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Evaluation of High Pressure Effect of Phonon Frequency Spectrum for Gold by Using Different Equations of State (EOS)

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Abstract:

Theoretical study was made on the high pressure dependence of lattice frequencies and distribution function for Gold through analyzing phonon frequency spectrum (pfs) by using Grüneisen approximation in two equation of state Birch- Murnghan (B-M EOS) and modify Lenard –Jones (mL –J EOS).

The change in specific volume of crystal induce a change in the frequencies of lattice vibrations in a very complex manner. Present work shows how this complexity can be overcome by using Grüneisen approximation.

Comparison of obtained results, in the present work, with literature emphasize the importance of considering pressure dependence of Grüneisen parameter in evaluating gold (pfs) under high pressure. This may be attributed by the effect of filled 4f and 5d orbitals.

Keywords: lattice vibration, distribution function, pfs, Grüneisen approximation, specific volume, lattice vibration, EOS.

حساب تأثير الضغط العالي على طيف التردد الفونوني للذهب باستخدام معادلات حالة مختلفة

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مديرية تربية محافظة نينوى

الملخص :

تم في هذا البحث إجراء دراسة نظرية لتغير ترددات اهتزاز شبيكة الذهب وتغير كثافة الأنماط مع الضغط من خلال تحليل طيف التردد الفونوني للذهب. باستخدام تقريب كرونشين في معادلات حالة مختلفة (برخ- مرنكهان ولينارد- جونس المحورة).

إن تغير ترددات اهتزاز الشبيكة تأتي من خلال التغير في الحجم البلوري من خلال إجراءات معقدة. لذا يعرض هذا البحث إمكانية التغلب على هذه الصعوبات من خلال استخدام تقريب كرونيشين ومعادلة الحالة لبرخ- مرنكهان ومعادلة الحالة لينارد- جونس المحورة.

تظهر النتائج التي تم الحصول عليها في هذا البحث، مقارنة مع نتائج الأبحاث العلمية ضرورة احتساب تغير معامل كرونشين مع الضغط عند احتساب تأثير الضغط العالي على طيف التردد الفونوني للذهب، ولعل ذلك يعزى لتأثير المدارات الالكترونية 4f, 5d.

الكلمات الدالة: ترددات الشبيكة، دالة التوزيع، طيف التردد االفونوني، تقريب كرونيشين، الحجم النوعي، اهتزازات الشبيكة، معادلات الحالة.

INRODUCTION:

One of the interesting phenomena that may take place under applied high pressure is a sudden change in the arrangement of the atom. The Gibbs free energies of the different possible arrangement of atom vary under compression, and in some stage it becomes favorable for the material to change the type of atomic arrangement (Hänstrom, 2000).

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The equation of state (EOS) of system describes the relation among thermodynamic variables such as pressure, temperature and volume. It provides numerous pieces of information relating to the nonlinear compression of a material at high pressure and has been widely applied in engineering and other scientific research. Recently, Rapid advances in computation capabilities and accurate high pressure experimental techniques have given a strong improvement theoretical work (Abdullah and AL-Sheikh, 2008).

For practical applications, an ideal EOS of state should have the following four merits. (Jiuxun, 2005)

(i)-The energy should be analytic U=U (v).

(ii)-The EOS should be both pressure analytic P=P(v) and volume V=V (p).

(iii)-It should satisfy the following spinodal condition

$B \alpha (P-P_{sp})^{1/2}$ with $(P-P_{sp})$

(iv)-It should have high energy precision with simple form and a small number of parameters, and allow one to predict the compression curve for materials at high pressure using only the parameters determined from experimental data at low pressure.

Reported results of Synchrotron X-ray diffraction experiments on gold samples contained within a helium or methanol pressure medium in a diamond anvil cell. The quasi-hydrostatic ruby fluorescence scale (Takemura, 2001), was used for pressure determination over the range(0-75) GPa at 300 K in the helium experiment (Mao et al, 1986). Helium is well known to provide the most nearly hydrostatic pressure environment at pressures above 15 GPa (Mao, et al, 1988). That the stress distribution was in fact very close to hydrostatic was verified using several different criteria, including ruby peak widths and splitting's, X-ray diffraction peak width and lattice parameter variance from multiple diffraction lines.

