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Research paper

Mechanical stability criterions of cubic Na_2He up to 500 GPa

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Abstract

The Cauchy pressure Cp was usually used to explain the atomic bonding character in a compound, while the mechanical stability criterions are usually used to study the stability of the structure under external compression. Using the elastic constants reported recently by Zahidur Rahaman et al. in Chinese Journal of Physics, 56 (2018) 231-237, as well as different mathematical formula, we reported on the Cauchy violation and the generalized mechanical stability criterions of cubic Na2He compound under high hydrostatic compression from 100 GPa to 500 GPa. For pressures ranging from 100 to 500 GPa, all values of both Cauchy pressure Cp and the generalized mechanical stability criteria G are negative. In addition we calculated the Debye temperature θD of Na_2He compound using Siethoff's approach. The results obtained are slightly lower than those obtained from the Debye approach reported by Zahidur Rahaman et al.

Keywords: *High Hydrostatic Compression; Cauchy Violation for Cubic Crystals; Generalized Mechanical Stability Criterions.*

1. Introduction

Helium with symbol (He) is chemically inert element because of its closed-shell electronic configurations [1]. After hydrogen (H), helium is the second most abundant element in the universe, it is present in significant quantities in normal stars [2].
It is well known that the axial pressures as well as the hydrostatic compression have significant effects on the structural, electronic, mechanical, thermodynamical, and magnetic properties of materials [1-8].
Using density functional theory (DFT) calculations, Zahidur Rahaman et al. [1] studied the pressure-dependent elastic constants, mechanical moduli and thermodynamic properties of cubic Na_2He compound in pressure ranging from 100 to 500 GPa. They found good accordance between the theoretical and experimental lattice parameters.
Using a variable-composition evolutionary structure prediction algorithm, as implemented in the USPEX computer code, Dong et al. [2] have investigated the structural phase stability of helium (He)-sodium (Na) system at normal conditions and at high pressures. They found that under high compression (p >113 GPa), the Na_2He compound becomes stable at the fluorite-type structure. They found also that the presence of helium atoms causes strong electron localization. Amari and Daoud [9] investigated the elastic constants and thermodynamic properties as well as the structural phase transition of TmAs material, while Benamrani et al. [10] studied the structural phase transition and both elastic and thermodynamic properties of scandium mono-phosphide (ScP) semiconducting compound.
Some other works [11], [12] investigated the phase transition of materials under sufficient high pressure compression using the generalized mechanical stability criteria.
In the present work, we attempt to the Cauchy violation and the generalized mechanical stability criterions of cubic Na_2He compound under high hydrostatic compression from 100 to 500 GPa using the elastic constants reported by Zahidur Rahaman et al.[1].

2. Theory, results and discussion

At equilibrium (zero-pressure), the Cauchy pressure C_p of the cubic crystals is given as follows: $C_p = C_{12} - C_{44}$, while the mechanical stability criterions are expressed as follows: $C_{11} > 0$, $C_{11} + 2C_{12} > 0$, $C_{11} - C_{12} > 0$, and $C_{44} > 0$ [1]. Under high pressure (under hydrostatic compression), the previous conditions should be written as a function of pressure. The new Cauchy pressure should be written $C_p = C_{12} - C_{44} - 2P$ [13, 14], where P is the pressure. The new stability criteria for cubic crystals were obtained by writing the elastic energy of deformation in terms of the Lagrangian strain [15]. The well-known stability conditions for a cubic crystal under hydrostatic compression can be obtained as [15]:

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$$K = (B_{11} + 2B_{12})/3 > 0,\ G = B_{44} > 0 \text{, and } G' = (B_{11} - B_{12})/2 > 0 \quad (1)$$

Where, B_{11}, B_{12}, and B_{44} are given as a function of pressure P as follows: $B_{11} = (C_{11} - P)$, $B_{12} = (C_{12} + P)$, and $B_{44} = (C_{44} - P)$ [15]. So with consequence, under hydrostatic compression, the generalized mechanical stability criteria must be applied, and the expressions of the Eq. (1), becomes [11, 16-18]:

$$K = (C_{11} + 2C_{12} + P)/3 > 0,\ G = (C_{44} - P) > 0 \text{, and } G' = (C_{11} - C_{12} - 2P)/2 > 0 \quad (2)$$

