NEUTRON THERMALIZATION IN CRYSTALLINE MEDIA - CALCULATION OF FERMI AGE TO THERMAL ENERGY

by

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ABSTRACT

A study is made of neutron slowing down and thermalization in crystalline media in the range of energies, less than 1 ev., where crystal binding effects are significant. Equations are presented, with various approximations, for the energy transfer cross section and the average logarithmic energy decrement per collision in this region. The validity of these equations and approximations is discussed and numerical results are presented. With these results, the Fermi Age from indium resonance to thermal is calculated for graphite and beryllium, and found to be 53.7 and 8.94 sq. cm. respectively. A detailed calculation is also made of the age from fission to indium resonance, in beryllium, and found to be 70.1 cm^2. The results obtained are compared to existing experimental and theoretical values, and discrepancies, where they occur, are discussed.

Thesis Supervisor: Dr. Irving Kaplan

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I. Introduction:

The study of neutrons slowing down in the energy range less than one ev., and their approach to thermal equilibrium with the moderator, constitutes a portion of the field of neutron thermalization. In this region the binding energies of the atoms in the moderator material are comparable with the neutron energy so that, in the slowing down treatment, the moderator atoms can no longer be considered free. In this treatment, only moderators in crystalline form will be considered; the extension of this treatment to liquid systems (H_2O, D_2O) is further complicated by the necessity for considering, not only atomic binding, but also molecular energy levels and molecular motion in liquid systems.

For energies less than one ev., the neutron is considered to interact with the crystal lattice as a whole, and consequently slowing down theory developed for high energy neutrons, in which the scattering atoms are assumed free, is unsuitable. The presence of crystalline has the effect of reducing the average logarithmic energy decrement per collision (ξ) below that value calculated for a free atom. This decrease is partially due to the fact that neutrons can gain, as well as loose, energy in interactions with the crystal lattice. The energy units transferred in crystal interactions are called phonons, and are somewhat analogous to photon transfers in atomic and nuclear interactions.

The procedure to be followed in this treatment is to present expressions for the energy transfer cross section $\sigma(E,E',T,\Omega)$; that is, the cross section, at a given temperature T, for a neutron initially at energy E, to be scattered at an angle Ω, and have energy E' after the collision. By integrating over all angles, the above cross section can be reduced to $\sigma(E,E',T)$. With this cross section, and a prescribed spectrum for the energy of the transferred phonons, the average logarithmic energy decrement per collision can be calculated as a function of neutron energy, moderator temperature, and crystalline properties, in the region of crystalline binding effects. With $\xi(E,T)$ known, the Fermi age from indium resonance (1.46 ev.) to an appropriate lower limit can be calculated with the familiar Fermi age integral from age-diffusion theory. Although the exact value of this lower limit, corresponding to thermal energy, is open to question, a value of 5kT is used for the final result; values of age as a function of the lower limit of the age integral are also presented.

Detailed calculations are given for the age, from indium resonance to thermal, in beryllium and graphite; however, the methods and equations used, with appropriate modifications, are applicable to most crystalline substances.

For completness, a detailed calculation was made of the age from fission to indium resonance in beryllium.

In this calculation, effects of the variation in scattering cross section and of the fission spectrum were considered.

II. Energy Transfer Cross Section

In the past many authors, using various approximations, have derived expressions for the energy transfer cross section in the crystalline binding region. Weinstock[1], in 1944, derived an expression for the cross section for one phonon processes in monoatomic, polycrystalline solids. Later Cassels[2] extended the theory to include spin and isotope effects. More recently, the theory has been generalized, to include multi-phonon processes, by Squires[3], Kothari and Singwi[4], Placezk[5], Glauber[6] and others.

2.1 Method of Kothari and Singwi

The following discussion is based primarily on the work of Kothari and Singwi, and the complete mathamatical details may be found in reference 4. The inelastic scattering cross section, in the range of crystalline binding, is composed of a coherent and incoherent contribution. The coherent cross section is related to the interference scattering of slow neutrons, while the incoherent contribution is related to diffuse scattering from spin, isotope, and magnetic disorder.

This can be expressed as

$$\sigma_s = \sigma_{coh} + \sigma_{incoh} \qquad [1]$$

In the treatment to follow, the Fermi pseudopotential approximation[7] is used in which the short range potential between neutron and scattering nucleus is replaced by a point interaction of the form

$$V(\bar{r}_n, \bar{r}) = \frac{2\pi a_n}{m} \delta(\bar{r}_n - \bar{r}) \qquad [2]$$

where $\bar{r}_n$ and $\bar{r}$ are the position vectors of the nucleus and neutron respectively, m is the neutron mass, and a_n is the bound scattering length adjusted so that scattering from isolated fixed nuclei is correctly represented by the Born approximation.

With the above Fermi approximation, and the methods of quantum mechanics, it is shown[4] that the differential incoherent cross section; per unit solid angle, per scattering nucleus, for a process in which l phonons are absorbed, neglecting magnetic effects; is given by

$$d\sigma_{incoh,+l} = \frac{s}{4\pi k_1 l!}\left(\frac{1}{MN}\right)^l \sum_{q_i=0}^{l} k_2(\bar{k}_1 - \bar{k}_2 \cdot \epsilon_s)^{2l} \exp\left[-\frac{\hbar^2}{M}(k_1-k_2)^2\right] \cdot \prod_{i=1}^{l} q_i^{-1}\left(e^{q_i/T} - 1\right) \qquad [3]$$

Using the Debye model of a crystal, replacing the sum over q_i by an integration, letting q_i take on positive as well as negative values to account of emission as well as absorbtion of phonons, and integrating over all solid angles, one obtains the following expression for the incoherent cross section corresponding to the emission or absorbtion of l phonons:

$$\sigma_{\text{incoh, } l} = \frac{s}{2k^2 l!}\left(\frac{2}{2M}\right)^l \prod_{i=1}^{l} \int_{-1}^{+1} q_i\left[\coth\left(q_i/2T\right)-1\right] dq_i \int_{k_2-k_1}^{k_2+k_1} t^{2l+1} \cdot \exp\left(-\frac{bF t^2}{M}\right) dt \qquad [4]$$

In equation [4], all energies are expressed in terms of the Debye energy of the crystal, $k\Theta_D$, where k is Boltzmann's constant and Θ_D is the characteristic temperature of the phonon spectrum in the Debye model. In this model, $k\Theta_D$ is also the maximum phonon energy. Also

k_1^2 = the initial neutron energy in terms of the Debye energy, i.e. $E/k\Theta_D$,

k_2^2 = the neutron energy after collision, i.e. $E'/k\Theta_D$,

M = ratio of moderator to neutron mass,

s = 4π times the difference between the mean square and squared mean scattering lengths, i.e. $4\pi[\overline{(a^2)} - (\bar{a})^2]$,

q_i = energy of transferred phonon in terms of the Debye Energy

T = moderator temperature in terms of the Debye temperature,

$t^2 = (k_1-k_2)^2$.

The exponential, appearing in eq.[4], is known as the Debye Waller factor; and in the Debye approximation

$$F = 1/2 \int_0^1 q \coth(q/2T)\, dq.$$

The initial and final neutron energies, k_1^2 and k_2^2, are related by

$$k_1^2 - k_2^2 = \sum_{i=1}^{l} q_i, \qquad [5]$$

and the total incoherent cross section is given by

$$\sigma_{incoh} = \sum_{l=1}^{\infty} \sigma_{incoh,l} \qquad [6]$$

In a similar manner, it is shown that the coherent cross section can be expressed as

$$\sigma_{coh} = \sum_{l=1}^{\infty} (\sigma^{o}_{coh,l} + \sigma'_{coh,l}) = \sigma^{o}_{coh} + \sigma'_{coh} \qquad [7]$$

where

$$\sigma^{o}_{coh,l} = \frac{\sigma}{2k_i^2 l!}\left(\frac{3}{2M}\right)^{l} \prod_{i=1}^{l} \int_{-1}^{+1} q_i [\coth(q_i/2T) - 1]\, dq_i \int_{k_2-k_1}^{k_2+k_1} t^{2l+1} \cdot$$

$$\cdot \exp\left(-\frac{6Ft^2}{M}\right) dt \qquad [8]$$

and

$$\sigma'_{coh,l} = \frac{\sigma}{2k_i^2 l!}\left(\frac{3}{2M}\right)^{l} \sum_{r} \frac{Z_r}{r} \prod_{i=1}^{l} \int_{-1}^{+1} q_i [\coth(q_i/2T) - 1]\, dq_i \cdot$$

$$\cdot \int_{k_2-k_1}^{k_2+k_1} \exp\left(-\frac{6Ft^2}{M}\right) t^{2l} \sin(rt)\, dt \qquad [9]$$

$S=4\pi(\bar{a})^2$, and Z_r is the number of nuclei at lattice distance r.

If equation [8] is compared to equation [4], one notes that the two expressions are identical aside from the factor S/s. With this fact and eq. [1], the total scattering cross section can be written as

$$\sigma_s = (s+S)\sum_l \sigma_l'' + \sigma_{coh}' \quad , \qquad [10]$$

where σ_l'' is given either by eq.[4] or [8] with the factor s or S omitted respectively, and σ_{coh}' is obtained by summing eq.[9] over all values of l. The assumption made by Placzek, to simplify eq.[10], is that σ_{coh}' can be neglected in comparison with $(s+S)\sigma''$. This is called the incoherent approximation, and its validity will be discussed later.