The latter approach should be an especially sensitive indicator of non- hydrostatic stresses in gold because of its large elastic anisotropy (Meng, et al, 1993) and the demonstrated effects of non-hydrostatic stress on lattice parameter variance (Duffy, *et al*, 1999).

In present work, an evaluation of the effect of pressure on lattice vibration and mode density for gold has been achieved, by using B-M, mL-J EOSs and Grüneisen approximation. Present results, in comparison with literature, show the importance of considering pressure dependence of Grüneisen parameter, in evaluating effect of pressure on (pfs) for gold.

THORTICAL DATLES

Equation of State

1-Birch-Murnaghan EOS (Birch, 1947)

(Boetteger *et al.* , 2012) describe anew SESAME-type EOS, suitable for use in hydrodynamic calculations for gold. The third-order Birch-Murnaghan equation of state (Birch, 1947)

$$\mathrm{P}(V)=\frac{3}{2}B_o\left[\left(\frac{V_o}{V_\mathrm{P}}\right)^{7/3}-\left(\frac{V_o}{V_\mathrm{P}}\right)^{5/3}\right]\left\{1-\left(\frac{3}{4}\right)\left(4-B_o'\right)\left[\left(\frac{V_o}{V_\mathrm{P}}\right)^{2/3}-1\right]\right\} \quad (1)$$

This EOS based upon the assumption that the strain energy of a solid undergoing compression can be expressed as a Taylor series in the finite strain.

Where

V_o : volume at atmospheric pressure; V_p : volume at pressure P

B_o' : pressure derivative of B_o

2-Modified Lenard–Jones EOS (Jiuxun, 2005)

The modified Lenard- Jones EOS (mL- J) is

$$\mathrm{P}_{\mathrm{mLJ}}=\frac{\mathrm{B_o}}{\mathrm{n}}\left(\frac{\mathrm{V_o}}{\mathrm{V_p}}\right)^{\mathrm{n}}\left[\left(\frac{\mathrm{V_o}}{\mathrm{V_p}}\right)^{\mathrm{n}}-1\right] \quad (2)$$

Where: $n=\frac{1}{3}B_o'$; $B_o'=\frac{dB}{dP}$

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Equation (2) is just the two-parameter EOS, we proposed (mLJ EOS). It can be shown to have almost all of the merits mentioned in the introduction, and the precision is higher than those for several popular EOSs.

Grüneisen Parameter

The Grüneisen parameter (γ), is a valuable quantity in solid-state geophysics because it can be used to set limitations on the pressure and temperature dependence of the thermal properties of the mantle and core, and to constrain the adiabatic temperature gradient. It is dimension less and, for a wide range of solids, has an approximately constant value, varying only slowly with the pressure and temperature (Anderson, 1989).

The Grüneisen parameter (γ) is of considerable importance to earth scientist because it sets limitations on the thermoelastic properties of the lower mantle and core. There are several formulations of the Grüneisen parameter in frequent use which not only give different values for (γ) at ambient pressure but also predict averring dependence of (γ) as a function of compression (Vocadlo *et al.*, 2000).

The Grüneisen parameter variation with the pressure according to (Boehler, 1983).

$$\gamma_p = \gamma_o \left(\frac{V_p}{V_o} \right)^q \qquad (3)$$

Where γ_0 : Grüneisen parameter at atmosphere pressure

γ_p : Grüneisen parameter at pressure P

q : second Grüneisen parameter atmospheric pressure that equal to one unit (Boehier and Ramakrishnan,1980).

