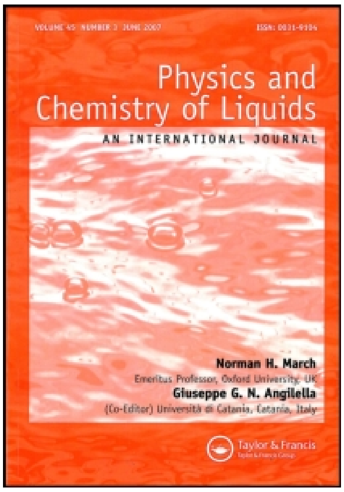

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Wave-Number Dependent Viscosity of Liquid Metals

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LETTER
Wave-Number Dependent Viscosity of Liquid Metals

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Two approaches to the wave-number dependent viscosity $\eta(q)$ of liquid metal Rb are compared. The first is based on the two-component theory of a liquid metal, and expresses $\eta(q)$ in terms of the ionic static structure factor $S(q)$ plus elastic scattering data. The second describes the ion-ion interaction by an effective pair potential, mediated by the conduction electrons. Some preliminary results for liquid Ga are also briefly referred to.

KEY WORDS: Effective ion-ion interaction, molecular dynamics, two-component theory.

The purpose of this note is to make contact between two different approaches to the wave-number dependent shear viscosity $\eta(q)$ of a liquid metal, with specific reference to liquid Rb. The first of these approaches, due to Tosi, Parrinello and March[1], treats the liquid metal, say Rb, as a two-component system of Rb^+ ions and electrons e. The second method, typified by the work of Balucani, Vallauri and Gaskell[2], regards the liquid as having only one component, essentially a collection of suitably screened ions, interacting via an effective pair potential $\phi(r)$ which is mediated by the electrons.

Taking the two approaches in turn, the two-component approach allows the q-dependent viscosity $\eta(q)$ (cf. Eq. (2) below) to be expressed in terms of the ionic static structure factor $S(q)$ by

$$\eta(q) = \pi\rho^2 k_B T \frac{S(q, 0)}{[S(q)]^2}, \tag{1}$$

the approximations underlying the simple formula (1) being set out in Ref. 1. Here, $S(q, \omega)$ is the dynamical structure factor of the ions, and it is to be emphasized that in Eq. (1) only the $\omega = 0$ limit of $S(q, \omega)$ appears, apart from the static structure factor $S(q)$ which is the integral of $S(q, \omega)$ over all energy transfers.

While the discussion of the elastic scattering of neutrons, embodied in $S(q, 0)$ in Eq. (1), is still a difficult problem for analytic liquid state theory, Barker *et al.*[3] have reported measurements of such elastic scattering from liquid Rb and liquid Ga (see also Ref. 1).

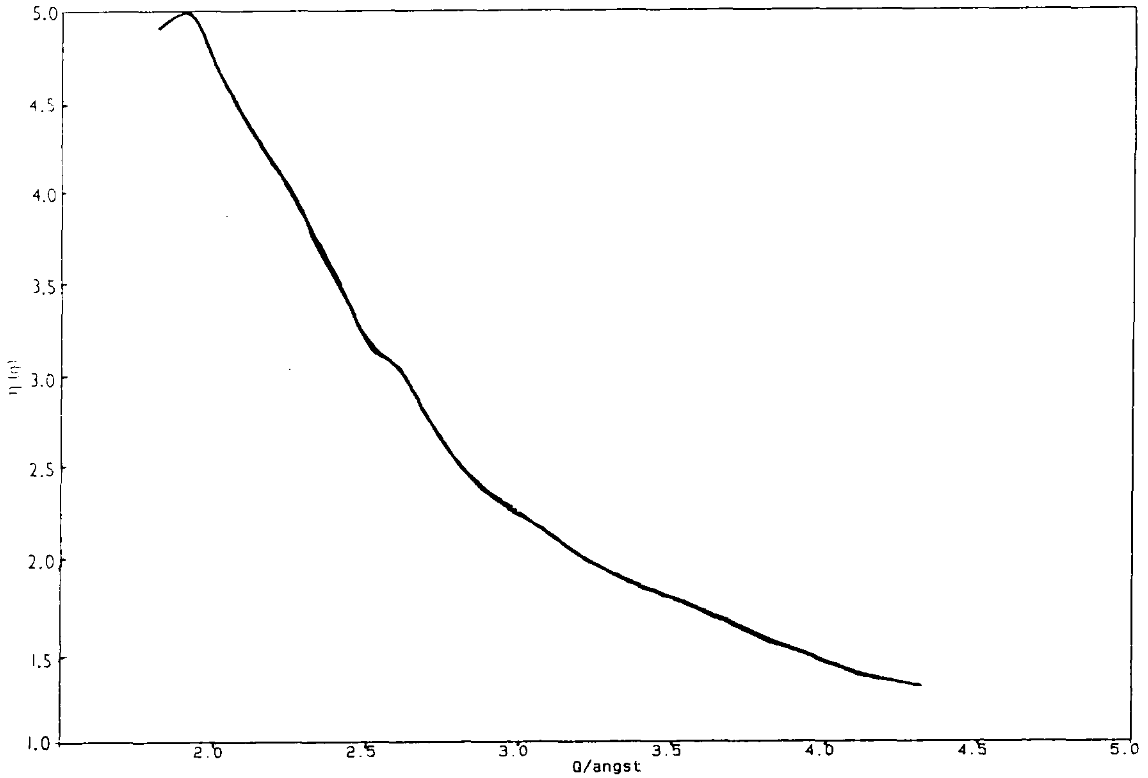

Figure 1 Plot of 'sound-wave' viscosity, generalized to be wave-number dependent (cf. Eq. (2)). The curve is obtained using experimental data for elastic scattering[3] and for static structure[4] in Eq. (1). The units of $\eta(q)$ are arbitrary, while the wave number is in reciprocal Å. Note that the range of wave number is restricted by the experimental data. Also, the 'peak' shown in $\eta(q)$ is anticipated to be within the experimental error, and therefore not a real feature of the wave number dependence of the 'sound-wave' viscosity.