With the incoherent approximation, eq.[10] may be re-written as

$$\sigma_s = (s+S)\sum_l \sigma_l'' = \sum_{l=0}^{\infty} \sigma_l \qquad [11]$$

where

$$\sigma_l = \frac{s+S}{2k^2 l!}\left(\frac{3}{2M}\right)^l \prod_{i=1}^{l} \int_{-1}^{+1} q_i\left[\coth\left(q_i/2T\right)-1\right] dq_i \int_{k_2-k_1}^{k_2+k_1} t^{2l+1} \cdot$$

$$\exp\left(-\frac{6Ft^2}{M}\right) dt \qquad [12]$$

F is given by

$$F = 1/2 \int_0^{\prime} q \coth(q/2T)\, dq, \qquad [13]$$

and the relationship between k_1^2, k_2^2, and q_i is given by eq.[5].

In a separate paper[8], Kothari and Singwi have evaluated the first three terms in the phonon expansion[11]. The one phonon cross section (the cross section for the absorbtion or emission of one phonon by a neutron) is obtained by setting l=unity in eq.[12], and using eqs. [13] and [5]. After integration over t, in eq.[12], one obtains the following expression for the one phonon cross section as a function of initial and final neutron energy, and moderator temperature:

$$\sigma_1(k_1^2,k_2^2) = \frac{(S+S)M}{96 k_1^2 F^2}(k_2^2-k_1^2)\left[\coth\left(\frac{k_2^2-k_1^2}{2T}\right)-1\right]\left\{\left[1+\frac{6F}{M}(k_2-k_1)^2\right]\times\right.$$

$$\left.\exp\left[-\frac{6F}{M}(k_2-k_1)^2\right]-\left[1+\frac{6F}{M}(k_2+k_1)^2\right]\exp\left[-\frac{6F}{M}(k_2+k_1)^2\right]\right\} \qquad [14]$$

and

$$\sigma_1(k_1^2) = \int_{k_1^2-1}^{k_1^2+1} \sigma_1(k_1^2,k_2^2)\, dk_2^2 \qquad [15]$$

Equation [15] must be solved, for each value of k_1^2, by performing the indicated integration over k_2^2 numerically.

It should be noted that the one phonon cross section is given by eq.[14] only in the region $k_1^2-1 \leq k_2^2 \leq k_1^2+1$, and is equal to zero otherwise.

In a similar manner, the two phonon cross section is obtained by setting l=2 in eq.[12]; the resulting expression is

$$\sigma_2(k_1^2,k_2^2)=\frac{(5+5)M}{384\,k_1^2F^3}\Big\{\Big[1+\frac{6F}{M}(k_2-k_1)^2+\frac{1}{2}\Big(\frac{6F}{M}\Big)^2(k_2-k_1)^4\Big]\exp-\Big[\frac{6F}{M}(k_2-k_1)^2\Big]$$

$$-\Big[1+\frac{6F}{M}(k_2+k_1)^2+\frac{1}{2}\Big(\frac{6F}{M}\Big)^2(k_2+k_1)^4\Big]\exp-\Big[\frac{6F}{M}(k_2+k_1)^2\Big]\Big\}\times$$

$$\int_0^{2-|k_2^2-k_1^2|} dv\Big[\coth\Big(\frac{k_2^2-k_1^2+v^2}{4T}\Big)-1\Big]\Big[\coth\Big(\frac{k_2^2-k_1^2-v^2}{4T}\Big)-1\Big]\times$$

$$\Big[(k_2^2-k_1^2)^2-v^2\Big] \qquad [16]$$

and

$$\sigma_2(k_1^2)=\int_{k_1^2-2}^{k_1^2+2}\sigma_2(k_1^2,k_2^2)\,dk_2^2 \qquad [17]$$

As in the previous case, the above integral is evaluated numerically for various values of k_1^2. The two phonon cross section is given by eq.[16] only in the range $k_1^2-2 \leq k_2^2 \leq k_1^2+2$, and is equal to zero otherwise. This is equivalent to specifying the maximum energy of the transferred phonon as $k\Theta_D$.

The elastic scattering cross section can be obtained simply be setting l=0 in eq.[12]; the result is

$$\sigma_{el} = \sigma_o = \frac{(s+S)M}{24k_1^2F}\left(1-\exp-[24Fk_1^2/M]\right) \qquad [18]$$

For neutron energies of the order of $k\Theta_D$,$(k_1^2=1)$, higher phonon processes (greater than two) become increasingly important. Because of the highly complex nature of the phonon cross section for three and greater phonon transfers, and because it would be necessary to evaluate these cross sections to obtain accurate results in this energy region, an Einstein approximation of the crystal is expected to yield better results for k_1^2 greater than unity.

Using an Einstein crystal model, Kothari and Singwi[8] derive an energy transfer cross section from eq.[12]. The assumption is made that all phonons have the same energy, $k\Theta_E$, where k is Boltzmann's constant and Θ_E is the Einstein temperature of the crystal. Further, since the total number of modes corresponding to each polarization is N, one obtains

$$\sum_i f(q_i) = Nf(1) \qquad [19]$$

Using the above relations for an Einstein model, and eq.[12], Kothari and Singwi[8] present the following expression for the cross section in which l phonons are absorbed and m phonons are emitted:

$$\sigma_{l,m} = \frac{(s+S)(1-e^{-1/T})^{-m}(e^{1/T}-1)^{-l}}{24k_1^2(l+m)!\,M^{l+m}} \int_{k_2-k_1}^{k_2+k_1} t^{2(l+m)+1} \exp\left[-\frac{6Ft^2}{M}\right] dt \qquad [20]$$

All symbols have the same meaning as previously, except that all energies are now expressed in terms of the Einstein energy, $k\Theta_E$. Also,

$$F = 1/6 \coth 1/2T \qquad [21]$$

and

$$k_2^2 - k_1^2 = l - m \qquad [22]$$

After integrating eq.[20] with respect to t, and with eqs.[21] and [22]; the energy transfer cross section, in the case in which l phonons are absorbed and m phonons emitted; is given in the Einstein approximation by

$$\sigma_{l,m} = \frac{(s+S)M}{24k_1^2 F}(1+e^{-1/T})^{-m}(e^{1/T}+1)^{-l}(e^{-\alpha}[1+\alpha+\alpha^2/2!+\cdots$$

$$+\alpha^{l+m}/(l+m)!])_b^a \qquad [23]$$

where

$$a = (\coth 1/2T)\frac{[k_2-k_1]^2}{M} \qquad [24_a]$$

and

$$b = (\coth 1/2T)\frac{[k_1+k_2]^2}{M} \qquad [24_b]$$

Equations [23] and[24] will be used in the region E greater than $k\Theta_D$ to give a more accurate representation of the cross section for multi-phonon processes.

2.2 Method of Nelkin

M.S. Nelkin[9]; from the derivation of Glauber[6], using the Fermi pseudopotential, the incoherent approximation, the Debye crystal model, and neglecting polarization of the phonons; presents the following expression for the energy transfer cross section in the crystalline binding region:

$$\sigma(E\rightarrow E') = \frac{\sigma_o}{4\pi}\left(\frac{E'}{E}\right)^{1/2} \int_{-\infty}^{+\infty} dt \int_{-1}^{+1} dx \exp(it[E'-E])\cdot\exp(\gamma/M\, x [g(t)-g(0)]) \qquad [25]$$

where

$$\gamma = E'+E-2x(EE')^{1/2} \qquad [26]$$

In the Debye approximation, g(t) is given by

$$g(t) = 3/\Theta_D^3 \int_0^{\Theta_o} w\, dw[(\bar{n}+1)\cdot\exp(iwt)+ \bar{n}\cdot\exp(-iwt)], \qquad [27]$$

and

$$\bar{n} = [\exp(w/T) -1]^{-1} \qquad [28]$$

In eqs. [25] to [28], E is the initial neutron energy, E' is the neutron energy after collision, σ_o is the bound atom cross section, T is the moderator temperature, and w is the frequency of the transferred phonon. Nelkin uses a system in which $\bar{h}=k=1$, where $\bar{h}$ is $1/2\pi$ Planck's constant and k is Boltzmann's constant. Although the form may be different, eq.[25] presented by Nelkin[9], corresponds to eqs. [11] and [12] presented by Kothari and Singwi[4].

Placzek[5], recognizing the poor convergence of the phonon expansion of the inelastic scattering cross section at energies of the order of, and greater than, the Debye energy, suggested expanding the inelastic cross section in powers of 1/M. This expansion converges rapidly, for energies in the region of interest, provided that M is large compared with unity and T/Θ_D.

Following the suggestion of Placzek, Nelkin expanded the function $\exp[\gamma/M(g[t]-g[0])]$ in powers of 1/M. If only first order terms are retained, the expression for the inelastic scattering cross section, from eq. [25], is

$$\sigma(E\rightarrow E') = \frac{\sigma_o 3T}{M\Theta_D^3}\left(\frac{E'}{E}\right)^{1/2}\cdot(E'+E)\left(\frac{E'-E}{T}\left[\exp\left(\frac{E'-E}{T}\right)-1\right]^{-1}\right) \quad [29]$$

for $|E'-E|\leq\Theta_D$, and is zero otherwise.

The validity of eq.[29] as a representation of the energy transfer cross section will be discussed later.

2.3 Discussion and Evaluation of Energy Transfer Cross Sections

In this section, the methods and accompanying assumptions used by Nelkin, and Kothari and Singwi in deriving expressions for the energy transfer cross section will be reviewed and discussed.

The incoherent approximation was made by both authors in their work. This approximation corresponds to neglecting the correction term to the coherent scattering contribution, σ'_{coh}, in eq.[10]. R.C. Bhandari[10] has evaluated this correction term for the elastic, and one phonon partial cross sections, i.e. l=0,l=1, for beryllium. In the low energy region (0.00104 ev.), below the Bragg cutoff, the values for the one phonon cross section, with and without the incoherent approximation, differ markedly. But in the energy range of interest in age calculations(greater than 5kT), there is essentially no difference between the computed cross sections. Moreover, when the total inelastic scattering cross section is computed, by summing over all values of l, the difference between the two values, even at low energy, is only a few percent. Although the use of the incoherent approximation does not accurately describe the behavior of the partial phonon cross sections at low energies, it yields a fairly accurate representation of integrated quantities,eg.,the total inelastic scattering cross section. However, the use of the incoherent approximation results in a value of the elastic scattering cross section which is too large.

