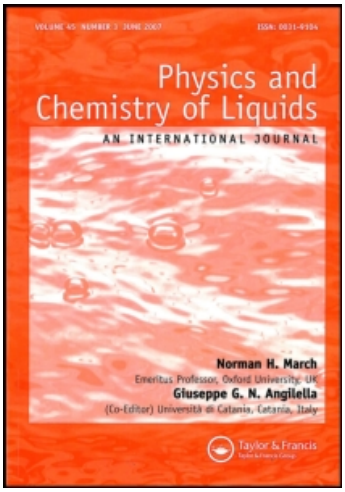

Physics and Chemistry of Liquids
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713646857

Neutron and X-ray diffraction from liquid Rb

N. H. March[abc]; I. Nagy[cd]; P. M. Echenique[ce]
[a] Physics Department, University of Antwerp, Antwerp, Belgium [b] University of Oxford, Oxford, UK [c] Donostia International Physics Center (DIPC), San Sebastian, Spain [d] Department of Theoretical Physics, Technical University of Budapest, Budapest, Hungary [e] Departamento de Fisica de Materiales, Facultad de Ciencias Quimicas, Universidad del Pais Vasco, San Sebastian, Spain

To cite this Article March, N. H. , Nagy, I. and Echenique, P. M.(2008) 'Neutron and X-ray diffraction from liquid Rb', Physics and Chemistry of Liquids, 46: 5, 481 — 483
To link to this Article: DOI: 10.1080/00319100802247555
URL: http://dx.doi.org/10.1080/00319100802247555

Physics and Chemistry of Liquids
Vol. 46, No. 5, October 2008, 481–483

Taylor & Francis
Taylor & Francis Group

LETTER

Neutron and X-ray diffraction from liquid Rb

N.H. March[abc], I. Nagy[cd]* and P.M. Echenique[ce]

[a]*Physics Department, University of Antwerp, Antwerp, Belgium;* [b]*University of Oxford, Oxford, UK;* [c]*Donostia International Physics Center (DIPC), San Sebastian, Spain;* [d]*Department of Theoretical Physics, Technical University of Budapest, Budapest, Hungary;* [e]*Departamento de Fisica de Materiales, Facultad de Ciencias Quimicas, Universidad del Pais Vasco, San Sebastian, Spain*

(*Received 22 May 2008; final version received 6 June 2008*)

Motivated by the recent X-ray diffraction experiments by Matsuda, Tamura, and Inui (Phys. Rev. Letters **98**, 096401 (2007)). on liquid Rb, it is stressed that important information about electron–ion and electron–electron correlations is embodied in a comparison of their X-ray data with the neutron observations of Franz, Freyland, Glaser, Hensel, and Schneider (J. Phys. (Paris) Colloq. **8**, 194 (1980)). Electron diffraction experiments on liquid Rb would also be important, if feasible.

Keywords: liquid Rb; correlations; X-ray diffraction; neutron diffraction

The exceptionally detailed X-ray diffraction data on expanded liquid Rb by Matsuda *et al.* [1] (referred to as MTI below) prompt us to make a number of observations.

(i) First of all, MTI mention differences from the neutron scattering results of Franz *et al.* [2] but do not elaborate on the reasons for that. We therefore stress below the interesting electron–ion (ei) and electron–electron (ee) structural information embodied, at least in principle, in the comparison of the MTI X-ray data with the counterpart neutron observations.

(ii) Comparison with the theory of expanded jellium is pressed by MTI. Already, one feature for the heavier alkali fluid metal Cs is available, which introduces the shrinking of the discontinuity in the electron momentum distribution $n(k)$ at the Fermi momentum k_F as the density is lowered. Using the experimental results analysed by Warren [3] for the magnetic susceptibility of Cs along the liquid–vapour coexistence curve towards the critical point, Chapman and March [4] demonstrated that the above discontinuity in $n(k)$ was quite markedly different from jellium (0.2 instead of 0.6) at the cross-over between the regime of Pauli paramagnetism and the low-density Curie limit. W.W. Warren (Personal communication to N.H. March) subsequently confirmed the theoretical estimate in [4] for the magnitude of the discontinuity. This shows that at this cross-over point, both electron–electron and electron–ion interactions play important quantitative roles in determining the magnitude of the discontinuity in $n(k)$ in

*Corresponding author. Email: nagy@phy.bme.hu

ISSN 0031–9104 print/ISSN 1029–0451 online

DOI: 10.1080/00319100802247555
http://www.informaworld.com

expanded liquid Cs, and one can safely assume that an analogous situation will obtain in fluid metallic Rb.

