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Comparative Theoretical Study for (Ni) Phonon Frequency Spectrum Under High Pressure Using Different EOSs

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Abstract – **In the present work evaluation of the effects of high pressure on phonon frequency spectrum for nickel has been performed by using different equations of state (EOSs) through evaluating lattice vibrations frequencies shift and variations of mode density under high pressure by using Grüneisen approximation. Results obtained for variation of compressed volume $\left(\frac{V_p}{V_0}\right)$ with pressure, in the present work, by using Birch-Murnaghan EOS, Modified Lennard-Jones EOS, Vinet EOS (B-M, mGL-J, Vinet) EOSs reveal more agreement, with experimental data, than with theoretical results given in literature. Variation of Grüneisen parameter (γ) under high pressure has been considered in our calculations. Comparison of Ni phonon frequency spectrum under high pressure with considering and ignoringγ variation has been given too.**

Keywords – **Nickel, Phonon Frequency Spectrum, EOSs, Grüneisen Approximation.**

I. Introduction

Today, nickel–containing materials are used in building, water supply systems, food preparations, energy industry, chemical industry, transport industry, electronic components, medical equipments.

Nickel has a unique combination of properties (high melting point, 1453℃, adherent oxide flims, resists alkalis, ductile, alloys readily-solute and solvent, magnetic at room temperature, catalytic). The addition of nickel to copper improves its strength and durability also the resistance to corrosion, erosion and cavitations in all natural water including seawater and brackish, treated or polluted waters. The alloys also show excellent resistance to stress corrosion cracking and befouling gives a material ideal for application in marine chemical environments for ship and boat hulls, desalination plants, heats exchange equipment, seawater and hydraulic pipeline, oil rigs and platforms, fish farming cages, seawater intake screens, etc.

Addition of Ni to –Iron and manganese give standard alloys to which the material may be ordered in wrought and cost forms (Bradly, 2011). Nickel- cadmium batteries can be discharged and recharged more times than lead-acid batteries before battery cell failure occurs. The study is based on the equations of state (EOS) at high pressure is of fundamental interest because they permit interpolation and extrapolation into the regions in which the experimental data are not available adequately. (Al-saqa and Al-sheikh, 2013). The EOS is a relations to analyze the thermo physical properties of different classes of solids. It provides useful information about the relationship between pressure (P), volume (V) and temperature (T) that helps to understand the behavior of materials under the effect of high pressure and high temperature.

The aim of present work is to combine Grüneisen approximation with different EOSs in order to evaluate the effect of high pressure on phonon frequency spectrum of nickel (Ni) and compare the results obtained by these different EOSs in this work, with each other.

II. Theoretical Details

There are three different EOSs usedin this work which are**:**

The Modified Lennard-Jones EOS which is based on the generalized Lennard- Jones potentials is (jiuxun, 2005):

$$P_{ML-J} = \frac{B_o}{n}\left(\frac{V_o}{V}\right)^n\left[\left(\frac{V_o}{V}\right)^n - 1\right] \quad (1)$$

Where n $= \frac{1}{3}B'_{oT}$

B_{oT} is the bulk modulus at atmosphere.

B'_{oT}isthe first-order pressure derivative of bulk modulus at atomsphere. V_o is the volume at atmosphere. V_P is the volume at pressure P.

Birch-Murnaghan EOS which is based on finite strain theory is (Birch, 1947):

$$P_{BM} = \frac{3}{2}B_{oT}\left[\eta^{-7/3} - \eta^{-5/3}\right]\left\{1 - \left(\frac{3}{4}\right)(4 - B'_{oT})\left[\eta^{-2/3} - 1\right]\right\} \quad (2)$$

here $\eta = \frac{V_p}{V_0}$

$\eta =$ **compressed volume** $\left(\frac{V_p}{V_0}\right)$

The Vinet EOS which based on interatomic potential is (Vinet*et al.*,1987)**.**The long use and wide application of this EOS has engenderd for it a certain authority in the literature. Nevertheless, this EOS rests on the assumption of Eulerian strain

$$\in(\eta) = \frac{1}{2}(1 - \eta^{-2/3}) \quad (3)$$

III. Solids Under High Pressure

When a crystal is subjected to high pressure the following effects may occur (Sheerwood, 1972):

1) Strain may develop in the crystal which may change the symmetry of the crystal and/or cause mixing between modes and both of these effects may cause inactive modes to become active.

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2) Frequency shifts nearly always occur to high frequency due to change in volume.
3) Changes may occur in intensities of bands due to the pressure induced dipole moment and polarizability changes.
4) Strain may disorder the crystal and, if this happened, the translations symmetry of the crystal vanished and K ≠ 0 could become active.
5) High pressure have been found useful in speeding the growth of single crystals.