Consequently the total cross section computed is also too large, and attains a value, in the high energy limit, of 6.2 b in beryllium. Bhandari, without the incoherent approximation, calculated a lower value for the elastic scattering cross section in beryllium; when this value is combined with the inelastic cross section, to give the total cross section, the value obtained in the high energy limit of the crystalline binding region is 5.9 b in good agreement with the experimental value[23]. As will be seen later, this difference in total cross section will give values of ξ, with and without the incoherent approximation, which differ by approximately 5% maximum.

"For the few crystals for which the frequency spectrum has been carefully calculated from force constants, it is found that the spectrum deviated markedly from the usual smooth Debye curve. However, since we are interested only in integrated properties, the error involved in assuming the Debye frequency spectrum appears to be quite small...."[4]

In the phonon expansion, the Einstein model is used to calculate the energy transfer cross section in that energy region where multi-phonon processes make a significant contribution. It is conceivable that the Einstein model could give fairly good results when the neutron energy is several times greater than the Einstein energy of the crystal. However, in the low energy region, the Einstein model could not give accurate results, since it is

impossible, in this model, for any energy transfer to occur once the neutron energy is less than the Einstein energy (0.064ev. in beryllium). Physically, this is not so.

The inverse mass expansion used by Nelkin[9], and originally suggested by Placzek[5], converges rapidly provided that the ratio of moderator to neutron mass (M) is large compared with unity and T/Θ_D. Consequently, this approach would be useful for heavy crystalline moderators at moderate temperatures. For Magnesium (mass number=24) Placzek has calculated the first three terms in the mass expansion for $E=\Theta_D/36$, and $T/\Theta_D=2.05$. He found that the term of order $1/M^2$ was only half a percent of the term of order $1/M$. To obtain similar accuracy from a phonon expansion, it was necessary for Squires[2] to calculate six terms.

Unfortunately, moderators used in nuclear reactors, of necessity, have low mass numbers; therefore it is questionable whether the mass expansion used by Nelkin, in which terms of higher order than $1/M$ are neglected, is sufficiently accurate. For the moderator materials of interest here (graphite and beryllium) the condition for rapid convergence, M much greater than unity, does not apply. For the case of beryllium, Kothari and Singwi[4] have calculated the term of order $1/M^2$ in the mass expansion, and found it to be negative and approximately 10% of the term of order $1/M$ in magnitude, for neutrons of energy equal to 0.009 ev.

Therefore, by neglecting higher order terms in the mass expansion, the inelastic cross section computed by Nelkin is approximately 10% too high. M.V. Kazarnovski[11] asserts that neglecting terms of greater order than 1/M in the mass expansion is equivalent to neglecting multiple phonon and thermal effects. This statement is questionable, since it is difficult to attach direct physical interpertation to the separate terms in the mass expansion. It should be noted that in the high energy limit, Nelkin's expression for the energy transfer cross section, eq.[29], converges to the bound atom cross section σ_o. This is not a serious limitation, as will be shown later, since the quantity σ_o will cancel out of the expression for the average logarithmic energy decrement per collision. In a later work[12], Nelkin has replaced σ_o by the free atom cross section when using the energy transfer cross section in spectrum calculations. In this case

$$\sigma_{free} = \sigma_o(1+1/M)^{-2} \qquad [30]$$

Nelkin does not expect the expression he presents for $\sigma(E \rightarrow E')$, eq. [29], to represent the detailed behavior of the inelastic cross section at all energies; however, he does believe that it will give physically reasonable results for integrated quantities.

The phonon expansion of Kothari and Singwi is expected to yield more accurate results than the inverse mass expansion of Nelkin. This is especially true at neutron energies below the Debye energy of the crystal, where multi-phonon processes are unimportant and the inelastic cross section can be well approximated by the sum of the one and two phonon cross sections. At energies greater than the Debye energy, one should calculate the contribution from higher phonon processes because the convergence of the phonon expansion is relatively poor. Kothari and Singwi[8] have estimated that the contribution of the two phonon cross section to the average logarithmic energy decrement per collision is 6.4% at $E=k\Theta_D$ and 45% at $E=2k\Theta_D$ in beryllium. Since the expressions for higher phonon processes are so complex, Kothari and Singwi feel that the contribution of multi-phonon processes to the energy transfer cross is adequately represented by the Einstein crystal model at neutron energies greater than $k\Theta_D$. The fact that the Einstein model is not applicable at low neutron energies does not preclude its yielding physically reasonable results at higher energies.

III. Average Logarithmic Energy Decrement per Collision

Once expressions for the energy transfer cross section have been obtained, one can calculate the average logarithmic energy decrement per collision, ξ. In the general case, this is given by

$$\xi(E) = \frac{\int_A^B \sigma(E \rightarrow E') \ln[E/E']\, dE'}{\int_A^B \sigma(E \rightarrow E')\, dE'} \qquad [31]$$

where the limits of integration, A and B, are functions of E, and depend on the specific form of $\sigma(E \rightarrow E')$. This point will be clarified by specific examples to be presented later.

3.1 Method of Kothari and Singwi

With the phonon expansion of Kothari and Singwi[8], equation [31] becomes

$$\xi(k_1^2) = 1/\sigma_s \left\{ \int_{k_1^2-1}^{k_1^2+1} \sigma_1(k_1^2,k_2^2) \cdot \ln[k_1^2/k_2^2]\, dk_2^2 + \int_{k_1^2-2}^{k_1^2+2} \sigma_2(k_1^2,k_2^2) \times \ln[k_1^2/k_2^2] dk_2^2 \right\} \qquad [32]$$

where $\sigma_1(k_1^2,k_2^2)$ and $\sigma_2(k_1^2,k_2^2)$ are given by eqs. [14] and [16] respectively.

The total scattering cross section, σ_s, is given by

$$\sigma_s(k_1^2) = \sigma_o(k_1^2) + \sigma_1(k_1^2) + \sigma_2(k_1^2) \qquad [33]$$

where σ_o, σ_1, and σ_2 are given by eqs. [18], [15], and [17] respectively. In eq. [32], the first term on the right hand side corresponds to one phonon transfer, and the second term to two phonon transfer processes.

Within the range of neutron energies where the Einstein approximation is used, ξ is given by

$$\xi(k_1^2) = \frac{1}{\sigma_s} \sum_n \left([\sigma_{o,n} + \sigma_{1,n+1}] \cdot \ln \frac{k_1^2}{k_1^2 - n} + \sigma_{n,o} \cdot \ln \frac{k_1^2}{k_1^2 + n} \right) \qquad [34]$$

where the partial cross sections are given by eq. [23] with the appropriate values of l and m. $\sigma_{o,n}$ is the cross section for a process in which zero phonons are absorbed by the neutron, and n phonons are emitted; similarly, $\sigma_{1,n+1}$ corresponds to the absorbtion of one phonon and the emission of n+1 phonons. $\sigma_{n,o}$ is the cross section for the absorbtion of n phonons and the emission of zero phonons. The first two terms on the right hand side of eq. [34] correspond to processes in which there is a net transfer of n phonons, of energy $k\Theta_E$, <u>from</u> the neutron; the last term corresponds to the transfer of n phonons <u>to</u> the neutron.

Kothari and Singwi[8] assert that only cross section terms of the form indicated in eq.[34], with n running from zero to two, make a significant contribution to ξ.

Kothari and Singwi[8] have made the long and tedious calculations necessary to evaluate ξ from eqs. [32] and [34]. The calculation has been made for beryllium with $\Theta_D = 1000^\circ K$ and $\Theta_E = 740^\circ K$; the moderator temperature, T, was taken to be $300^\circ K$. $\xi(E)$ was plotted in the low energy range using the Debye model, eq.[32], and in the high energy region with the Einstein model, eq.[34]. The two curves intersected at $E/k\Theta_D = 1.63$, and were smoothly joined in this region to yield a best value of ξ over the entire energy interval. This curve of ξ vs. E, for beryllium, is reproduced figure 1, curve B; the values are normalized by dividing by the free atom value, ξ_o.

3.2 Method of Nelkin

With eq.[31], and Nelkin's expression for the energy transfer cross section, one obtains for ξ

$$\xi(E) = \frac{1}{\sigma_s} \int_{E-\theta_D}^{E+\theta_D} \sigma(E \rightarrow E') \cdot \ln \frac{E}{E'} \, dE' \qquad [35]$$

where $\sigma(E \rightarrow E')$ is given by equation [29].

After substituting

$$z = \Theta_D/E$$

$$y = E-E'/\Theta_D \qquad [36]$$

$$\varphi = \Theta_D/2T$$

in eq.[35], the following expression is obtained for the slowing down power in the crystalline binding region:

$$\xi\sigma_s = \frac{-3\sigma_o}{M\varphi z}\int_{-1}^{+1} dy(1-yz)^{-3/2}(1-yz/2)\cdot\ln[1-yz]\cdot g(2\varphi y) \qquad [37]$$

where

$$g(x) = x(e^x-1)^{-1}. \qquad [38]$$

If the factors in the integrand are expanded in a power series, multiplied out, and integrated term by term, the following expression results*:

$$\xi/\xi_o = 1 - (4.5\beta_3[\varphi])z + (1.175)z^2 - (7.19\beta_5[\varphi])z^3 +$$
$$+ (1.205)z^4 - (9.66\beta_7[\varphi])z^5 + (1.207)z^6 +$$
$$-(11.97\beta_9[\varphi])z^7 + \ldots. \qquad [39]$$

---

* The first five terms are given by Nelkin in ref. 9; the remaining three terms were evaluated by the author using Dr. Nelkin's original calculation sheets.

where

$$\beta_n(\varphi)=\int_0^1 t^n\cdot\coth(\varphi t)\cdot dt=\frac{1}{n\varphi}+\frac{\varphi}{3(n+2)}+\frac{\varphi^3}{45(n+4)}+\frac{2\varphi^5}{945(n+6)}+$$

$$-\frac{\varphi^7}{4725(n+8)}+\cdots. \qquad [40]$$

The quantities φ and z are defined in eq.[36]. In eq.[39], $2\sigma_o/M$ was replaced by $\xi_o\sigma_s$ so as to give the proper value of ξ in the limit when E approaches infinity, i.e., z approaches zero. With a value of $\Theta_D = 1000^oK$ and $T=300^oK$, ξ/ξ_o was computed as a function of neutron energy. The results of this computation are presented in figure 1, curve A.