In the Mie – Grüneisen theory of thermal expansion of solids, the Grüneisen parameter (γ) is defined by (Dlouh, 1964).

$$\gamma = \frac{\alpha_V . B_T}{C_V . \rho} = \frac{\alpha . B_S}{C_P . \rho} \qquad (4)$$

Where

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α_V –Volume=me coefficient of thermal expansion; B_T – Isothermal bulk modulus
C_P, C_V– are the specific heat at constant pressure and constant volume; ρ – Density
Grüneisen approximation

The connection between the frequencies (ν) and (ν_P) of corresponding vibration at specific volumes V and V_P, using Grüneisen approximation, given by the following expression (Dlouha, 1964)

$$\upsilon_p = \upsilon \left(\frac{V_p}{V_o} \right)^{-\gamma} \tag{5}$$

Where:

ν – Frequency at atmospheric pressure

ν_P – Frequency at pressure P; V_o – volume at atmospheric pressure

V_p – volume at pressure P; γ – Grüneisen approximation

While the relation between the function $g(\omega, V_p)$ for volume v and the analogical function $g(\omega, V_p)$ for volume V_p is

$$g(\omega, V_p) = \left(\frac{V_p}{V_o} \right)^{\gamma} g\left[\omega \left(\frac{V_p}{V} \right)^{\gamma}, V_p \right] \quad .... \tag{6}$$

COMPUTATION AND RESULTS

Fig (1) shows Au phonon frequency (pfs) at atmospheric pressure, room temperature (Gulseren, 1992).

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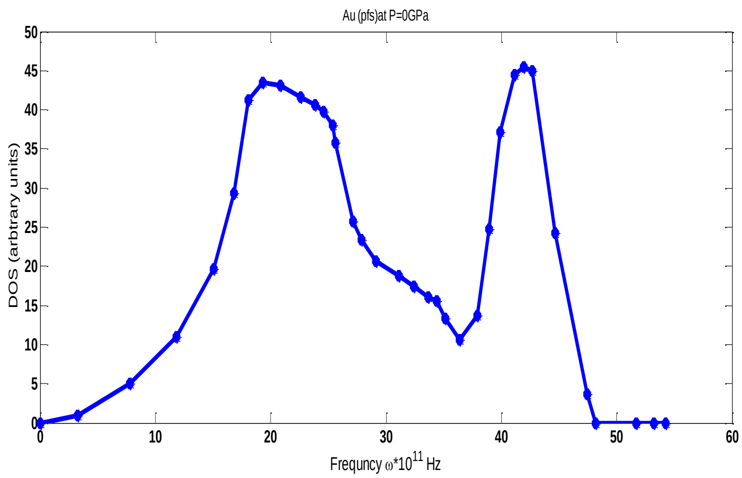

Fig (1): phonon frequency spectrum (pfs) for gold at atmospheric pressure (Gulseren, 1992).

The frequency distribution function of gold has been calculated by (Gulseren, 1992) based on the Z- neighbor model in which the inter atomic forces are restricted to interaction with the first and second neighbors, is shown in Fig(1). This has been calibrated using (matlab program) where the corresponding g (ω) value for each (ω) is tabulated in (Table-I).

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Table- I: Lattice vibrations and its corresponding mode density for Au as obtained