IV. Phonon Frequency Spectrum Under High Pressure- Grüneisen Approximation

Each change in the specific volume $V_0$of a crystal excites a change in the equilibrium positions of the particles and consequently also a change in the frequency spectrum. Even if we confine ourselves to isotropic change in volume frequencies of the vibrations will change as a functions of the changes of at least two elastic constants, each of which will generally have a different dependence on the specific volume. Thus it is obvious that a change in specific volume of the crystal is reflected in a change of its frequency spectrum in a very complex manner. However If, we consider all the difficulties in calculating the frequency spectrum of a crystal, it is unthinkable to perform further calculations for different specific volumes. To show how these difficulties can be overcome at least approximately. A suitable approximations of the changes in frequencies due to changes in the specific volume of a crystal is the Grüneisen approximations from which the following expression is obtained for the connection between frequencies(ν_0) and (ν_P') of corresponding vibrations at specific volume V_0 and V_P (Dlouha J.; (1964)

$$\nu_P = \nu_0 \left(\frac{V_P'}{V_o}\right)^{-\gamma} \quad (4)$$

Where γ is the so –called **Grüneisen parameter.**

While the relation between mode density g(V_o,V_o) at atmospheric and g(V_P, V_P) at pressure P, is given as

$$g(V_P,V_P) = \left(\frac{V_P}{V_0}\right)^{\gamma} g(v_{o,V_o}) \quad (5)$$

V. The Grüneisen Parameter

Grüneisen parameter is very important for the thermal equation of state of materials at high pressures, as it treats thermal effects at high pressures It is dimensionless and, for a wide range of solids, has an approximately constant value.

The Grüneisen parameter has both a microscopic and macroscopic definition (Grüneisen, 1912), yet the physical connection between them has been the source of much confusion.

The macroscopic definition is in terms of familiar thermodynamic properties, which in principle may be evaluated experimentally

$$\gamma_{th} = \frac{\alpha_v B_T}{C_{v,}\rho} \quad (6)$$

Where :
$\boldsymbol{\alpha_V}$ is the volume coefficient of thermal expansion.
$\mathbf{C_V}$ is specific heat at constant volume.
$\boldsymbol{\rho}$ is the density.
$\mathbf{B_T}$ is the isothermal bulk modulus.

The microscopic definition arises from a considerations of the motion of atoms in a solid and their vibrational frequencies. It was in fact original definition proposed by (Grüneisen, 1912), who postulated that the vibrational frequenciesof the individual atoms in solid, varied with the volume,V ,via the relation

$$\gamma_{i(q)} = -\frac{\partial \ln \omega_{(q)}}{\partial \ln V} \quad (7)$$

Where $\boldsymbol{\omega(q)_i}$ is the frequency of with mode of vibration, which itself is a function of wave vector ($\mathbf{q_i}$) in the first Brillion zone and **V** is volume. (Boehler and Ramakrshnan, 1980) reported a relation for pressure dependence of Grüneisen parameter as

$$\gamma_P = \gamma_0 \left(\frac{V_P}{V_0}\right)^q \quad (8)$$

Where

$\boldsymbol{\gamma_{o,}\gamma_p}$ Grüneisen parameter at atmospheric and under high pressure respectively, **q-** second Grüneisen parameter which has been considers of an equal unity or a constant value.

V. Calculations and Results

Pressure Dependence of $\left(\frac{V_P}{V_0}\right)$

Calculation of (V_p/V_0) variations with the pressure, for Ni, has been achieved by using (B-M, mGL-J and Vinet) EOSs with values of (**B_{oT}= 1888.51 kbar ,B'_{oT}= 4.624 kbar**), for nickel (Kuchhal and Dass, 2003).

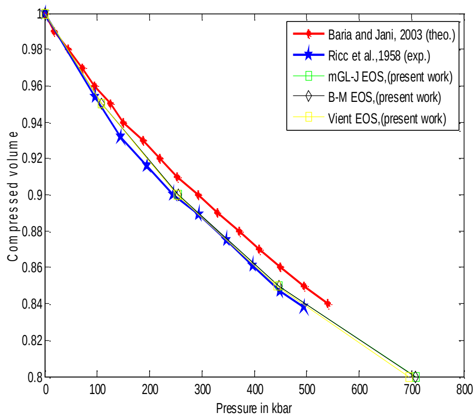

Fig. 1. shows results obtained in the present work for Ni, by using (B-M, mGL-J, Vinet) EOSsin comparison with the theoretical results of (Barie and Jaine, 2003) and experimental data of (Ricc*et. al.*, 1958)

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VI. Evaluations of Phonon Frequency Spectrum for Nickel Under High Pressure

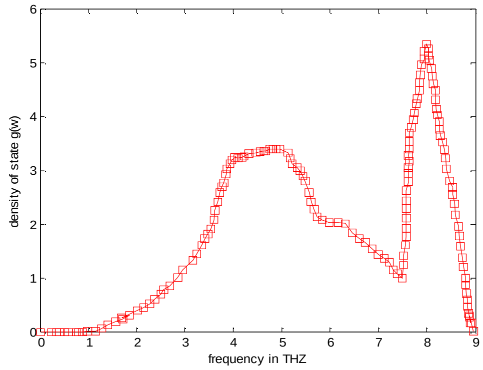

Fig. 2. Shows experimental phonon frequency spectrum for Ni at ambient conditions(Miller and house, 1971)

On calibrating $g(\nu_i)$ for the corresponding (ν_i) values from Fig.2, and using $\frac{V_P}{V_o}$ values of Fig.1 for (mGL-J, B-M, Vinet) EOSs respectively in equation (5)And (6) with the corresponding values of pressuee from equations (1,2,and 4) respectively, Figs.3 shows variation of phonon frequency spectrum, for nickel, under high pressure, by using different equations of state. It is obvious from **Fig.3** that frequencies shift to high values as pressure increases in accordance with the theoretical predictions given in solid under high pressure article of this paper.

