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# The structure of molten bismuth–lead alloys

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In order to extend the efforts to derive an effective pair potential for liquid metals to more complicated systems, neutron diffraction measurements of $S(Q)$ for bismuth–lead alloys were performed on the liquid and amorphous diffractometer (LAD) at the Rutherford–Appleton Laboratory. The measurements were performed for different Bi–Pb compositions at different temperatures approaching the melting point for each alloy The main efforts were focused on investigating the variation of the position and height of the first peak of the structure factor and its shoulder as a function of composition and temperature. The results suggest singularity in evolution of the nearest neighbour arrangement when the composition approaches the eutectic point

## 1. Introduction

In recent years, there has been significant interest in the determination of the structure and of the interatomic pair potential for simple metals and liquid binary alloys. Successful attempts to derive the interatomic pair potential from the structure factor have been reported. Particularly, the interatomic pair potentials for liquid lead [1] and liquid bismuth [2] were obtained. So the next step is to derive the interatomic pair potential for Pb–Bi alloys from their structure factors. This paper reports measurements of the structure factors for liquid Pb, Bi and some of the Pb–Bi alloys at temperatures close to the melting point.

## 2. Experimental procedure

The neutron diffraction measurements were performed on the liquid and amorphous diffractometer (LAD) at the Rutherford–Appleton Laboratory. The standard data treatment and the usual corrections offered by the GENIE software package were applied to extract the final structure factors from the raw data. The measurements reported in this paper were performed on the liquid samples just above their melting points as described in table 1.

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## 3. Results and discussion

Figure 1 shows the structure factors, $S(q)$, of Pb–Bi alloys as function of bismuth concentration. The measurements were performed up to a momentum transfer of 25 $Å^{-1}$. It is interesting to see the development of the shoulder of the main peak of the structure factor as a function of bismuth concentration, as well as the change in the height of the main peak. This feature is discussed below. The structure factor for liquid lead agrees very well with the one obtained by Dahlborg et al. [3] and with the structure factor calculated by molecular dynamics simulation with the interatomic pair potential proposed by Dzugutov et al. [1]. Figure 2 shows the comparison of the structure factor obtained in this measurement with the molecular dynamics simulation of Dzugutov [2] and confirms the correctness of this pair potential. The structure factor of pure bismuth disagrees in detail – as shown in fig. 3

Table 1
Parameters of the measured samples

| Sample | $T$ (K) | Number density (Å$^{-3}$) |
|---|---|---|
| Pb | 623 | 0.03095 |
| $Pb_{70}Bi_{30}$ | 493 | 0.03077 |
| $Pb_{45}Bi_{55}$ | 413 | 0.03025 |
| $Pb_{20}Bi_{80}$ | 493 | 0.02958 |
| Bi | 548 | 0 02891 |

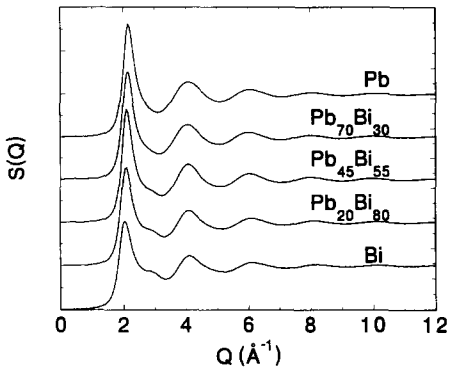


Fig 1. Structure factor, $S(Q)$, of Pb–Bi alloys for different concentrations of bismuth.

with the previous measurements made by Dahlborg and Davidovic [4]. The largest difference appears just around the shoulder and the second peak of the structure factor. The discrepancy between the MD-fitted structure factor and the neutron diffraction data in the region of the shoulder was suggested [2] to arise from many-body forces. The new results, which give much

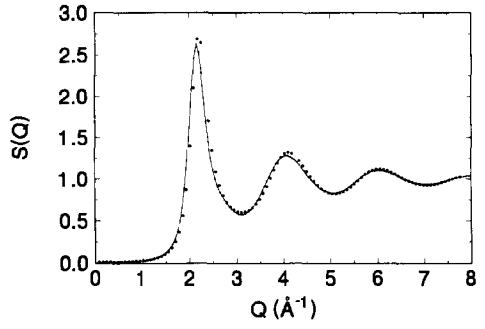


Fig 2. Structure factor of liquid lead at 623 K measured in this study (solid line with vertical bars corresponding to statistical errors) compared with the results of the earlier molecular dynamics simulation [2] (dots).