(iii) Using experimental neutron data for expanded Cs again along the liquid–vapour coexistence curve by Jüngst *et al.* [5], one of us [6] had earlier fitted their data for the density d in terms of coordination number z by

$$d = az + b, \tag{1}$$

where $a = 230$ and $b = -80$, both in kg m^{-3} (see also [7]). This Equation (1) yielded $z = 2$ for the coordination number of fluid Cs at the critical density, consistent with the results extracted from neutron experiments by Winter and Hensel [8]. Though X-ray data were used, somewhat less appropriately as referred to again below, in [1] the same essential conclusion (see low-density limit of z plotted by MTI in their Figure 3) was reached for Rb.

We now elaborate a little further on some of the above summary points. Beginning with comparison of MTI between X-ray and neutron scattering data, it is highly relevant to refer to the recent theoretical study of Leys and March [9], who implement quantitatively the general distinction made in the early work of Egelstaff *et al.* [10]. Essentially, a liquid metal-like expanded Rb treated in [1] is a two-component system of ions and (quantal) electrons. Thus like the classical molten salt NaCl, three partial structure factors are required to completely define the two-component fluid. We denote these below as the nuclear–nuclear (nn) piece $S_{nn}(k)$, the electron–ion (ei) contribution $S_{ei}(k)$ and the electron–electron (ee) partial structure factor $S_{ee}(k)$. Naturally therefore, three experiments are needed to extract this complete structural information. Already Franz *et al.* [2] have measured $S_{nn}(k)$ directly by neutron diffraction. It is encouraging for such partial structure factor analysis that MTI stress marked differences between the neutron measurements [2] and their X-ray data [1].

In this same context, Leys and March [9] considered Mg and used computer simulation for $S_{ei}(k)$, plus the correlation study of Cusack *et al.* [11] for $S_{ee}(k)$. Equally to the point of this Letter is the fact, already stressed in [10], that neutron, X-ray and electron diffraction data combined would, in principle, allow the 'experimental' extraction of $S_{ei}(k)$ and $S_{ee}(k)$. We recommend that attention be given to whether electron diffraction experiments could be carried out along the same thermodynamic path that Matsuda and co-workers utilise in their Figure 1.

Acknowledgements

The contribution of N.H. March to the present study was carried out during a visit to DIPC, San Sebastian. N.H. March wishes to thank Professors P.M. Echenique and A. Rubio for generous hospitality. Support from the Basque UPV/EHU (Grant No. 9/UPV 00206.215-13639/2001), the Spanish MEC (Grant No. FIS2004-06490-C03-00), the EU Network of Excellence NANOQUANTA (Grant No. NMP4-CT-2004-500198) and the OTKA (Grant No. T049571) is acknowledged.

References

[1] K. Matsuda, K. Tamura, and M. Inui, Phys. Rev. Lett. **98**, 096401 (2007).

[2] G. Franz, W. Freyland, W. Glaser, F. Hensel, and E. Schneider, J. Phys. (Paris) Colloq. **8**, 194 (1980).

[3] W.W. Warren, Phys. Rev. B **29**, 7012 (1984).
[4] R.G. Chapman and N.H. March, Phys. Rev. B **38**, 792 (1988).
[5] S. Jüngst, B. Knuth, and F. Hensel, Phys. Rev. Lett. **55**, 2160 (1985).
[6] N. H. March, Phys. Chem. Liquids **20**, 241 (1989); J. Math. Chem. **4**, 271 (1990).
[7] G.R. Freeman and N.H. March, J. Phys. Chem. **98**, 9486 (1994).
[8] R. Winter and F. Hensel, Phys. Chem. Liquids **20**, 1 (1989).
[9] F.E. Leys and N.H. March, J. Phys. A: Math. Gen. **36**, 5893 (2003).
[10] P.A. Egelstaff, N.H. March, and N.C. McGill, Can. J. Phys. **52**, 1651 (1974).
[11] S. Cusack, N.H. March, M. Parrinello, and M.P. Tosi, J. Phys. F: Metal Phys. **6**, 749 (1976).