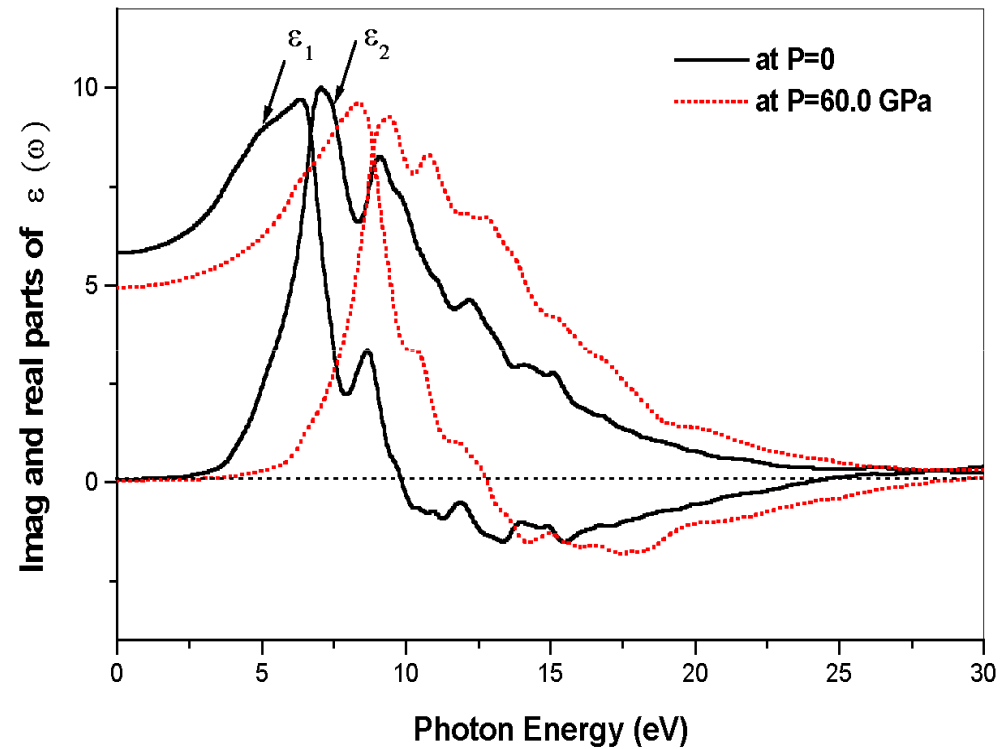


Fig .7: Calculated EVGGA- real and imaginary parts of the dielectric function of SiGe₂N₄: (solid line) at P=0 GPa and (dotted line) at P=60GPa.

Optical properties

- Investigations performed with 256 k-pts in IBZ
- EV-GGA was used

- **Analysis of absorptive part $\epsilon_2(\omega)$**
- Threshold for direct optical transition (fund absor edge) at 3.21eV
- The main peak 7.12 followed by two other peaks 9.05 and 12.24eV
- Under pressure all peaks, positions of all peaks are shifted

- **Analysis of real part**
- At high freq the zero crossing of $\epsilon_1(\omega)$ corr to screened plasma freq 24.7eV
- The $\epsilon_1(0)$ is the static optical dielectric constant ϵ_∞ 5.85eV
- The behaviour of static dielectric const (static refractive index) is linear
- A linear fit gives $\frac{1}{n_0} \frac{dn}{dp}$ and $\frac{v_0}{n_0} \frac{dn}{dv}$ with $-1.29 \cdot 10^{-3} \text{ GPa}^{-1}$ and 0.38

Optical properties

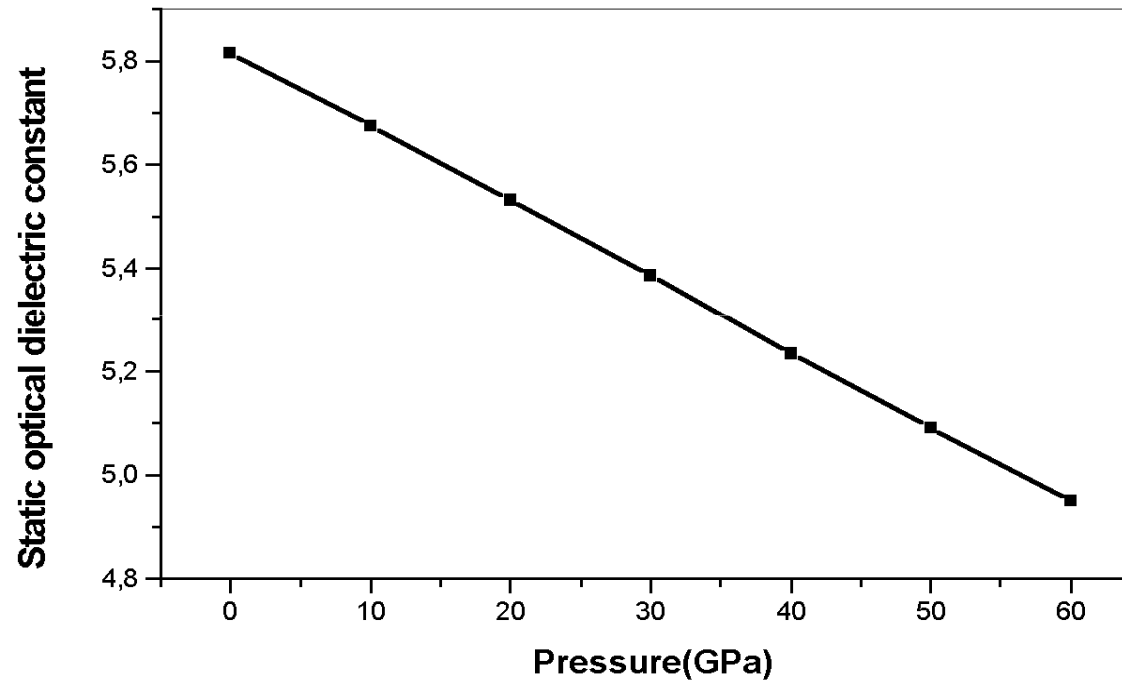


Fig. 8: Pressure dependence of the static optical dielectric constant ϵ_{∞} of SiGe₂N₄ within EVGGA

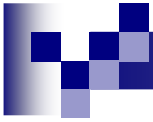


Conclusions



Conclusion

- The calculated ground state properties such a_0 , B_0 and B' agree quite well with available theoretical results.
- The calculated Band Struct show that SiGe₂N₄ is a direct band gap
- Dielectric function was investigated and analyzed to identify the optical transitions
- To the best of our knowledge, there are no earlier studies on the elastic constant as well as the effect of pressure on the electronic structure and imaginary part of the dielectric constant, we feel that our calculations can be used to cover the lack of data for this compound.



Merci pour votre attention