It should be noted that in Nelkin's inverse mass expansion, when terms of higher order than 1/M are neglected, the only material property affecting ξ/ξ_o is the Debye temperature. The factor 1/M, in eq.[37], is incorporated into ξ_o. The calculation was originally made for beryllium; however if the Debye temperature of graphite is taken to be 1000^oK,[13] the results of fig. 1, curve A, can also be applied to graphite. Actually, due to the highly anisotropic crystal lattice of graphite, the calculation of ξ/ξ_o is not so straightforward as is indicated above; however the use of 1000^oK for the Debye temperature of graphite does have some experimental and theoretical basis. A further discussion of the effect of the anisotropic nature of the graphite lattice, on the

calculation of the slowing down properties, will be presented later.

3.3 Results of Gurney

In 1946, R.Gurney, using an Einstein crystal model, calculated the average logarithmic energy decrement per collision in beryllium and graphite. The details of his calculation were not available, but his equations indicate that only processes in which energy was lost by the neutron were considered. His equation is presented in the following form:

$$\xi(E)=\frac{\sum_n (J_n \cdot \ln[E/E-nk\Theta_E])}{\sum_n J_n} \qquad [41]$$

The exact form of J_n is not given, but it is believed that J_n corresponds to the partial cross section for the emission of n phonons of energy $k\Theta_E$.

Gurney calculated $\xi(E)$, using an Einstein model with $\Theta_E=742^\circ K$ and $T=300^\circ K$, in beryllium. The results of this calculation are reproduced in fig. 1, curve C. He also applied the Einstein model to graphite using $\Theta_E^{\perp}= 452^\circ K$ as characterizing lattice vibrations perpendicular to the graphite lattice planes, and $\Theta_E^{''}= 1553^\circ K$ for vibrations parallel to lattice planes. A value of ξ was evaluated corresponding to each direction, and the total ξ was obtained by simply adding the two, i.e. $\xi_T = \xi_\perp + \xi_{''}$.

The validity of Gurney's method is questionable, since it is doubtful whether the anisotropic nature of the graphite crystal lattice can be treated in such a simple manner. Gurney's results, for graphite, are presented in fig. 2, curve C. In both cases, the plots are normalized by dividing by the free atom value, ξ_0.

3.4 Discussion and Evaluation

In figure 1, results are presented for $\xi(E)/\xi_0$ in beryllium; as determined by the methods of Nelkin (curve A), Kothari and Singwi (curve B), and Gurney(curve C); with Θ_D=1000°K, Θ_E= 742°K, and T=300°K. The dashed portions of the curves are extrapolated to obtain values of ξ/ξ_0 at low energies. All the curves approach unity at large values of E.

The reason for Gurney's values (curve C) being higher than the others is twofold: first, cross sections were not known very accurately when the calculation was made (1946), and second, an Einstein model is used in which energy gain processes are neglected. This would give a higher value of ξ/ξ_0 than that calculated by Kothari and Singwi, using an Einstein model for E greater than $1.63k\Theta_D$, who included energy gain processes (see eq.[34]).

There is no obvious reason for Nelkin's method (curve A) to yield values of ξ/ξ_0 which are lower than those of Kothari and Singwi. However, it is believed that the neglecting of higher order terms in the mass expansion; in the case of

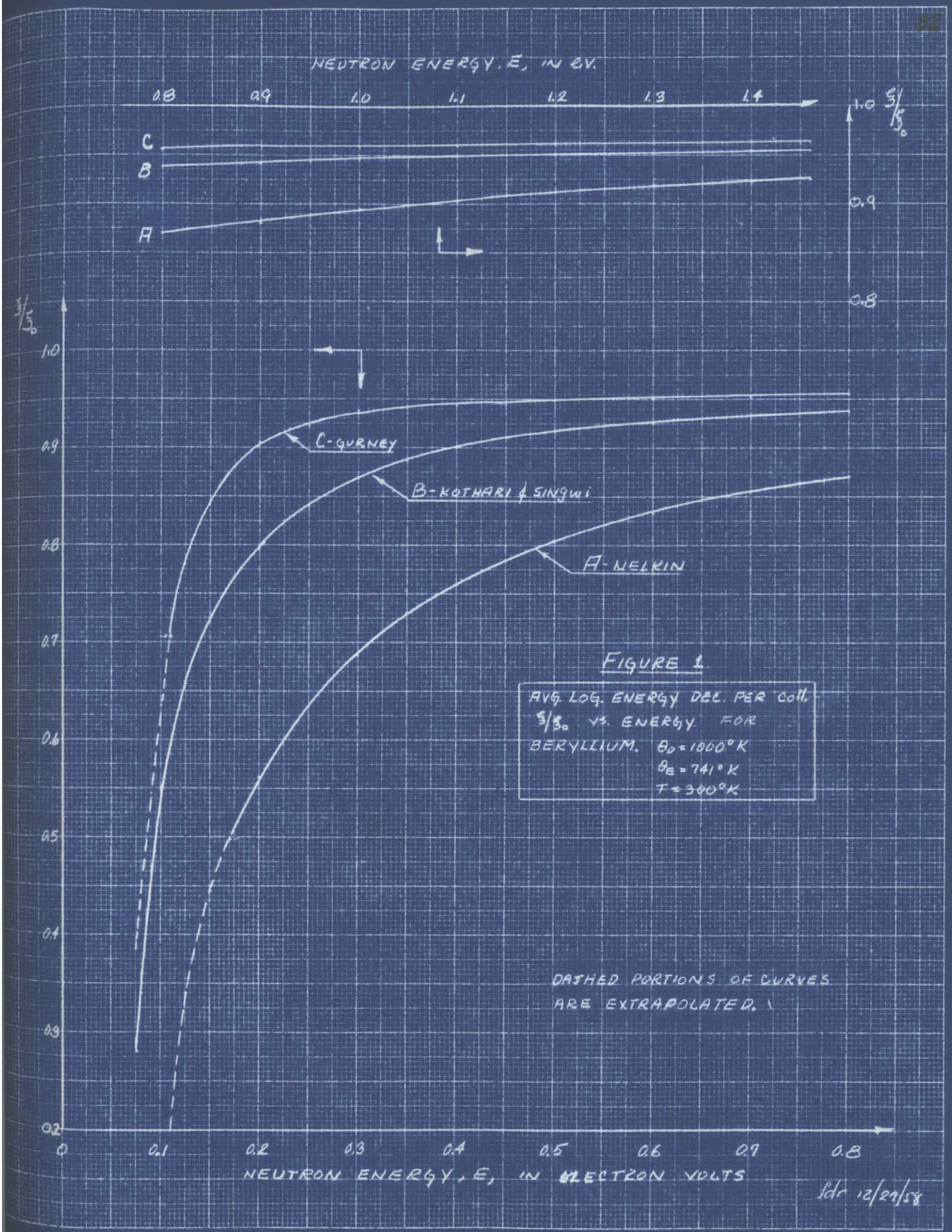

FIGURE 1

AVG. LOG. ENERGY DEC. PER COLL. ξ/ξ_0 VS. ENERGY FOR BERYLLIUM. $\theta_D = 1800°K$, $\theta_E = 741°K$, $T = 300°K$

DASHED PORTIONS OF CURVES ARE EXTRAPOLATED.