Sr. No.	$\omega_i \times 10^{11}\,\sec^{-1}$	$g(\omega_i)$	Sr. No.	$\omega_i \times 10^{11}\,\sec^{-1}$	$g(\omega_i)$
1	0	0	31	35.1323	13.1215
2	1.7297	0.4144	32	36.3800	10.4512
3	3.2042	0.7827	33	37.0605	11.7403
4	5.4159	2.7164	34	37.9112	13.4899
5	7.7977	4.9263	35	38.4216	19.1989
6	9.7826	7.8729	36	38.9319	24.8158
7	11.8242	10.9116	37	39.4991	31.8140
8	13.6957	15.7919	38	39.8960	37.1547
9	15.1134	19.6593	39	40.5766	41.4825
10	16.0208	24.6317	40	41.1437	44.4291
11	16.8147	29.4199	41	41.4839	45.0737
12	17.4953	35.1289	42	41.8809	45.4420
13	18.0057	41.2063	43	42.3346	45.1657
14	19.2533	43.4162	44	42.6749	44.9816
15	20.8412	43.1400	45	43.0718	40.5617
16	21.7486	42.3112	46	43.4121	36.7864
17	22.5992	41.4825	47	43.9225	32.0902
18	23.8469	40.6538	48	44.2060	28.9595
19	24.58.41	39.7330	49	44.4896	26.1971
20	25.3781	38.0755	50	44.6030	24.1713
21	25.6616	35.6813	51	45.2268	20.0276
22	26.3422	30.8932	52	45.8507	15.5157
23	27.1928	25.4604	53	46.3043	12.2007
24	27.8733	23.5267	54	46.5879	9.8987
25	28.6106	21.6851	55	46.9282	7.5046
26	29.1210	20.4880	56	47.4953	3.4530
27	31.0491	18.8306	57	47.9490	0.8748
28	32.4102	17.4494	58	48.1758	0
29	33.6578	15.884	59	51.6919	0
30	34.3951	15.5157	60	54.2439	0

from Fig. (1)

To evaluate the effect of high pressure on Au pfs. Eq(1) has been combined with eq. (4) and (5) and applied on data tabulated in Table-I, With values of B_o , $B_o^{'}$ and γ as tabulated in (Table II).

Table-II: value of B_o , $B_o^{'}$ and γ for Au.

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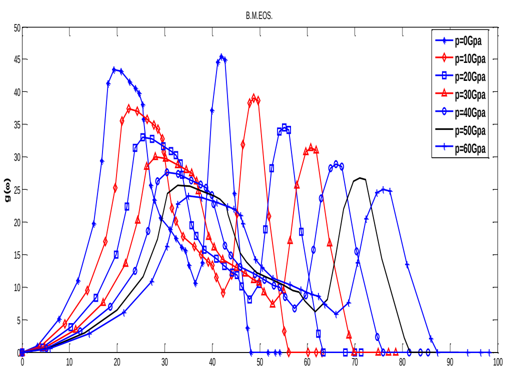
B_o GPa	$B_o^{'}$	γ	Ref.
166.6	5.5	2.5	Duffy, *et al., 1999a*

Fig. (2A) shows Au pfs evaluated at different applied pressure as calculated by using B-M EOS and Grüneisen approximation.

Similarly, on coupling eq.2 with eqs (5, 6) and data of tables I, II.

Fib. (2B) shows variation of Au pfs with pressure as evaluated by using mL –J EOS and Grüneisen approximation.

–A– **–B–**



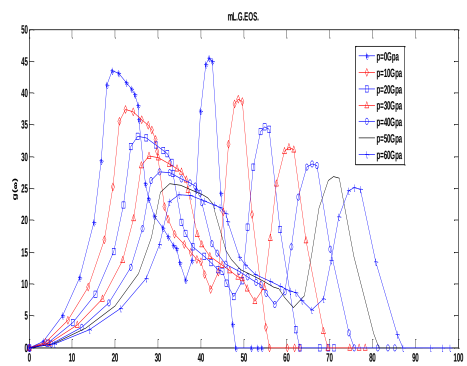


Fig (2): variation of Au (pfs) with the pressure by using different EOSs

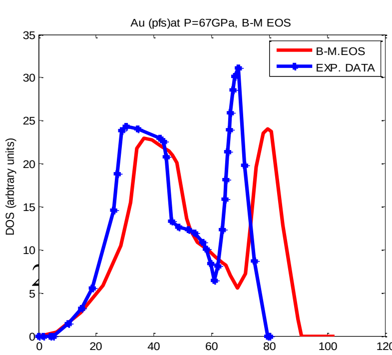
A- B-M EOS B- mL-J EOS

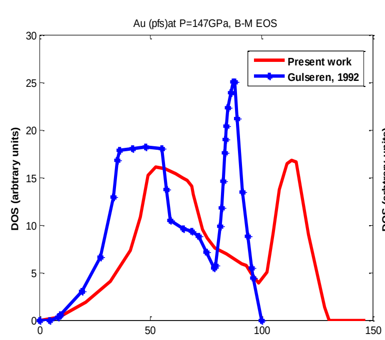
Using first principle calculations (Gulseren, 1992) calculated Au phonon frequency spectrum at specified pressure.

