

Partial Structure Factors of Liquid Na-K and AI-Mg Alloys(Physics)

| 著者 | WASEDA Y., OHTANI M., SUZUKI K. |
|-------------------|---|
| journal or | Science reports of the Research Institutes, |
| publication title | Tohoku University. Ser. A, Physics, chemistry |
| | and metallurgy |
| volume | 26 |
| page range | 179-179 |
| year | 1976 |
| URL | http://hdl.handle.net/10097/27834 |

Effective Interionic Pair Potentials and Properties for Liquid Sodium and Potassium

Y. Waseda and K. Suzuki

Acta Metallurgica, 21 (1973), 1065.

Effective interionic pair potentials for liquid sodium and potassium have been derived from recent X-ray diffraction data using the Born-Green and Percus-Yevick equations. The results, in good agreement with pseudopotential or molecular dynamics calculations, were obtained in the case of the Born-Green equation.

Self-diffusion coefficients of these metals were calculated from the Born-Green pair potential and the pair correlation function using the kinetic theory of fluids. The contributions of the hard, soft and cross-effect between the hard and soft forces to the self-diffusion coefficient were discussed. In addition, viscosity coefficients and surface tensions were calculated. In all cases, adequate agreement with experimental data was obtained.

Partial Structure Factors of Liquid Na-K and Al-Mg Alloys

- Y. WASEDA, M. OHTANI and K. SUZUKI
- Z. Naturforschung, 28a (1973), 1002.

Three partial structure factors $S_{ij}(Q)$ have been evaluated from the scattered X-ray intensities of liquid Na-K and Al-Mg alloys assuming that the $S_{ij}(Q)$ are independent of the relative abundance of the respective elements in the alloys. The functions $S_{ii}(Q)$ and $S_{jj}(Q)$ and the reduced radial distribution functions $G_{ii}(r)$ and $G_{jj}(r)$ obtained in this work are very similar to those observed in the respective pure liquid metals. In both cases, $S_{ij}(Q)$ and $G_{ij}(r)$ have maxima which lie in between those of the pure elements. From these results, liquid Na-K and Al-Mg alloys are interpreted as random mixing fluids.

A comparison between the partial structure factors obtained in this work and those calculated from the hard sphere model was made. Adequate agreement was obtained on the low angle side of the first peak, but agreement on the whole pattern is not necessarily found. The electrical resistivity was calculated using Faber-Ziman's theory and compared with experimental data.

Interionic Potentials in Liquid Metals Including Liquid Noble and Transition Metals

Y. WASEDA and K. SUZUKI

Phys. Stat. Sol. (b), 57 (1973), 351.

The Born-Green equation has been analyzed numerically to derive the effective interionic pair potentials from the structural data observed by X-ray or neutron diffraction experiments for liquid metals (Mg, Zn, Hg, Al, Ga, In, Tl, Sn, Pb, Sb, Bi), noble metals (Cu, Ag, Au), and transition metals (Fe, Ni) using a linearized simultaneous equation method. In all cases the potentials were found to be insensitive to temperature and to have long-ranged oscillations. But the damping behaviour