sdr 12/29/58

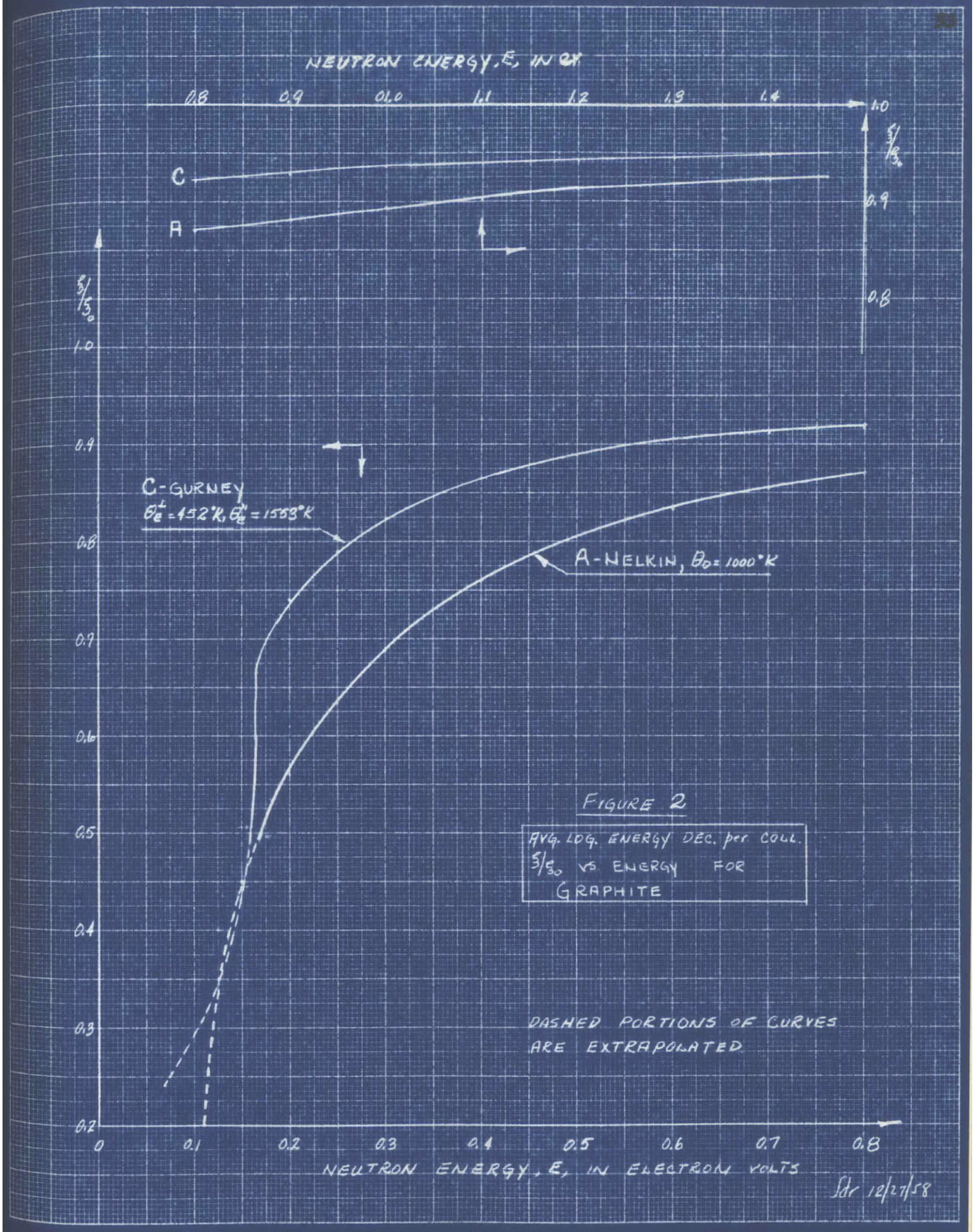

FIGURE 2

AVG. LOG. ENERGY DEC. per COLL. ξ/ξ_0 VS. ENERGY FOR GRAPHITE

DASHED PORTIONS OF CURVES ARE EXTRAPOLATED

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low mass number materials (beryllium), where the condition for rapid convergence ($M \gg 1$) is not satisfied; may yield values of ξ/ξ_o which are too low.

It should be noted that the series expansion, presented by Nelkin, eq.[39], for ξ/ξ_o, converges quite slowly at low energies. This is a result of the mathamatical form in which the coefficient of $1/M$, in the inverse mass expansion, is presented rather than the failure to satisfy the condition for rapid convergence. The form in which Nelkin presents his results lends itself, rather easially, to numerical computation, while the equations of Kothari and Singwi, eq. [32] and [34] are exceedingly cumbersome to manipulate. In spite of this, it is believed that the method of Kothari and Singwi yields the most accurate results for ξ/ξ_o in beryllium.

In figure 2, results are presented for ξ/ξ_o in graphite as determined by Gurney,, and as calculated from Nelkin's equation with $\Theta_D = 1000^oK$ and $T = 300^oK$.

Unlike beryllium, which has a hexagonal close-packed lattice, carbon atoms are situated in planes in the graphite crystal lattice; this gives rise to a highly anisotropic material. Consequently, the graphite texture has a considerable effect on its slowing down, and diffusion properties.

As stated previously, no reason can be seen as to why the method used by Gurney to compute $\xi(\epsilon)$, for graphite, is appropriate. It seems unreasonable that the ξ for polycrystalline substances should be equal to the algebraic sum of values computed for vibrations perpendicular and parallel to the lattice planes. The details of Gurney's calculation were not available, but his result does exhibit the proper over all trend. Gurney's results are presented in fig.2, curve C. The explanation of the high value of ξ obtained by Gurney, assuming that his method is correct, is the same as that used to explain the high values found for beryllium.

In order to explain the specific heat of graphite at low temperatures, Krumhansl and Brooks[15] have constructed a model in which Debye temperatures of 900°K and 2500°K are assigned to vibrations perpendicular and parallel to the lattice planes respectively. Based on this model, Kothari and Singwi[16] have attempted to make theoretical estimates of the scattering cross section in graphite. Using the incoherent approximation, and the Debye model, they have calculated the one and two phonon cross sections corresponding to vibrations both perpendicular and parallel to the lattice planes. The total scattering cross section, for polycrystalline graphite, was taken to be the sum of these partial cross sections. The calculation was made for low energy neutrons (10A°), but unfortunately their results do not agree very well with the experimental values,(BNL-325).

Kothari and Singwi attribute this discrepancy to the effect of texture and microstructure in graphite. Another source of error may lie in the fact that the incoherent approximation is not particularly well suited for estimation of the elastic scattering cross section, and McReynolds et.al.[17] assert that elastic scattering predominates strongly over inelastic scattering in graphite.

At present, there appears to be no satisfactory method for considering the anisotropic nature of the graphite crystal lattice in the computation of the energy tansfer cross section or ξ . Since the binding energy between atoms within a crystal plane is far greater than that between planes, the average logarithmic energy decrement per collision should be significantly greater in interactions perpendicular to the lattice planes than parallel to them. As a first approximation, it is assumed that almost the entire contribution to ξ comes from vibrations perpendicular to lattice planes. For greater ease in calculation, Nelkin's eq.[39] is used with $\Theta_D = 1000^\circ K$. (Krumhansl and Brooks give $900^\circ K$ as the Debye temperature corresponding to vibrations perpendicular to the lattice planes; an additional $100^\circ K$ was added to partially correct for interactions parallel to the lattice planes. Reference 13 also quotes $\Theta_D = 1000^\circ K$ for graphite). Based on this approximation, the values of ξ/ξ_0 obtained are presented in fig.2, curve A.

For neutron energies greater than approximately 0.2 ev., a certial portion of the interactions involve collisions in which an atom is displaced from its lattice site. For these events, ξ is greater than any of the previously discussed theories would predict, since they do not account for such events. The frequency of such events increases with neutron energy so that, at the upper end of the energy range considered, the values of ξ/ξ_o, for each method presented, should be increased. A quantitative estimate of this correction has not been made, but the existance of this effect should be noted since its omission adds another approximation to the results already derived.

IV. Computation of Fermi Age from Indium Resonance to Thermal

After obtaining $\frac{\xi(E)}{\xi_o}$ in the crystalline binding region, one can calculate the Fermi age, τ. The age will be computed from indium resonance to thermal; consequently, τ will be taken as zero at E=1.46 ev.

4.1 Method

The age to thermal is given by

$$\tau = \int_{E_t}^{1.46} \frac{D}{\xi N \sigma_s} \cdot \frac{dE}{E} = \int_{E_t}^{1.46} \frac{1}{3\xi N^2 \sigma_{tr} \sigma_s} \cdot \frac{dE}{E} \qquad [42]$$

where N is the number of moderator atoms per cc., D is the diffusion coefficient, and σ_{tr} is the transport cross section. The value of the lower limit of the age integral, E_t, is somewhat arbitrary, and the difficulties associated with its choice will be discussed later.

For the case of small absorbtion, σ_{tr} is taken as $\sigma_s(1-2/3A)$, where σ_s is the total (elastic+inelastic) scattering cross section. With this substitution, eq.[42] becomes

$$\tau=\int_{E_t}^{1.46}\frac{1}{3N^2\sigma_s^2(1-2/3A)\xi}\cdot\frac{dE}{E} \qquad [43]$$

Taking σ_s as constant in the range 1.46 ev. to E_t[23], one obtains, for the age from indium resonance to thermal

$$\tau=\frac{1}{3\xi_o(1-2/3A)N^2\sigma_s^2}\int_{E_t}^{1.46}\frac{1}{\xi(E)/\xi_o}\cdot\frac{dE}{E}. \qquad [44]$$

Let

$$C=\frac{1}{3\xi_o(1-2/3A)N^2\sigma_s^2} \qquad [45]$$

and

$$I(E_t)=\int_{E_t}^{1.46}\frac{1}{\xi(E)/\xi_o}\cdot\frac{dE}{E} \qquad [46]$$

Then

$$\tau(E_t)=C[I(E_t)] \qquad [47]$$

$I(E_t)$ must be evaluated by numerically integrating eq.[46]. This is done in the following way:

$$I(E_t)=\sum_{j=1}^{n} \frac{1}{[\overline{\xi/\xi_o}]_j} \cdot \ln \frac{E_{j-1}}{E_j} \qquad [48]$$

where $E_o = 1.46$ ev., and $[\overline{\xi/\xi_o}]_j$ is the average value of ξ/ξ_o in the energy interval E_j to E_{j-1}. The upper limit of the summation, n, is a function of E_t which is, in turn, the lower energy limit of the nth group.

With the values of ξ/ξ_o obtained from figures 1 and 2, $I(E_t)$ was calculated for graphite and beryllium from eq.[48]. The details of this calculation, corresponding to each curve in figs. 1 and 2, are presented in tables I through IV. For each calculation, values of $I(E_t)$ are obtained by adding the last column in each table up to the group in which $E_t = E_j$; these values are presented at the bottom of each table as a function of E_t which is now expressed as a function of moderator temperature.

