Pressure Dependence of the Recoilless Fraction For 14.4keV Transition of Fe^{57} in Copper

Adnan M. Al-Sheikh
Department of Physics
College of Science
Mosul University

Mumtaz M. Saleh
Department of Physics
College of Education
Mosul University

Yahya N. Al-Jamal
Department of Physics
College of Science
Mosul University

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ABSTRACT

The effect of pressure on the recoilless fraction (f) for the gamma-ray transition 14.4keV emitted by Fe^{57} as an impurity in copper, using phonon frequency spectrum (pfs) analysis and Debye model calculations, has been studied. The variation in Grüneisen parameter (γ) and Debye temperature (θ_D) with pressure are included as an improvement over previous studies. The theoretical results which have been obtained are in good agreement with the experimental values.

اعتماد الجزء الخالي من الارتداد، للإشعاع 14.4keV المنبعث من الحديد Fe^{57} في النحاس على الضغط

الملخص

تم في هذا البحث دراسة تأثير الضغط على الجزء الخالي من الارتداد (f) للانتقال 14.4keV للحديد Fe^{57} كشوائب في النحاس باستخدام تحليل الطيف الفونوني للنحاس بالإضافة إلى استخدام نموذج ديباي. ان تغيرات معامل Grüneisen وتغيرات درجة حرارة ديباي مع الضغط، قد تم اخذها بنظر الاعتبار وهذا يعد تطويراً للدراسات السابقة مما جعل نتائجنا اكثر توافقاً مع النتائج التجريبية.

INTRODUCTION

For optical transitions the recoil of an atom due to emission of radiation does not destroy resonance with another atom since typically the recoil energy (E_R) of the atom is less than the natural line width of the radiation (Γ). This is not true for nuclear transitions. When $E_R >> \Gamma$, as is true for nuclear transitions, no resonance is possible. Thus for Fe^{57} ($t_{1/2} = 10^{-7}$ sec; $\Gamma = 4.5 \times 10^{-9}$ eV) the recoil of energy of the atom upon emission of the 14.4 keV gamma-ray is 1.9×10^{-3} eV, thus $E_R >> \Gamma$, while for an optical transition of 5000 °A and $t_{1/2} = 10^{-8}$ sec ($\Gamma = 4.5\times10^{-8}$) $E_R \cong 6\times10^{-11}$ eV and $E_R << \Gamma$.

The Mössbauer effect arises from the experimental fact that for an atom embedded in a solid there exists a finite probability that a nuclear transition will occur with out recoil. This recoilless radiation makes it possible to achieve resonance with the atom similarly placed in another solid. The recoilless fraction arises from those nuclear which the lattice is in the same quantum state after the transition as before the transition, i. e., no phonon is emitted. Thus the f-value for a certain initial lattice state $\{n_s\}$ is (Moyzis, 1968).

$$f_{\{n_s\}} = \left| < \{n_s\}_g \left| H_i \right| \{n_s\}_e > \right|^2 \qquad \text{.................. (1)}$$

where,

$\}n_s\} = n_s$ phonon in sth lattice mode.

g and e – subscripts denote the ground and excited states of the lattice.

H_i – Non-relativistic interaction Hamiltonian responsible for the decay.

The effect of pressure on f-fraction in solids has been studied by many workers (Dlouha, 1964 ; Mahesh, 1975 ; Sharma and Al-Sheikh, 1979 ; Pottel et al., 1989 and Al-Khero, 2000). The pressure dependence of f-fraction for 14.4 keV gamma-ray transition of Fe^{57} as an impurity in cooper host, at room temperature has been studied by (Moyzis et al., 1968).

In the present work, this dependence incorporated using the experimental pfs of Cu (Sina, 1966), Fig.1. The relative recoilless fraction f_p / f_o were calculated including the Grüneisen parameter change with pressure. Debye model calculations using Debye temperature (θ_D) as it varies with pressure (θ_p) and Grüneisen parameter were also made. Including the variation of Grüneisen parameter and θ_D with pressure is an improvement for the effects of pressure on f-fraction studies.