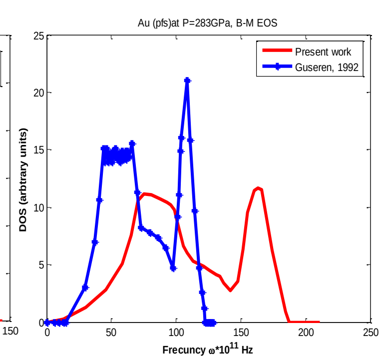
Fig. (3A, B, C) shows a comparison between present results given in Fig. (2A) and (Gulseren, 1992) results at specified pressure values.

While Fig. (4A, B, C) shows a compassion between specified present results given in Fig. (2B) with (Gulseren, 1992) results.

A B







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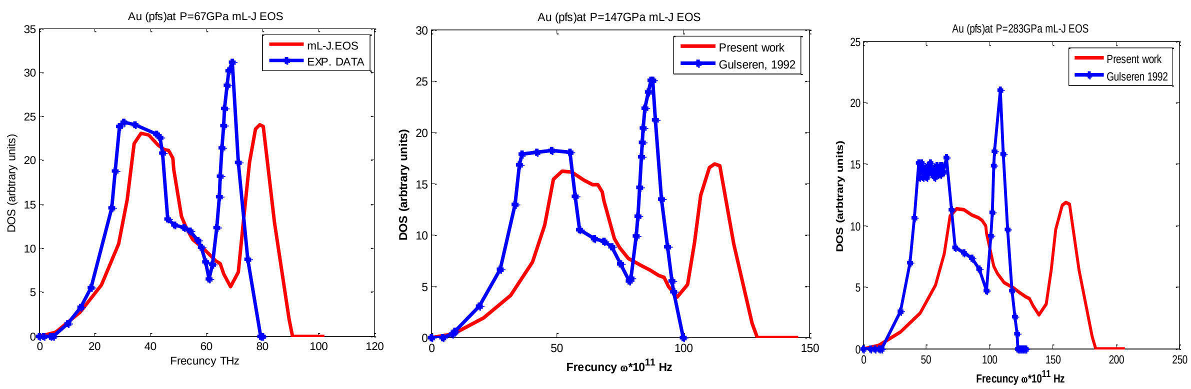
C

A B
C

Fig(3): comparison, between present work and literatures, of (pfs) at room temperature for Au under (A) 67GPa, (B) 147GPa, (C) 283GPa using B-MEOS



A . B C

Fig (4): comparison, between present work and literatures, of (pfs) at room temperature for Au under (A) 67GPa, (B) 147GPa, (C) 283GPa using mL-J EOS

Variation of γ –parameter with high pressure:

To improve present results given in Fig.(3A, B, C) and Fig.(4A, B, C) it is reasonable to consider, in calculations, pressure dependence of γ – parameter as given in eq(4).

Combing eq.(4) with eq.(5) and eq.(6), and evaluating pressure from eq.(2) one time and from eq.(3) another time, Figs.(5A, B, C)and Figs.(6A, B, C)show a comparison between (Gulseren, 1992) results and present results, using γ approximation and considering γ parameter depends, for Au phonon frequency spectrum under specified pressure.