Correspondingly, values of C, eq.[45], were calculated for graphite and beryllium using the following physical properties:

TABLE I

Details of calculation of age from indium res. to thermal, in beryllium and graphite, using results of Nelkin: Figs. 1 & 2, curve A

Group	E_{j-1} ev.	E_j ev.	$\left[\overline{\xi/\xi_s}\right]_j$	$\left[\overline{\xi_s/\xi}\right]_j$	$\frac{E_{j-1}}{E_j}$	$\ln\frac{E_{j-1}}{E_j}$	$\left[\frac{\overline{\xi_s}}{\xi}\right]_j \ln\frac{E_{j-1}}{E_j}$
1	1.46	1.20	0.919	1.089	1.217	0.1961	0.2135
2	1.20	1.00	0.904	1.106	1.200	0.1821	0.2015
3	1.00	0.80	0.880	1.136	1.250	0.2230	0.2532
4	0.80	0.70	0.862	1.159	1.142	0.1328	0.1539
5	0.70	0.60	0.846	1.182	1.168	0.1551	0.1834
6	0.60	0.50	0.821	1.219	1.200	0.1821	0.2220
7	0.50	0.40	0.785	1.273	1.250	0.2230	0.2840
8	0.40	0.30	0.727	1.374	1.333	0.2870	0.3941
9	0.30	0.25	0.660	1.514	1.200	0.1821	0.2757
10	0.25	0.20	0.599	1.670	1.250	0.2230	0.3722
11	0.20	0.182	0.542	1.846	1.099	0.0944	0.1742
12	0.182	0.156	0.498	2.025	1.174	0.1602	0.3245
13	0.156	0.129	0.411	2.435	1.200	0.1821	0.4430
14	0.129	0.104	0.242	4.130	1.243	0.2172	0.8950

E_t ev.	0.182 (7kT)	0.156 (6kT)	0.129 (5kT)	0.104 (4kT)
$I(E_t)$	2.728	3.052	3.496	4.390

TABLE II

Details of calculation of age from indium res. to thermal, in beryllium, using results of Kothari and Singwi; Fig.1, curve B.

Group	E_{j-1} ev.	E_j ev.	$\left[\frac{\bar{\xi}}{\xi_0}\right]_j$	$\left[\frac{\bar{\xi}_0}{\xi}\right]_j$	$\frac{E_{j-1}}{E_j}$	$\ln\frac{E_{j-1}}{E_j}$	$\left[\frac{\bar{\xi}_0}{\xi}\right]_j \ln\frac{E_{j-1}}{E_j}$
1	1.46	1.00	0.951	1.050	1.460	0.3784	0.3975
2	1.00	0.70	0.940	1.060	1.430	0.3565	0.3795
3	0.70	0.50	0.925	1.081	1.400	0.3360	0.3638
4	0.50	0.40	0.910	1.099	1.250	0.2230	0.2450
5	0.40	0.30	0.886	1.129	1.330	0.2850	0.3218
6	0.30	0.25	0.858	1.164	1.200	0.1822	0.2120
7	0.25	0.20	0.821	1.219	1.250	0.2230	0.2720
8	0.20	0.182	0.787	1.270	1.100	0.0952	0.1149
9	0.182	0.156	0.753	1.328	1.174	0.1602	0.2125
10	0.156	0.129	0.703	1.421	1.205	0.1863	0.2650
11	0.129	0.104	0.615	1.625	1.243	0.2172	0.3530
12	0.104	0.0776	0.445	2.245	1.337	0.2900	0.6510

E_t ev.	0.182 (7kT)	0.156 (6kT)	0.129 (5kT)	0.1038 (4kT)	0.0776 (3kT)
$I(E_t)$	2.307	2.519	2.784	3.137	3.788

TABLE III

Details of calculation of age from indium res. to thermal, in beryllium, using results of Gurney: Fig. 1, curve C.

Group	E_{j-1}	E_j ev.	$\left[\frac{\bar{\xi}}{\xi_o}\right]_j$	$\left[\frac{\bar{\xi_o}}{\xi}\right]_j$	$\frac{E_{j-1}}{E_j}$	$\ln\frac{E_{j-1}}{E_j}$	$\left[\frac{\bar{\xi_o}}{\xi}\right]_j \ln\frac{E_{j-1}}{E_j}$
1	1.46	1.00	0.962	1.040	1.460	0.3784	0.3915
2	1.00	0.80	0.957	1.045	1.250	0.2230	0.2330
3	0.80	0.50	0.950	1.051	1.600	0.4690	0.4935
4	0.50	0.40	0.946	1.057	1.250	0.2230	0.2355
5	0.40	0.30	0.934	1.070	1.333	0.2870	0.3070
6	0.30	0.20	0.921	1.086	1.500	0.4060	0.4410
7	0.20	0.182	0.895	1.118	1.099	0.0944	0.1112
8	0.182	0.156	0.870	1.149	1.174	0.1602	0.1841
9	0.156	0.129	0.827	1.210	1.200	0.1821	0.2200
10	0.129	0.104	0.734	1.361	1.243	0.2172	0.2955
11	0.104	0.776	0.538	1.858	1.337	0.2900	0.5380

E_t ev.	0.182 (7kT)	0.156 (6kT)	0.129 (5kT)	0.104 (4kT)	0.0776 (3kT)
$I(E_t)$	2.213	2.397	2.617	2.912	3.450

TABLE IV

Details of calculation of age from indium res. to thermal, in graphite, using results of Gurney: Fig. 2, curve C

Group	E_{j-1} ev.	E_j ev.	$\left[\overline{\frac{\xi}{\xi_o}}\right]_j$	$\left[\overline{\frac{\xi_o}{\xi}}\right]_j$	$\frac{E_{j-1}}{E_j}$	$\ln\frac{E_{j-1}}{E_j}$	$\left[\overline{\frac{\xi_o}{\xi}}\right]_j \ln\frac{E_{j-1}}{E_j}$
1	1.46	1.00	0.944	1.059	1.460	0.3784	0.4010
2	1.00	0.80	0.927	1.079	1.250	0.2230	0.2408
3	0.80	0.60	0.914	1.094	1.333	0.2870	0.3138
4	0.60	0.50	0.898	1.113	1.200	0.1821	0.2030
5	0.50	0.40	0.879	1.139	1.250	0.2230	0.2540
6	0.40	0.30	0.844	1.184	1.333	0.2870	0.3400
7	0.30	0.25	0.807	1.239	1.200	0.1821	0.2258
8	0.25	0.20	0.765	1.308	1.250	0.2230	0.2915
9	0.20	0.182	0.720	1.389	1.099	0.0944	0.1310
10	0.182	0.156	0.579	1.725	1.174	0.1602	0.2762
11	0.156	0.129	0.414	2.415	1.200	0.1821	0.4390
12	0.129	0.104	0.326	3.068	1.243	0.2172	0.6660
13	0.104	0.776	0.265	3.775	1.337	0.2900	1.0880

E_t ev.	0.182 (7kT)	0.156 (6kT)	0.139 (5kT)	0.104 (4kT)	0.0776 (3kT)
$I(E_t)$	2.401	2.677	3.116	3.782	4.870

For beryllium

$$\text{density} = 1.85 \text{ gm/cc}$$
$$A = 9$$
$$N = 0.1238 \cdot 10^{24} \text{ atoms/cc}$$
$$\sigma_s = 5.95 \text{ b}$$
$$\xi_o = 0.207$$

For graphite

$$\text{density} = 1.60 \text{ gm/cc}$$
$$A = 12$$
$$N = 0.0803 \cdot 10^{24} \text{ atoms/cc}$$
$$\sigma_s = 4.75 \text{ b}$$
$$\xi_o = 0.158$$

With eq. [45], and the above data, C for beryllium and graphite were calculated to be

$$C_{Be} = 3.21 \text{ cm}^2$$
$$C_C = 15.38 \text{ cm}^2.$$

From eq.[47]; with the values of $I(E_t)$ presented in tables I to IV, and the values of C_{Be} and C_C given above; $\tau(E_t)$ was evaluated, corresponding to the methods of Kothari and Singwi, Nelkin, and Gurney for evaluating ξ/ξ_o, for graphite and beryllium. The results of this calculation are presented in table V (beryllium) and VI (graphite).

For purposes of comparison, results are also presented, for $\tau(E_t)$, when ξ/ξ_o is taken to be independent of energy and equal to unity.

TABLE V

Results of calculation of age from 1.46 ev. to E_t in beryllium.

E_t in ev.	$\tau(E_t)$ in cm^2.			
	Nelkin Table I	Kothari & Singwi Table II	Gurney Table III	$\frac{\xi}{\xi_o}$=const.
0.182:(7kT)	8.76	7.40	7.10	6.66
0.156:(6kT)	9.80	8.09	7.70	7.19
0.129:(5kT)	11.21	8.94	8.40	7.79
0.104:(4kT)	14.10	10.08	9.35	8.50
0.0776:(3kT)	-----	12.17	11.09	9.40

DENSITY=1.85 gm/cc

Temp. = 300°K

ξ_o = 0.207

TABLE VI

Results of calculation of age from 1.46 ev. to E_t in graphite.

E_t in ev.	$\tau(E_t)$ in cm^2.		
	Nelkin Table I	Gurney Table IV	$\frac{\xi}{\xi_o}$=cons't=1
0.182 :(7kT)	41.9	36.9	32.0
0.156 :(6kT)	46.9	41.0	34.4
0.129 :(5kT)	53.7	47.8	37.2
0.104 :(4kT)	67.4	58.2	40.6
0.0776:(3kT)	----	74.9	45.1

density=1.60 gm/cc

Temp. =300°K

ξ_o =0.158

In this case, eq. [44] can be integrated directly to give

$$\tau(E_t) = C \cdot \ln[1.46/E_t] \qquad [49]$$

All calculations were made for a moderator temperature of $300^{\circ}K$.

4.2 Results and Discussion

At this point one is faced with the problem of choosing an appropriate value of E_t, corresponding to thermal energy. The value of E_t to use as a lower limit of the age integral appears to be that value of energy at which the epithermal reactor spectrum (approximately 1/E) joins the Maxwell-Boltzmann spectrum. In reality, this joining is continuous, so that E_t is not clearly defined. From both experimental and theoretical studies of reactor spectra[18,19], this transition energy is estimated to be approximately 4 to 5kT, where T is the moderator temperature, (the difference between neutron and moderator temperature, caused by spectrum hardening due to large thermal absorbtion, has been neglected). For the work to follow, a value of E_t equal to 5kT, as suggested by Cohen[19], will be used.