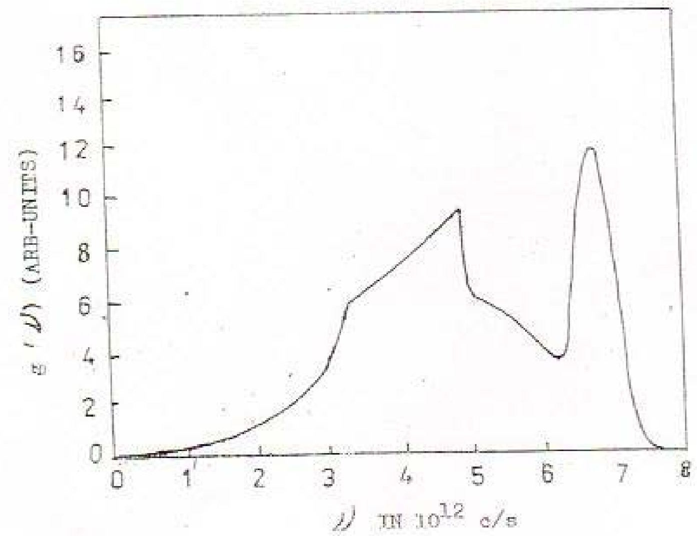

Fig. 1: Phonon frequency spectrum for Cu.

THEORY

1. Recoilless fraction:

At room temperature the recoilless fraction (f_o) for a simple cubic lattice in harmonic approximation is given as (Wertheim, 1964).

$$f_o = \exp\left[-\frac{E_R}{N\hbar}\int_o^{\omega_{max}}\frac{g(\omega)}{\omega}\coth\left(\frac{\hbar\omega}{2K_BT}\right)d\omega\right] \qquad \text{.................. (2)}$$

with

$$N = \int_o^{\omega_{max}}\frac{g(\omega)}{\omega}d\omega$$

E_R – is the recoil energy of free nucleus.

The integral in equation (2) are evaluated by numerical integration over the pfs. The alternative form of equation (2) which are more suitable for numerical evaluation are obtained by adopting it for specific pfs, and using $\omega = 2\pi\nu$, to a good approximation are expressed as summation over all such pfs. These are:

$$f_o = \exp\left[-\frac{A}{\Phi}\sum_i\frac{g(\nu_i)}{\nu_i}\coth\left(\frac{a\nu_i}{T}\right)\right] \qquad \text{..................... (3)}$$

with

$$\Phi = \exp\sum_{i=1}^{n} g(\nu_i) \ ,$$

$$A = \frac{E_R}{2\pi\hbar} \quad , \quad a = \frac{\pi\hbar}{K_B}$$

The dependence of f-fraction on pressure is obtained through the shift in the phonon frequency (ν) due to change in the specific volume of solid when pressure is applied. In Grüneisen approximation this change is given as (Dlouha, 1964).

$$\nu_{ip} = \nu_i\left(\frac{V_p}{V_o}\right)^{-\gamma} \qquad \text{................. (4)}$$

where γ is the Grüneisen parameter. For Cu, γ=1.96 (Condon and Obishw,1967) and:

$$\frac{V_p}{V_o} = \left(1+\frac{P}{234}\right)^{-0.176} \qquad \text{................ (5)}$$

where p is the pressure in kbar (Moyzis, 1968).

Combining equations (3) and (5) one obtain the f-fraction f_p at pressure p.

$$f_p = \exp\left[-\frac{A}{\Phi}\sum_i\frac{g(\nu_i)}{\nu_{ip}}\coth\left(\frac{a\nu_{ip}}{T}\right)\right] \qquad \text{.............. (6)}$$

2. Grüneisen Parameter:

The complicated change of phonon spectrum under pressure was not yet studied either theoretically or experimentally. An important thermodynamics parameter of solids, which can change with pressure is the Grüneisen parameter, (Barron et al, 1982;

Dorogokuptes, 2000), which related to coefficient of volume expansion (α_p) and the compressibility (K_t) as (Antonov, et al.,1990;Landsberg, 1990).

$$\gamma = \frac{\alpha V}{K_t C_v} \qquad \text{.............. (7)}$$

where

$$\alpha_p = \frac{1}{V}\left(\frac{\partial V}{\partial t}\right)_p \ , \ K_t = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_t \qquad \text{.............. (8)}$$

If the first law of thermodynamics is involved :

$$\gamma = \frac{V}{\left(\frac{\partial u}{\partial p}\right)_v} \qquad \text{............. (9)}$$

Many solids have values of γ lying between values 1.0 and 3.0 at moderate temperatures.Examples are NaCl (1.36), Cu (1.96) and Na (1.25). Integration of equation (8) suggest an equation of state of such solids given by:

$$u = \frac{1}{\gamma} PV + F(v) \qquad \text{......... (10)}$$

where F(v) is a constant of integration.

Conversely, we shall find that simple theories of electrons in metals lead to an equation of state PV=gu, where g is a constant of order unity. Equation (9) enables one to infer that such system have constant Grüneisen parameter γ=g. Such inference are typical of thermodynamics arguments.