In analogy with the zero-stress criteria, the stability criteria of Eq. (2) are referred as spinodal, shear and Born criteria, respectively [11]. Using the elastic constants obtained by Zahidur Rahaman et al. [1], the values of the Cauchy pressure $C_p = C_{12} - C_{44} - 2P$ and the generalized mechanical stability criteria K_1, K_2, and K_3 were summarized in Table 1.

Table 1: Cauchy Pressure and the Generalized Mechanical Stability Criteria of Cubic Na_2He Compound. * C_{ij} Are from Ref [1]

p (GPa)	C_{11} (GPa) [1]	C_{12} (GPa) [1]	C_{44} (GPa) [1]	C_p(GPa)	K(GPa)	G(GPa)	G' (GPa)
100	407.05	187.55	36.54	- 48.99	294.05	-63.46	9.75
200	729.83	409.82	100.58	- 90.76	583.16	-99.42	-39.99
300	1018.2	628.55	170.20	- 141.65	858.43	-129.80	-105.17
400	1299.87	854.93	243.62	- 188.69	1136.58	-156.38	-177.53
500	1575.16	1081.55	321.77	- 240.22	1412.75	-178.23	-253.20

The evolutions of the Cauchy pressure C_p and the generalized elastic stability criteria under compression in the pressure ranging from 100 to 500 GPa of Na_2He compound were presented in Figure1 (curves (a) and (b), respectively).

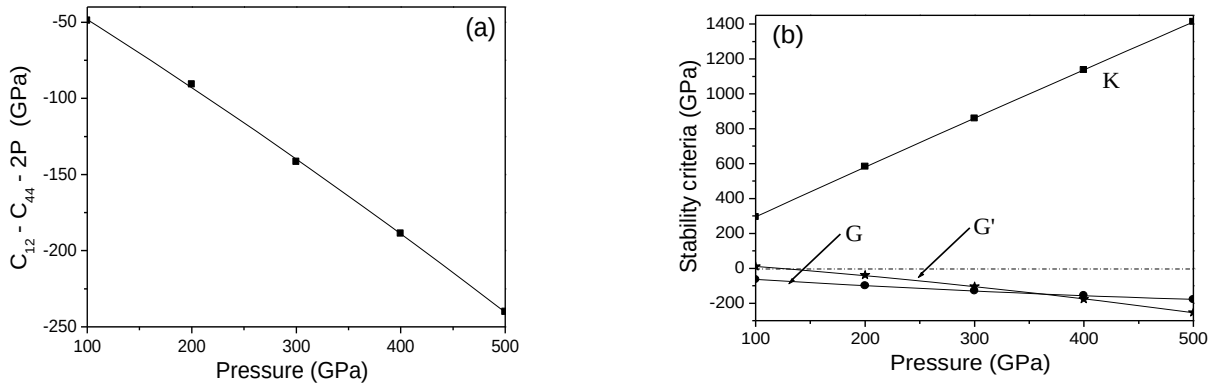

Fig. 1: (A) Cauchy Pressure C_p Versus Pressure for Na_2He Compound, (B) Generalized Stability Criteria Versus Pressure for Na_2He Compound.

The Debye temperature θ_D is an essential parameter in solid state physic [19-23]. For cubic crystals, the Debye temperature θ_D could be calculated using the following expression: $\theta_D = C_c s^{-1/6} (a G_c / M)^{1/2}$, while $G_c = \left[C_{44} \left[C_{44} (C_{11} - C_{12})/2 \right]^{1/2} (C_{11} - C_{12} + C_{44})/3 \right]^{1/3}$ [24-26], where, $C_c = (26.05 \pm 0.81)$ K (m kg $N^{-1})^{1/2}$ (the numerical value 26.05 ± 0.81 K (m kg $N^{-1})^{1/2}$ is valuable only for with cubic crystals), s is the number of atoms in the unit cell, a is the lattice parameter expressed in m, and M is the atomic weight (arithmetical average of the masses of the species), respectively [24-26].