For reasons discussed in section 3.4, it was concluded that, of the methods available for calculating $\bar{\xi}$, the method of Kothari and Singwi (eqs. [32] and[34]) should give the best results in the case of beryllium.

Therefore the value of τ from indium resonance to thermal, in beryllium, is that value of $\tau(E_t)$, calculated from the values of ξ/ξ_o presented by Kothari and Singwi, at $E_t = 5kT_o$. From table V, this value is 8.94 cm^2 for a density of 1.85 gm/cc.

Kothari and Singwi[8] also made a calculation of the age from 1.46 ev. to thermal, in beryllium, and obtain a value of 25 cm^2.* To obtain this value, $\xi(E)$ [presented here as curve B, fig. 1] is averaged over a Maxwellian distribution to obtain $\xi(T_o)$, where T_o is the temperature of the distribution, and in this case is equal to the moderator temperature. The Fermi age integral is now expressed in terms of T_o with a lower limit of 310°K (the moderator temperature is 300°K). To be consistent, the authors[8] should have used 300°K as a lower limit for the age integral, since this is the temperature at which the neutron distribution is in equilibrium with the moderator. However, this would have resulted in an age of infinity, since $\xi(T_o)$ goes to zero at $T_o = 300°K$. The use of 310°K for a lower limit appears to be merely an attempt to obtain a finite value for the age with little regard for the physical situation.

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* The value quoted in reference 8 is 20 cm^2, however a list of errata, distributed by the authors, indicate that this value should be 25 cm^2.

Moreover, the weighing of $\phi(E)$ with a Maxwellian distribution at all energies below 1.46 ev. seem incorrect, since neutrons of energy from 5kT to 1.46 ev. do not have such a distribution. It appears, therefore, that the value of 25 cm^2, for the age from indium resonance to thermal in beryllium, is incorrect and much too large.

At present, there are no experimental results with which to compare the value of 8.94 cm^2, calculated herein.

Also for reasons discussed in section 3.4, the values of $\tau(E_t)$, for graphite, presented in table VI, as calculated from eq.[39] with Θ_D= 1000°K appears to be the most satisfactory. At E_t= 5kT= 0.129 ev.(at T=300°K), τ= 53.7 cm^2. This value is in good agreement with the age measurement, from indium resonance to thermal, in graphite, of 57.5 $\pm$ 5 cm^2 (for density of 1.6) made by the French[20]. The agreement between the two values may be coincidental, since the approximation of applying Nelkin's simple equation to the complex crystal structure of graphite is rather crude. However, it does tend to indicate a certain degree of confidence in the method.

In view of the many approximations incorporated in the derivation of the equations from which the age calculations were made, it is difficult to estimate the accuracy associated with the values of age from indium resonance to thermal of 8.94 cm^2 and 53.7 cm^2 in beryllium and graphite respectively.

V. Calculation of Age from Fission to Indium Resonance in Beryllium.

For completeness, it was decided to make a detailed calculation of the age, in beryllium, from fission to indium resonance. This value; when added to the age from indium resonance to thermal, previously determined; will give the total Fermi age, in beryllium, from fission to thermal. Because such a calculation had recently been performed, in detail, for graphite, it was considered unnecessary to repeat it. However, the only previous calculation of age from fission to indium resonance, in beryllium, recorded in the literature, was made by Goldberger[21] in 1946. Since the cross section of beryllium and the details of the fission spectrum were not known too accurately in 1946, it was considered worthwhile to perform this calculation again.

The difficulties associated with such a calculation are unrelated to the problems encountered in the calculation of the age from 1.46 ev. to thermal. In this case, the neutron energies are large enough so that the moderator atoms can be considered free, and crystalline binding is no longer a problem. The value of ξ used is the free atom value, ξ_o, and is constant throughout the entire energy range considered. The difficulties encountered involve the variation of scattering cross section at high energy (0.04-12 Mev), and the energy distribution of fission neutrons.

5.1 Method

The procedure to be followed is first to calculate the age to 1.46 ev. for monoenergetic neutrons at various source energies in the range of the fission spectrum (this age will be a function of neutron energy), then to weigh the age, so determined, with the fission spectrum.

The age of neutrons of energy E_n, to 1.46 ev., is given by

$$\tau(E_n)=\int_{1.46\,ev.}^{E_n}\frac{D}{\xi_o N\sigma_s}\cdot\frac{dE}{E} \qquad [50]$$

In the case of small absorbtion, and taking $\sigma_{tr}=(1-2/3A)\sigma_s$, equation [50] becomes

$$\tau(E_n)=\frac{1}{3\xi_o(1-2/3A)N^2}\int_{1.46}^{E_n}\frac{1}{[\sigma_s(E)]^2}\cdot\frac{dE}{E} \qquad [51]$$

Actually, eq.[51] is only the integral contribution to the age, and a first and last flight corrections (to be discussed later) must be added. Equation [51] is numerically integrated in the following way:

$$\tau(E_n)=1/P\sum_{i=1}^{n}\frac{1}{(\overline{\sigma_s})_i^2}\cdot\ln\frac{E_i}{E_{i-1}} \qquad [52]$$

where

$$P=3\xi_o(1-2/3A)N^2. \qquad [52a]$$

E_o= 1.46 ev.; $(\overline{\sigma_s})_i$ is the average value of the scattering cross section in the energy range E_{i-1} to E_i; E_i is greater than E_{i-1}; and E_n is the upper limit of the integral in eq. [51], and corresponds to the source energy for monoenergetic neutrons.

To obtain the age of fission neutrons, which are distributed over a wide range of source energies, E_n, one performs the following integration:

$$\tau_f = \frac{\int_o^\infty \tau(E_n)\cdot f(E_n)\cdot dE_n}{\int_o^\infty f(E_n)\cdot dE_n} \qquad [53]$$

where $f(E_n)$ is the number of fission neutrons in the energy interval dE_n about E_n. Equation [53] is numerically integrated as follows:

$$\tau_f = \sum_{n=1}^{m} \overline{\tau}_n \cdot f_n \qquad [54]$$

where

$$\overline{\tau}_n = 1/2[\ \tau(E_n) + \tau(E_{n-1})], \qquad [55]$$

and f_n is the fraction of fission neutrons having energies between E_{n-1} and E_n; m is the total number of groups used in the calculation.

The first flight correction , for source neutrons of energy E_n, is given by

$$FFC_n = 1/3(1-2/3A)N^2[\sigma_s(E_n)]^2 \qquad [56]$$

For neutrons distributed in a fission spectrum, eq. [56] becomes

$$FFC = \xi\Sigma_s/P \sum_{i=1}^{m} \frac{f_i}{[\overline{\sigma_{s_i}}]^2} \qquad [57]$$

where P is defined by eq. [52], and the fission spectrum is normalized so that $\sum_{i=1}^{m} f_i = 1$.

The last flight correction, in the calculation of the age to 1.46 ev., is given by

$$LFC = \frac{1}{3(1-2/3A)N^2[\sigma_s(1.46)]^2} \qquad [58]$$

The total age from fission to indium resonance is then the sum of eqs. [54], [57], and [58], i.e.

$$\tau[\text{fiss.-In. res.}] = \tau_f + FFC + LFC \qquad [59]$$

5.2 Results and Discussion

With the aforementioned procedure, the age in beryllium from fission to 1.46 ev. was calculated. Twenty energy groups were used to cover the fission spectrum and describe the cross section variation. The fission spectrum used in the calculation was taken from ANL-5800[22] for thermal neutron fission in U^{235}. In the energy range greater than approximately 1.5 Mev., the scattering cross section was obtained by subtracting the (n,2n) and (n,α)

cross sections from the total cross section. All cross section values were obtained from BNL-325[23]. The complete details of the calculation of the Fermi age from fission to 1.46 ev., in beryllium, are presented in table VII.

With the properties of beryllium as given in sec. 5.1, the factor P is given by eq.[52$_a$]as

$$P_{Be} = 3(0.207)(0.926)(0.1238 \cdot 10^{24})^2 = 0.882 \cdot 10^{46}.$$

The last flight correction, from eq.[58], is 0.665 cm^2. Referring to table VII, the values in column 11 are obtained by summing the values in column 10 as indicated in eq.[52]. The values in column 11, $\tau(E_n)$, are plotted against E_n in figure 3. This plot shows that the approximation of $\bar{\tau}_n$ by an arithmetic mean, eq.[55], is fairly accurate. Values of $\bar{\tau}_n$, so calculated, are presented in column 12 of table VII. The fission spectrum, presented in column 13, was obtained from ref. 22. The integral contribution to the age is obtained by summing the values in column 14 according to equation [54]. Similarly, the first flight correction is obtained by summing col. [15] according to eq.[57]. The total age from fission to 1.46 ev., in beryllium, is given by eq.[59] as

$$\tau[\text{fiss.-In. res.}] = 64.30 + 5.126 + 0.665$$
$$= 70.1 \text{ cm}^2$$

TABLE VII

Details of calculation of age from fission to indium res. in beryllium (density= 1.85 gm/cc).