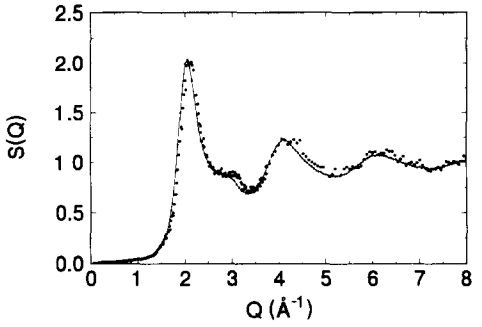


Fig 3. Structure factor of liquid bismuth at 548 K measured in this study (solid line with vertical bars corresponding to statistical errors) compared with the one measured by Dahlborg and Davidovic [4] (dots)

better precision in just that region, imply that the interatomic pair potential for liquid bismuth derived by Dzugutov [2] should be re-evaluated based on these data and the suggestion concerning the possible contribution of many-body forces should be re-examined, as already pointed out in ref. [5].

Figure 4 presents in detail the changes of the heights of the first and the second peaks of the structure factor as a function of bismuth concentration. The values are normalized to the height of the corresponding peak for pure lead. The second peak is almost constant, with the exception of the eutectic concentration where the value increases by about 6%. The main peak drops very

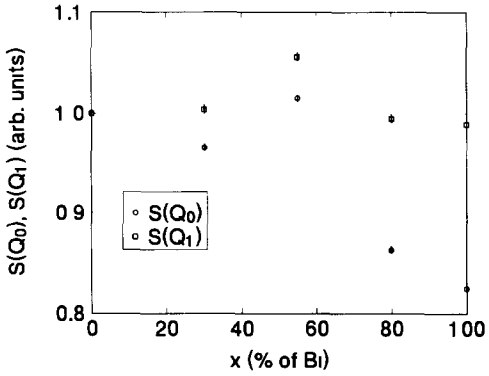


Fig 4. Variation of the peak heights – $S(Q_0)$ and $S(Q_1)$ – of the structure factor for liquid Pb–Bi alloys at temperatures just above the melting point. The values are normalized to the corresponding peak values for pure lead. Vertical bars are associated with the statistical error of the measured points

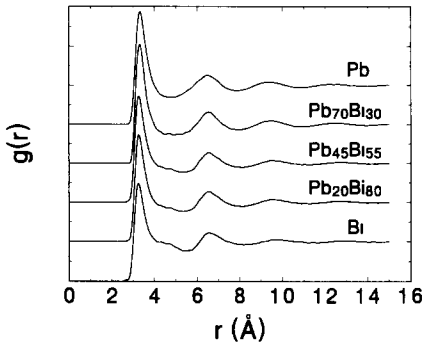


Fig. 5 Radial pair distribution function of Pb1–Bi alloys for different concentrations of bismuth

significantly (up to 18%) for bismuth concentrations above the eutectic point (54%). This change indicates a major rearrangement of the nearest neighbour shell in this region. Unfortunately, the experimental points are not dense enough to make a final conclusion.

Finally, fig. 5 show the radial distribution function as a function of the bismuth concentration. An evolution of the main peak, its shoulder, and changes in the shape of the second peak of $g(r)$ can be observed. The position, $r_0$, of the first peak of $g(r)$ decreases almost linearly from 3.325 Å for pure lead to 3.25 Å for pure bismuth, as displayed in fig. 6.

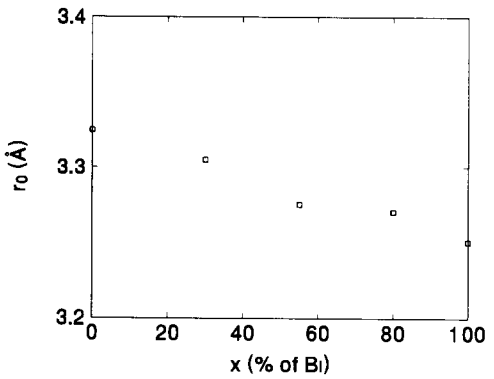


Fig 6. Positions of the first peak of the radial pair distribution function $g(r)$, $r_0$, as a function of alloy composition.

## 4. Conclusions

As was demonstrated in earlier MD studies on liquid lead and bismuth, the pair potentials in these two liquid metals are rather similar, while the local order is fundamentally different. This suggests that a continuous variation of the pair interaction should result in a discontinuous structural transformation. In a vague approximation, if the effects of short-range chemical ordering are ignored, the change in the interionic interaction can be induced by varying the composition of Bi–Pb liquid alloy. Our results indicate that the variation of the measure $S(Q)$ with concentration has a singularity at the eutectic point. This may be seen in fig. 4. However, other characteristics change continuously. More diffraction measurements for Bi concentrations between 55 and 80% would be needed to refine the described effect, which might be considerably washed out by the short-range chemical ordering. Also, new structure factor measurements on liquid Bi show the necessity for the reevaluation of the interatomic pair potential [2]. The diffraction results for Pb–Bi liquid alloys presented here provide an opportunity to carry out a detailed computer simulation study of these alloys.

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