Replacing the calculated elastic constants C_{ij} (p) and the lattice parameter a (p) reported in Ref [1] into the previous formula, the obtained values of θ_D for Na_2He compound are reported in table 2 and presented in Fig. 2, along the theoretical data of the Ref [1]. At pressure of 300 GPa, the value (1080.7 K) of θ_D obtained here is slightly lower than the value (1129.59 K) obtained by Zahidur Rahaman et al. [1] using the Debye approach, the deviation being ~ 4.33%.

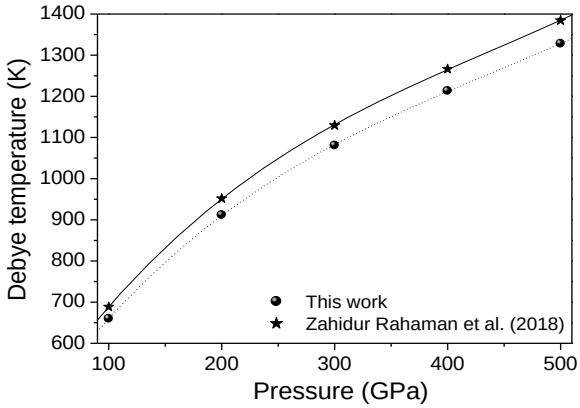

Fig. 2: Debye Temperature θ_D Versus Pressure for Na_2He Compound, Along the Theoretical Data of Zahidur Rahaman et al. [1].

Table 2: Debye Temperature θ_D of Na_2He Compound Versus Pressure

p (GPa)	100	200	300	400	500
θ_D (K)	659.9	911.6	1080.7	1213.2	1328.1

It is inferred from Fig. 2 that the Debye temperature θ_D of Na_2He compound increases non-linearly with increasing in pressure from 100 to 500 GPa. We note that a similar behavior was observed in comparison to data obtained for Cu_3N compound up to 30 GPa [3], for cubic zincblende boron nitride [12], for BeSe compound up to 50 GPa [20], for CaTe semiconducting material up to 27.8 GPa [25], for calcium oxide (CaO) compound [26, 27], for alkaline earth CaX (X = S, Se, Te) semiconducting materials [28], for both α-PbO_2 and β-PbO_2 materials [29], for cubic zincblende thallium-phosphide (TlP) up to 12 GPa [30], and for Ni_3Mo intermetallic compound up to 30 GPa [31]. The best fit of our data on θ_D (expressed in K) versus pressure p (expressed in GPa) for Na_2He compound is given as follows: $\theta_D = 301.1 + 4.25\ p - 0.007\ p^2 + 0.54 \times 10^{-5} p^3$.

3. Conclusion

Using the elastic constants reported by Zahidur Rahaman et al. in Chinese Journal of Physics, 56 (2018) 231-237, we studied the Cauchy violation and the generalized mechanical stability criterions of cubic Na_2He compound under high hydrostatic compression for pressures ranging from 100 to 500 GPa. We found that all values of the Cauchy pressure C_p are negative, which signifies that the cubic Na_2He compound from theoretical point behaves as brittle manner, and Na_2He compound becomes more brittle and stiffer with increasing pressure from 100 to 500 GPa. In addition all values of the generalized elastic stability criteria G are negative, which signifies that the cubic Na_2He compound from theoretical point is not mechanically stable in the pressure ranging from 100 to 500 GPa. Due to the lack of both experimental and theoretical data regarding the generalized mechanical stability criterions for cubic Na_2He compound under high hydrostatic compression, our results are predictions and still await experimental or other theoretical confirmation. Using Siethoff's approach, the Debye temperature θ_D of Na_2He compound increases non-linearly with increasing in pressure from100 to 500 GPa.

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