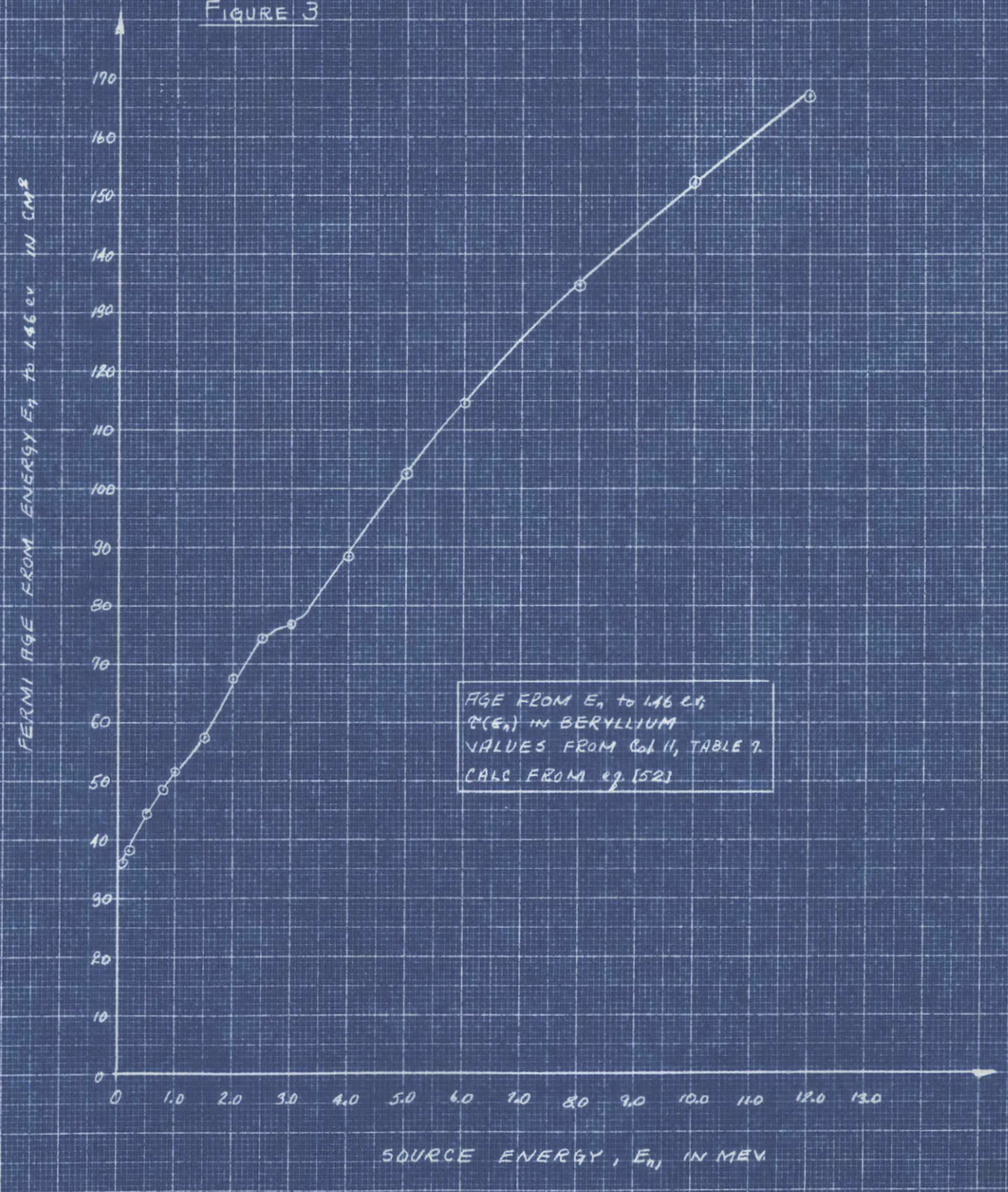
1	2	3	4	5	6	7	8
Group i orn	E_i mev.	E_{i-1} mev.	$\bar{\sigma}_{s_i}$: b	$(\bar{\xi})_i^2 \times 10^{48}$	$P(\bar{\sigma}_s)_i^2$	$\frac{1}{P(\bar{\sigma}_s)_i^2}$	$\frac{E_i}{E_{i-1}}$
1	0.04	1.46×10^{-6}	5.95	35.40	0.3120	3.210	2.74×10^{4}
2	0.10	0.04	5.85	34.20	0.3020	3.310	2.50
3	0.20	0.10	5.20	27.04	0.2385	4.190	2.00
4	0.50	0.20	4.20	17.62	0.1555	6.440	2.50
5	0.60	0.50	3.70	13.70	0.1210	8.260	1.20
6	0.65	0.60	5.70	32.50	0.2865	3.485	1.083
7	0.70	0.65	3.80	14.44	0.1270	7.87	1076
8	0.80	0.70	3.70	13.68	0.1205	8.30	1.143
9	0.85	0.80	3.90	15.20	0.1340	7.46	1.0625
10	1.00	0.85	3.40	11.65	0.1014	9.86	1.33
11	1.50	1.00	2.85	8.12	0.0716	13.99	1.50
12	2.00	1.50	1.80	3.24	0.0286	35.00	1.33
13	2.50	2.00	1.85	3.42	0.0316	31.60	1.25
14	3.00	2.50	3.00	9.00	0.0793	12.66	1.20
15	4.00	3.00	1.67	2.79	0.0246	40.6	1.33
16	5.00	4.00	1.33	1.77	0.0156	64.1	1.25
17	6.00	5.00	1.30	1.69	0.0149	67.1	1.20
18	8.00	6.00	1.27	1.61	0.0142	70.5	1.33
19	10.00	8.00	1.20	1.44	0.0127	78.8	1.25
20	12.00	10.00	1.18	1.40	0.0123	81.3	1.20

TABLE VII

continued

Group i or n	9 $\ln\frac{E_i}{E_{i-1}}$	10 $\frac{1}{P(\bar{\sigma}_s)_i^2}\ln\frac{E_i}{E_{i-1}}$	11 $\bar{\tau}(E_n)$ cm^{-1}	12 $\bar{\tau}_w$	13 f_n	14 $\bar{\tau}_w f_n$	15 $\frac{\xi_o}{P(\bar{\sigma}_s)_n^2} f_n$
1	10.20	33.10	33.10	33.10	0	0	0
2	0.9160	3.03	36.13	34.61	0.0139	0.481	0.0095
3	0.6930	2.91	39.04	37.59	0.0239	0.897	0.0205
4	0.9160	5.90	44.94	41.96	0.0950	4.000	0.127
5	0.1820	1.50	46.44	45.69	0.0351	1.608	0.060
6	0.0797	0.28	47.30	46.87	0.0357	1.670	0.0485
7	0.0731	0.58					
8	0.1336	1.11	48.41	47.86	0.0358	1.710	0.0621
9	0.0596	0.45	48.86	48.64	0.0178	0.865	0.027
10	0.2850	2.81	51.67	50.27	0.0527	2.650	0.108
11	0.4050	5.66	57.33	54.50	0.1621	8.840	0.480
12	0.285	9.98	67.31	62.32	0.1342	8.360	0.974
13	0.223	7.05	74.36	70.84	0.1054	7.460	0.690
14	0.182	2.30	76.66	75.51	0.0802	6.060	0.210
15	0.285	11.60	88.26	82.46	0.1032	8.500	0.857
16	0.223	14.30	102.56	95.41	0.0538	5.130	0.715
17	0.182	12.20	114.76	108.66	0.0269	2.920	0.373
18	0.285	20.10	134.86	124.81	0.0192	2.390	0.280
19	0.223	17.60	152.46	143.66	0.0042	0.598	0.0678
20	0.182	14.80	167.26	159.86	0.0011	0.169	0.0177
					Tot.	64.300	5.126

FIGURE 3



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The experimental value for the age from fission to indium resonance, in beryllium, is 80.2 ± 2 cm^2 (ref. 24). However, at energies greater than approximately 1.5 Mev., the (n,2n) and (n,α) cross sections become appreciable [see BNL-325]. These reactions, ocurring in the experimental sample, modify the original fission spectrum; consequently, one would not expect the measured age to agree with that value calculated with a fission spectrum. Meneghetti and Hummel[25] have estimated that the combination of (n,2n), and (n,α) reactions, in beryllium, tend to increase the original source neutrons by 8 or 9 percent. in an experiment. To determine the precise effect of this increase of source neutrons on the original fission spectrum, one would have to determine the energy distribution of the neutrons involved in these nuclear reactions. The analytical solution to this problem is highly complex and is not attempted herein.

Goldberger's[21] calculation, in 1946, resulted in a value of 81 cm^2 for the age from fission to In. resonance in beryllium, and Meneghetti and Hummel[25], assuming the scattering cross section equal to the total cross section, calculated a value of 89 cm^2. A calculation was also made[25] to determine what value of age to indium resonance would be measured in an experiment such as described in ref. 24. This calculation involved considering the effects of the (n,2n), and (n,α) reactions on the spectrum measured; the calculation employed only two groups of neutrons, and

the value obtained was 73 cm^2 (ref. 25).

In order to check Goldberger's value of 81 cm^2, an age calculation was made with the method described in sec. 5.1, from those cross sections, for beryllium, used at the time Goldberger made his calculation (1947)[26]. With the same fission spectrum as was used before (ref. 22), the integral contribution was found to be 78.3 cm^2. When the first and last flight corrections were added, the age from fission to indium resonance was found to be 83.5 cm^2. The difference between this value and the value of 81 cm^2, obtained by Goldberger, is probably due to the different fission spectrum and cross section values used in the respective calculations. Goldberger took his cross section values from report number MUC-HHG-7, while the values used for the comparison calculation were taken from ref. 26. Goldberger does not specify the fission spectrum that he used.

Since the numerical details of the calculations made by Meneghetti and Hummel[25] were not available, it is difficult to comment on the validity of their quoted values. They are presented here for purposes of comparison and completeness.

From the values obtained herein; for the age from fission to 1.46 ev. (sec. 5.2), and from 1.46 ev. to thermal (sec. 4.2); the total age from fission to thermal, in beryllium of density= 1.85 gm/cc, is

$$\tau[\text{fiss.-thermal}] = 70.1 + 8.94 = 79.0 \text{ cm}^2.$$

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