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A B C

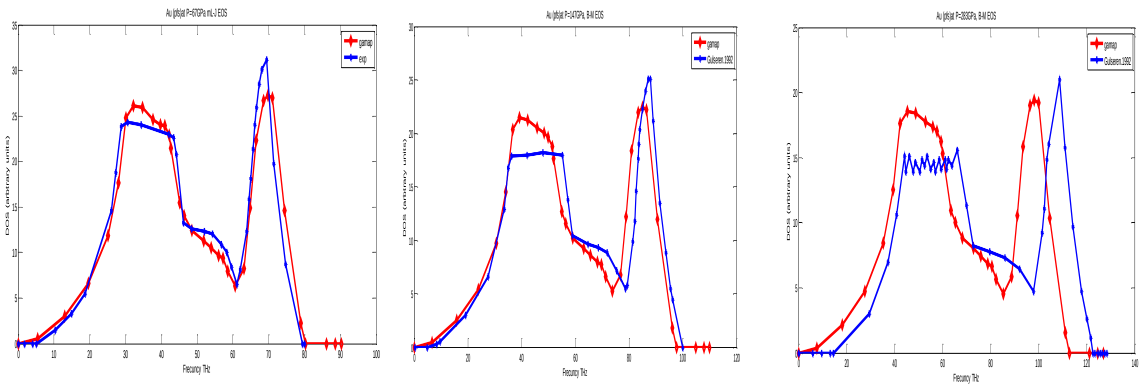
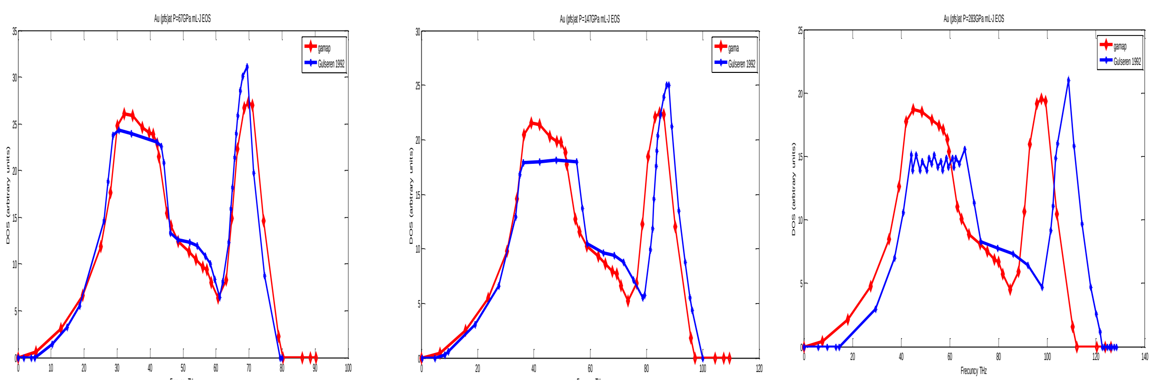


Fig (5): variation of (pfs) for Au with applied pressure (A) 67GPa, (B)147GPa, (C)283GPa evaluated in present work with that reported in literatures using (B-MEOS)

A B C



Fig(6) variation of (pfs) for Au with applied pressure (A) 67GPa, (B)147GPa, (C)283GPa evaluated in present work with that reported in literatures using (mL-JEOS)

Discussion:

This work shows, that Au lattice frequencies shift to higher frequencies under high pressure, while mode density spread to include new modes, Fig.2, This may be attributed as the effect of pressure cause inactive modes to become active modes.

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Present results, Fig (3 and 4), reveals that combining EOS. With Grüneisen, approximation is a useful approach for evaluating variation of phonon frequency spectrum under high pressure.

Figs (5 and 6) shows the importance of considering γ- parameter variation under high pressure, to improve the agreement between present work and results obtained by (Gulseren, 1992) which used first principle calculation. This may be attributed by the effect of filled 4f and 5d orbitals.

Furthermore, Figs. 6 shows better agreement with literatures by using mL-JEOS in Figs. (5). this may be interpreted as mL-JEOS derived on basis of interatomic potential while B-MEOS derived on basis of mechanical strain.

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