Equations (5 and 7) gives the Grüneisen parameter at pressure P as (Kumari and Dass, 1986).

$$\gamma_p = \frac{\alpha_p V_p}{K_t C_v}$$

or

$$\gamma_p = \gamma_o V_p \qquad \text{............ (11)}$$

K_t = isothermal compressibility.

This suggest an expression for f-fraction of equation (6) to be :

$$f'_p = \exp\left[-\frac{A}{\Phi}\sum_i \frac{g(v_i)}{v'_{ip}} \coth\left(\frac{a v'_{ip}}{T}\right)\right] \qquad \text{............. (12)}$$

with

$$v'_{ip} = v_i \left(\frac{V_p}{V_o}\right)^{-\gamma_p} \qquad \text{.............. (13)}$$

3. Debye Temperature:

The concept of Debye temperature (θ_D) is useful in connection with many topics in solid state physics. It is characteristic of each substance, appearing in Debye's theory of specific heat and given by :

$$\theta_D = \frac{\hbar\omega_D}{K_B} \qquad \text{………….(14)}$$

where ω_D is the maximum frequency of thermal vibration of the lattice.

The pressure dependence of θ_D is of much interest in this work, as it enables to predicts the variation of f-fraction with pressure given as (Kumari and Dass, 1986).

$$\theta_p = \theta_D \left(\frac{V_p}{V}\right)^{-\gamma} \qquad \text{………….(15)}$$

where

θ_D and θ_p are Debye temperatures at atmospheric pressure and at pressure P respectively.

In Debye approximation, f-fraction expressed as (Shepard and Mullen, 2000).

$$f_o = \exp\left[-\frac{E_R}{K_B\theta_D}\left(\frac{3}{2}+\frac{\pi^2 T^2}{\theta_D^2}\right)\right], T<\theta_D \qquad \text{………..(16)}$$

hence

$$f_p = \exp\left[-\frac{E_R}{K_B\theta_p}\left(\frac{3}{2}+\frac{\pi^2 T^2}{\theta_p^2}\right)\right] \qquad \text{………..(17)}$$

Considering, the variation of Grüneisen parameter with pressure equation (7) becomes as:

$$f_p' = \exp\left[-\frac{E_R}{K_B\theta_{p\gamma}}\left(\frac{3}{2}+\frac{\pi^2 T^2}{\theta_{p\gamma}^2}\right)\right] \qquad \text{……….(18)}$$

with

$$\theta_{p\gamma} = \theta_D \left(\frac{V_p}{V}\right)^{-\gamma_p} \qquad \text{……….(19)}$$

COMPUTATION AND RESULTS

Using fps for Cu, Fig. (1) by equations (3) and (6) we have determined f_p/f_o shown in Fig. (3) as (Rfp) at different values of pressure (kbars). Considering the influence of pressure on γ, Fig.(2). Equations(2) and(12) gives f_p'/f_o which are shown in Fig. (3) as (Rfpg). The results compared in Fig.(3) are in good agreement with experimental results (ExL, ExM, ExU), which represent different runs at the same pressure, of (Moyzis, 1968).

The Debye model gives f_p/f_o values according to equations (16) and (17). While f_p'/f_o given by equations (16) and (18). The result are shown in Fig. (4) as (Rfp) and (Rfpg) respectively. The variation of Debye temperature with pressure given by equations (15) (θ_P) and (19) ($\theta_{P\gamma}$) shown in Fig. (5), with θ_D=352 at atmospheric pressure (Sheoard and Mullen, 2000).

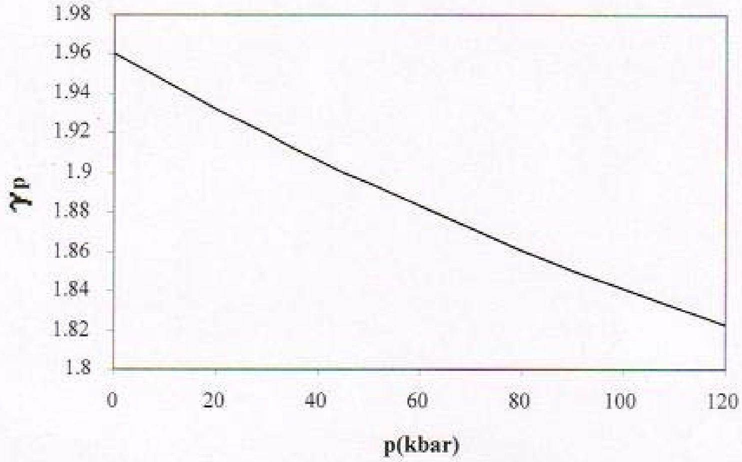

Fig. 2 : Variation of Grüneisen parameter with the pressure.