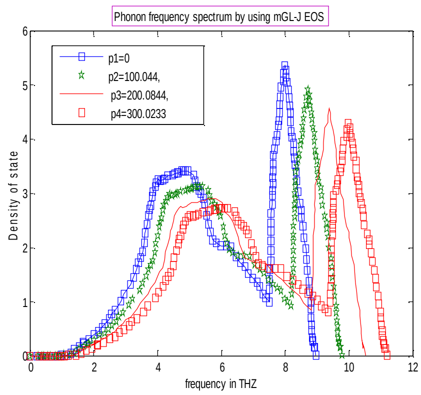

Fig. (3a)

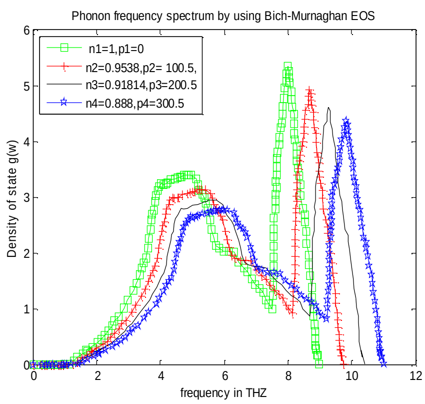

Fig. (3b)

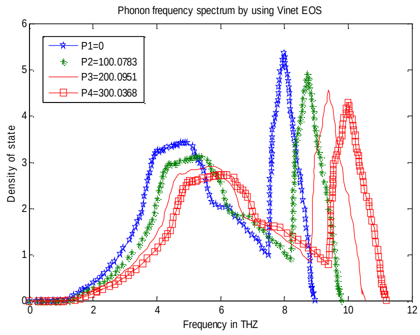

Fig. (3c)

Fig. 3. (a,b,c) Variation of phonon frequency, for Ni, with high pressure by using (mGL-J, B-M, Vinet) EOSs, withGrüneisen parameter is pressure independent

VII. Variations – of Grüneisen Parameter (γ) Under High Pressure

Fig. 4 shows variation of γ parameter, for Ni, under high pressure by using different EOSs, this variation has been calculated by substituting $\frac{V_p}{Vo}$ values of Fig.1 into eq.8

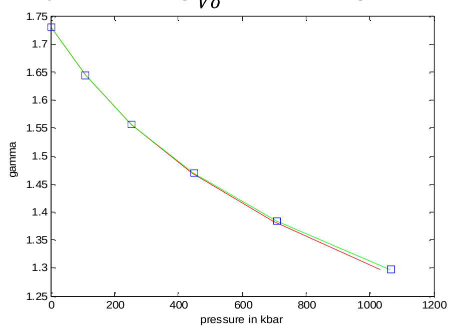

Fig. 4. Variation of parameter of γ parameter for Ni under high pressure

This variation may be reflected into variation of phonon frequency spectrum under high pressure. Fig.5 shows phonon frequency spectrum, for nickel, at 100 GPa evaluated by considering effect of γ variation with the pressure one time and neglecting, this variation another time.

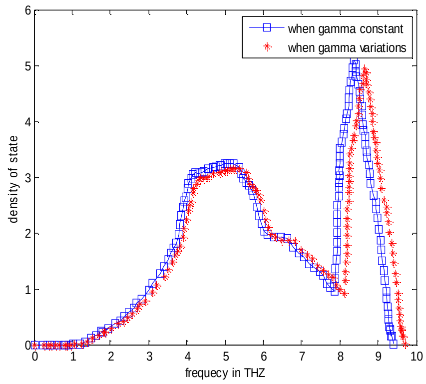

Fig. 5. Phonon frequency spectrum, for nickel, at (100 kbar) evaluated by considering effect of γ variation with the pressure one time and neglecting, this variation another time

VIII. Conclusion

The phonon frequency of Ni increases with the increases in pressure.as shown in Fig.3. and the phonon density of state spread up to high pressure domain as pressure increases. **The compression** curves which results from EOSs used in this work as shown in Fig.1 are coincide with experimental data (Ricc*et al*.,1958) and theoretical data (Baria and Jani, 2003) at relatively low pressure. But when pressure increase (p>100 kbar) the **vinet** EOS is most agreement with experimental data (Ricc*et al.*,1958) and show clear divergence from theoretical data (Baria and Jani, 2003). the reason for this behavior is that each equation of EOSs used in this work is derived from different theoretical bases. And in the same time both of (mGL-J EOS) and (B-M EOS) show good agreement with each other. By increasing pressure (p> 250 kbar) its obvious that all equations became more coincide with experimental data (Ricc*et al*.,1958).

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