Using recent liquid state static structure data of Hensel *et al.*[4] for the thermodynamic state of Rb characterized by temperature $T = 473$ K, together with the elastic scattering data of Barker *et al.*, Figure 1 shows $\eta(q)$ versus q over the available range of the elastic scattering data. Since, as discussed in Refs. 3 and 1, the elastic scattering reflects the peaks and valleys in $S(q)$ rather directly, it is clear that the structure in the 'sound-wave' viscosity $\eta(q)$ given in Eq. (1) is intimately related to the static structure factor $S(q)$.

Having discussed the sound-wave viscosity $\eta(q)$ from the fundamental standpoint of the two-component theory of a liquid metal, let us now turn to the second approach; that of treating liquid Rb as a one-component liquid of screened ions, with an effective pair potential $\phi(r)$ which is mediated by the conduction electrons. To date, to our knowledge, the q-dependent sound-wave viscosity has not been obtained from this approach with a realistic pair potential. However, the work of Balucani, Vallauri and Gaskell[2] has used the effective pair potential of Price[5], in conjunction with molecular

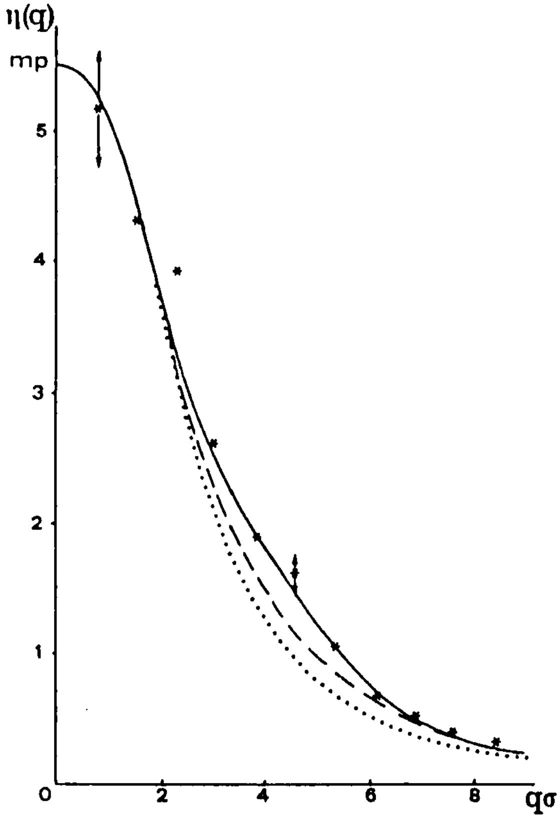

Figure 2 Shows the shear viscosity as calculated by molecular dynamics by Balucani *et al.*[2] using the effective interionic pair potential of Price *et al.*[5] The stars denote the molecular dynamics data of Ref. 2. The dotted and solid lines are from versions of the viscoelastic model[2]. The dashed line results from a 'two-exponential' memory function fit.[2] (N.B. Balucani *et al.* choose $q_0\sigma = 6.23$ in liquid Rb, with q_0 the principal maximum of the static structure factor.)

dynamics, to calculate the q-dependent shear viscosity $\eta_s(q)$. In the long wavelength limit $q \rightarrow 0$, the relation between η and η_s involves the bulk viscosity ζ through

$$\eta = \tfrac{4}{3}\eta_s + \zeta. \tag{2}$$

The form of the q-dependent shear viscosity $\eta_s(q)$ according to the work of Ref. 2 is reproduced in Figure 2. As in Figure 1 for $\eta(q)$, there is some semblance of structure in the q dependence of the shear viscosity $\eta_s(q)$.

Unfortunately, to date, much less is known about the bulk viscosity ζ than about the shear viscosity η_s. The hard sphere theory of Collins and Raffel[6], and Longuet-Higgins and Pople[7] directly relates the long wavelength limit values through

$$\frac{\eta_s}{\zeta} = \frac{3}{5} \tag{3}$$

but this result cannot be expected to be quantitative for a liquid metal like Rb with a relatively soft core. Neither can it be assumed that the q-dependence of ζ will closely follow that of η_s. Of course, one could subtract, effectively, the results of Figures 1 and 2 to determine the q-dependence of the bulk viscosity, but this will not be pursued here.

The present note is intended to point out the interest for first-principles liquid state theory of further work on the q-dependent viscosity. It is clearly of interest to bring into more intimate contact the two-component theory based on Eq. (1) and the conceptually attractive, simpler, one-component approach based on an effective pair potential. We are currently studying transport properties of the heavy alkali metals as they are taken up the coexistence curve towards the critical point, using the data of Hensel *et al.*[4]

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