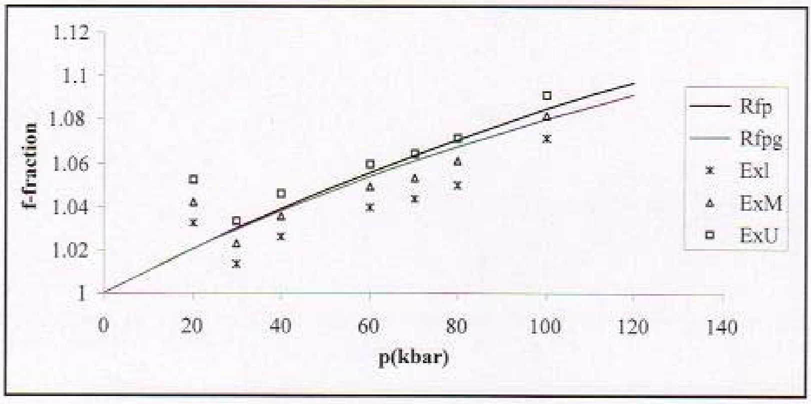

Fig. 3: Pressure dependence of f-fraction on pressure using pfs analysis.

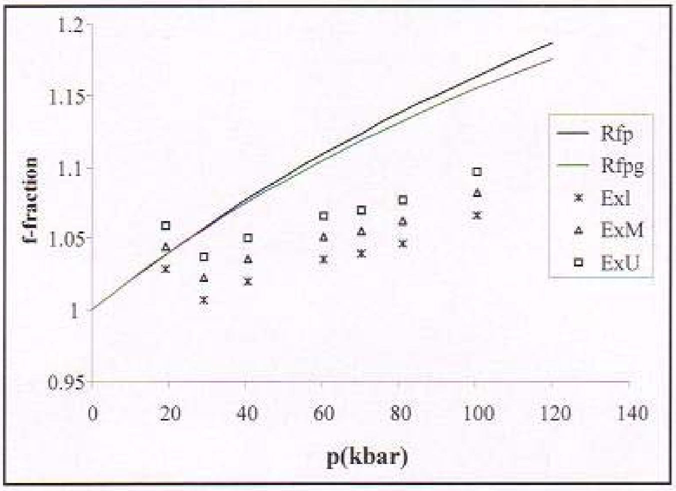

Fig. 4: Pressure dependence of f-fraction on pressure using Debye model.

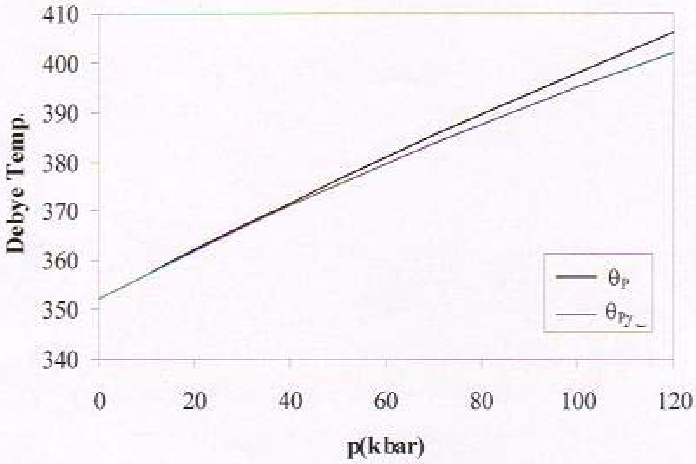

Fig. 5: Variation of Debye temperature with pressure.

DISCUSSION AND CONCLUSIONS

High pressure theoretical results on Fe^{57} in Cu reveal changes in f-fraction with increased pressure, Fig. (3) (Rfp). In particular the increase in the frequency is noticeable, indicating considerable changes in the phonon frequency distribution. It is evident, in this work that Grüneisen parameter (γ) for Cu decreases with pressure, Fig (2), this is in accordance with the volume dependence of Grüneisen parameter and it improved the agreement of our theoretical results with the experimental data (Moyzis, 1968) of f-fraction on using pfs analysis.

On the other hand, although using Debye model for f-fraction evaluation shows a poor agreement with the experimental data. These calculations show that (θ_D=352) as given by (Shepard and Mullen, 2000) is an improved values beside that Fig. 4 still evident that Grüneisen parameter decrease with pressure is a correct conclusion.

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