is made of eq. (18). If r is a uniformly distributed random number between 0 and 1, we have

$$r = \int_{q_{min}}^{q} P_a^{\pm}(q)dq \Big/ \int_{q_{min}}^{q_{max}} P_a^{\pm}(q)dq \qquad (19)$$

which may be solved for q. For weak nonparabolicity, fairly high lattice temperatures and not very high electric fields, eq. (19) yields approximately

$$q \approx q_{max}\sqrt{r}. \qquad \ldots (20)$$

The absorption and emission events are determined with the aid of eq. (16) by the usual procedure. (Fawcett *et al* 1970) q is determined from eq. (19) and β_0 is calculated from eq. (10). If another uniformly distributed random number is generated between 0 and 2π to fix the azimuthal angle ϕ, the final electron state after scattering is completely specified.

It may be noted that the sum of λ_a^+ and λ_a^- given by eq. (16) yields the expression for the total acoustic scattering rate in the elastic approximation, (Fawcett *et al* 1970). Furthermore, by setting $\alpha = 0$ in eqs. (10), (16) and (18) one readily obtains the expressions for a parabolic band structure.

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Partial structure factors for liquid alloys

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Recent studies (Gopala Rao & Murthy 1974, 1975a, 1975b) proved the usefulness of square well potential in the theoretical investigations of conducting fluids like liquid metals. In this note we propose to extend the same to binary liquid alloys, taking Na—K alloy as an example, for calculating the partial structure factors, S_{ij}, under the mean spherical model (MSM) approximation (Gopala Rao & Murthy, 1974)

As an extension of the MSM approximation for square well binary mixtures, we define,

$$C_{ij}(r) = C_{ij}^{hs}(r), \quad 0 < r \leqslant \sigma_{ij} \qquad \ldots (1)$$

$$= -\frac{u_{ij}(r)}{k_B T} = \frac{c_{ij}}{k_B T}, \quad \sigma_{ij} \leqslant r \leqslant A\sigma_{ij} \qquad \ldots (2)$$

$$= 0, \qquad r > A\sigma_{ij} \qquad \ldots (3)$$

with $\sigma_{ij} = (\sigma_i + \sigma_j)/2$. The superscript *hs* denotes the hard sphere solution of Percus-Yevick (PY) equation for binary mixtures (Lebowitz 1964) and c_{ij} and A are the depth and breadth, respectively, of the square well used. σ_i and σ_j are the hard sphere diameters of the species i and j respectively.

Using Lebowitz's (1964) solution of the PY equation for binary mixtures of rigid spheres to represent $C_{ij}(r)$ in the region, $0 < r \leqslant \sigma_{ij}$, and a square well potential to represent $C(r)$ in the region, $\sigma_{ij} \leqslant r \leqslant A\sigma_{ij}$, the Fourier transforms of $C_{ij}(r)$ can be written as,

$$\rho_i C_{ij}(k) = -\frac{24\eta_i}{(k\sigma_i)^6}\{a_i(k\sigma_i)^3[\sin k\sigma_i - k\sigma_i \cos k\sigma_i]\beta(k\sigma_i)^2[2k\sigma \sin k\sigma_b -$$

$$(k^2\sigma_i - 2)\cos k\sigma_i - 2] + \gamma[(4k^3\sigma_i - 24k\sigma_i)\times \sin k\sigma_i - (k^4\sigma_i - 12k^2\sigma_i + 24)\times$$

$$\cos k\sigma_i + 24]\} - \frac{24\eta_i\epsilon_{ii}}{k_B T}[-Ak\sigma_i \cos Ak\sigma_i + \sin Ak\sigma_i$$

$$+ k\sigma_i \cos k\sigma_i - \sin k\sigma_i]/(k\sigma_i)^3] \qquad \ldots (4)$$

and

$$C_{12}(k) = -\frac{4\pi}{k^6}\{(k^2[a_1 + 2b\sigma_1 + 4d\sigma_1^2(\sigma_{12} + 2\lambda)]$$

$$-24d\sigma_{12})k \sin k\sigma_{12} + (k^2[2b + 12d\sigma_1\sigma_2]$$

$$-k^4[a_1\sigma_{12} + b\sigma_1^2 + d\sigma_1^3(\sigma_{12} + 3\lambda)] - 24d)\times$$

$$\cos k\sigma_{12} + (24d - 12bk^2)\cos \lambda k + 24\lambda dk \sin \lambda k$$

$$+ \frac{4\pi\epsilon_{12}}{k^3 k_B T}[Ak\sigma_{12}\cos Ak\sigma_{12} + k\sigma_{12}\cos k\sigma_{12} + \sin Ak\sigma_{12} - \sin k\sigma_{12}] \qquad (5)$$

with $\eta_i = \pi\rho_i\sigma_i^3/6$, $\lambda = (\sigma_2 - \sigma_1)/2$ and ρ is the number density of the i-type atoms. The other constants, $\alpha, \beta, \gamma, \ldots$ etc. are as defined by Lebowitz (1964)

