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Abstract

Full Text

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PHYSICS

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ON THE STRUCTURE OF LIQUID NICKEL AND IRON

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The structure of nickel and iron was investigated by the method of X-ray structural analysis at temperatures 30–40° above the melting point. The carbon content in the metal after the experiments did not exceed 0.010%.

The intensity of the radiation scattered by the free surface of the liquid metal was recorded with a scintillation counter. For monochromatization and separation of the fluorescent radiation, a pulse analyzer and balanced filters were used. The recording was carried out successively at angles of incidence of the X-ray beam K_αMo on the surface of the specimen $\alpha = 7$ and 17°. At $\alpha = 7°$ the divergence angle of the primary beam was $3 \cdot 10^{-3}$ rad; at $\alpha = 17°$, $7 \cdot 10^{-3}$ rad; the area of the irradiated surface did not exceed 9 mm^2. The intensity was recorded by an automatic potentiometer during continuous rotation of the counter. Heating and melting of the metal were carried out by high-frequency currents in an atmosphere of pure helium. The temperature of the surface of the liquid metal was measured with a micro-optical pyrometer. The technique is described in more detail in (^{1}).

Fig. 1. Atomic distribution function of liquid nickel and liquid iron

Analysis of the intensity curves showed that the maxima of the curve $I(S)$, $S = 4\pi \sin\theta/\lambda$, for liquid iron are shifted toward smaller angles in comparison with the curve for nickel. This is revealed especially clearly when soft radiation is used (Table 1).

The atomic distribution functions were calculated on a Minsk-22 computer (Fig. 1). The differences in the shape of the curves are small and do not provide grounds for conclusions about differences in the atomic packings in liquid nickel and iron. Signifia pronounced asymmetry of the first maximum of the curve for iron, similar to that reported in work (^1), was not observed. This may be connected with insufficient monochromatization of the radiation in work (^1): in (^1) monochromatization was carried out with a single selectively absorbing filter instead of the balanced filters used in the present work.

If it is assumed that the atomic packings in liquid nickel and iron are of the same type, then the difference in the positions of the maxima of the intensity curves may be regarded as evidence that the most probable interatomic distances r_1 in iron are greater than in nickel. From the position of the first maximum of the intensity curve one can estimate the difference in distances: the quantity r_1 can be approximately determined from the formula $r_1 = A/S_1$, where A is a constant depending on the type of packing, and S_1 is the position of the first maximum of the intensity curve (^2). Assuming the packings to be of the same type, A may be taken to be the same for iron and nickel. In this case it is meaningful to analyze only the difference $\Delta r_1 = r_{1\mathrm{Fe}} - r_{1\mathrm{Ni}}$, since the constant A itself is not known exactly.

As can be seen from Table 1, the difference Δr is 0.10 Å, which is approximately twice as large as the difference in the shortest distances in solid nickel and iron at those temperatures at which both metals have the same structure—fcc.

The most probable interatomic distances determined from the position of the first maximum of the atomic distribution function for nickel and iron likewise differ by approximately 0.10 Å. It should be noted that in work (^4) the position of the first intensity maximum for iron is given in agreement with that obtained in the present work; however, the position of the first maximum of the distribution curve given in (^4), $r_1 = 2.52$ Å, is somewhat smaller than follows from the $4\pi r^2 \rho(r)$ curve shown in Fig. 1.

Table 1

Characteristics of short-range order

Metal	Melt near melting T: position of the 1st maximum $I(S)$, $2\theta_1$ in Fe radiation	Melt near melting T: position of the 1st maximum $I(S)$, $2\theta_1$ in Mo radiation	Melt near melting T: position of the 1st maximum $I(S)$, S_1, Å^{-1}	Melt near melting T: r_1, Å, determined from $I(S)$	Melt near melting T: r_1, Å, determined from $4\pi r^2\rho(r)$	Crystal, data (^3), $T =$ 1360°: phase	Crystal, data (^3), $T =$ 1360°: a	Crystal, data (^3), $T =$ 1360°: r_1, Å	Crystal, data (^3), $T =$ 1508°: phase	Crystal, data (^3), $T =$ 1508°: a	Crystal, data (^3), $T =$ 1508°: r_1, Å
Fe	54°30′±20′	19°±20′	2.98	2.59	2.58	γ	3.681	2.603	δ	2.9306	2.535
Ni	57°±20′	20°±20′	3.10	2.49	2.45	γ	3.615	2.556			

At present there are no well-founded considerations that could explain the different change in the interatomic distances in nickel and iron upon melting.

It may be assumed that the difference in the positions of the maxima of the $I(S)$ curves is connected with a difference in the types of packings—close to fcc in nickel and close to bcc in liquid iron. However, this assumption is not confirmed by analysis of the $4\pi r^2\rho(r)$ curve, both that shown in Fig. 1 and that obtained in (^4). For bcc packing, two coordination shells with 8 and 6 atoms, respectively, fall within the region of the first maximum. Therefore the first maximum for bcc packing should be more asymmetric than for fcc packing, where one coordination shell with 12 atoms falls within the region of the first maximum. As can be seen from Fig. 1, no such difference between the $4\pi r^2\rho(r)$ curves for iron and nickel is observed.

It is possible that in liquid iron there simultaneously exist regions with packings close to bcc and fcc structures.

Suggestions about the possibility of the coexistence of different types of atomic packings in metallic melts have been made repeatedly

($^{5-7}$). A neutron-diffraction study of liquid CuSn alloys, carried out using different copper isotopes (^{8}), showed that, in the split intensity maximum, one of the maxima is caused by scattering from tin-rich regions, and the other by copper-rich regions. These results may be regarded as reliable experimental evidence for the possibility of the coexistence of different types of atomic packings in two-component systems.

In works (^{5,6}), on the basis of an analysis of intensity curves obtained for liquid mercury and tin, it was concluded that in the melt there are regions with dense atomic packing and regions with a structure characteristic of the given metal at low temperatures (for tin) or high pressures (for mercury). However, such an interpretation of the intensity curves is not the only possible one: the presence of secondary maxima on the intensity curves may be a consequence of the preservation in the liquid, near the melting temperature, of the packing characteristic of the given crystal before melting (^{9}).

Thus, the assumption that different types of atomic packings exist in pure metals does not contradict the experimental facts, but it cannot be considered experimentally proven.

One may hope that increasing the resolving power of X-ray and neutron structural methods of investigation will make it possible to detect fine details of diffraction patterns, similar to what has been shown in works (^{10,11}) for liquid lead. Comparison of experimental intensity curves obtained with higher resolving power with intensity curves calculated for models consisting of packings of different types will make it possible to draw more substantiated conclusions about the presence of particular packings in a liquid metal.

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Note: Figure translations are in progress. See original paper for figures.