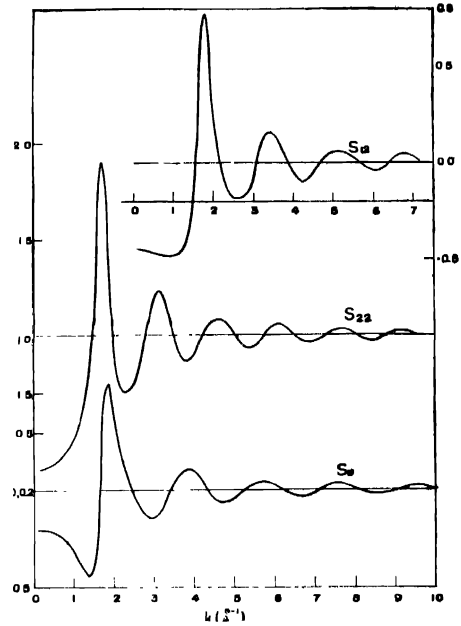
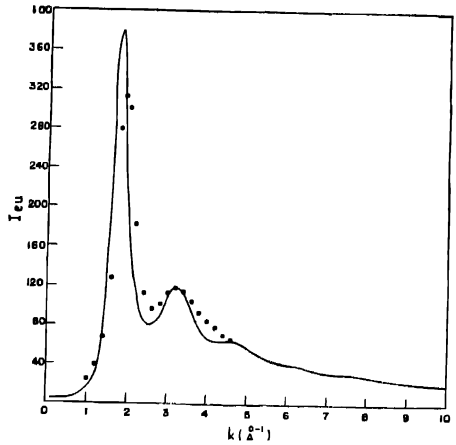


Fig. 1. Partial structure factors for liquid Na-K alloy at 373°K.



Fig, 2. Total intensity in electron units for Na-K alloy 37°K :——, theory;....., experiment.

(see also Ashcroft & Langreth 1967) The $C_{ij}(k)$ are related to S_{ij} as (e g. Ashcroft & Langreth, 1967),

$$S_{11}(k) = \{1-\rho_1 C_{11}(k)-\rho_1\rho_2 C_{12}^2(k)/[1-\rho_2 C_{22}(k)]\}^{-1} \quad \ldots (6)$$

$$S_{22}(k) = \{1-\rho_2 C_{22}(k)-\rho_1\rho_2 C^2_{12}(k)/[1-\rho_1 C_{11}(k)]\}^{-1} \quad \ldots (7)$$

$$S_{12}(k) = (\rho_1\rho_2)^{\frac{1}{2}} C_{12}(k)\{[1-\rho_1 C_{11}(k)][1-\rho_2 C_{22}(k)]-\rho_1\rho_2 C^2_{12}(k)\}^{-1} \quad \ldots (8)$$

and S_{ij} in turn are related to the total intensity of the scattered radiation as (Fournet 1957),

$$I_{en} = m_1 f_1^2 S_{11}+m_2 f_2^2 S_{22}+2(m_1 m_2)^{\frac{1}{2}} f_1 f_2 S_{12} \quad (9)$$

mi being the concentration of the species i in the mixture and f are the usual atomic scattering factors of i-type atoms

Eqs (4)–(8) have been used to compute the S_{ij} for liquid N_a—K alloy at 373K, the density being 0 87 gm/cm^3 ($m_1 = m_2 = 0\ 5$) and the results are shown in figure 1 The like potential parameters, σ, A, and ϵ used are those of the pure components (Gopala Rao & Murthy, 1974*c*), while the unlike parameters have been determined using the Lorentz-Bertherlot rules. Figure 2 shows the results obtained for the total intensity in comparison with the experimental results (Orton *et al* 1960) as reported by Enderby & North (1968) The measurement of agreement between theory and experiment is quite satisfactory, except an increase in the theoretical first peak height This may be due to the approximations involved, especially the Lorentz–Berthelot rules or to the experimental uncertainty As pointed out by Umar *et al* (1974), the X-ray data of Orton *et al* (1960) involves an underestimation of K scattering, which is a dominant feature around the first peak.

Thus the present model also represents the structure of liquid alloys quite satisfactorily.

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