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SHORT-RANGE ORDER IN TRANSITION METAL-METALLOID GLASSES

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A typical metallic glass consists of transition metal with about 15-25 at.% of one or more kinds of metalloids. Their structure and especially the nature of the short-range atomic arrangements is a problematic issue arising from difficulties in getting direct experimental information. The most direct information on the atomic structure of metallic glasses has been obtained from conventional X-ray and neutron scattering measurements in terms of the interference function. Although the interference functions contain information on both the short-range order and long-range order in these amorphous alloys, this information can only be extracted by complex procedures which involves theoretical models. However, even if all the individual partial structure factors are determined separately, only the average of the atomic configurations can be obtained - no detailed information on the probability distributions of different possible atomic configurations is available.

The hyperfine field distribution \( p(H) \) determined by Mössbauer spectroscopy gives valuable information in the study of short-range order because of its sensitivity to local environments. The evaluation of \( p(H) \) from the strongly broadened and overlapping lines of the Mössbauer spectra is a difficult task. The unknown intensities of the second and fifth lines may cause serious systematical errors in the determined \( p(H) \); especially the presence of paramagnetic components can be misinterpreted as a "tail" in \( p(H) \) (i.e. the distribution spreads to zero field) as it has been done for \( \text{Fe}_{75}\text{P}_{15}\text{C}_{10} \) /1/ and \( \text{Fe}_{32}\text{Ni}_{14}\text{P}_{12}\text{B}_{6} \) (MG 2826A) /2/. The systematical errors related to the overlap of the lines can be avoided with the simple procedure described in Ref. 3. In some cases (e.g. \( \text{Fe}_{80}\text{B}_{20} \) the \( p(H) \) distributions determined by different methods agree reasonably well with each other /3,4,5/. These distributions are often structureless and can be approximated by a Gaussian form, i.e. it can be characterized with two parameters: with the average hyperfine field and with the width of the distribution.

The interpretations of the measured \( p(H) \) are widely different. Recently, the \( p(H) \) of amorphous \( \text{Fe}_{80}\text{B}_{20} \) was successfully explained /4/ in the model of dense random packing of hard spheres (DRPHS). In this interpretation the \( p(H) \) distribution is attributed to the fluctuating number of iron neighbours resulting in a contribution of \( \Delta H \approx 24.5 \text{ kOe} \) by each close-contact iron atoms to the hyperfine field at a given iron site and the close-contact coordination probabilities were taken from the Bernal liquid-structure model /6/. Similar interpretation of \( p(H) \) was given for other metallic glasses, as well /7/.

However, serious objection can be raised against such an interpretation of the \( p(H) \) distribution: there is no evidence for the supposed strong neighbour contribution to the hyperfine field. Contrary, in metallic glasses as in crystalline intermetallic compounds the iron hyperfine field is proportional to the iron magnetic moment /8/ which is determined mostly by the metalloid neighbourhood. For example, in crystalline \( \text{Fe}_{2}\text{B} \) and \( \text{FeB} \) the iron atoms with 3 B and 10 Fe; 4 B and 10 Fe; 6 B and 10 Fe nearest neighbours have a hyperfine field of 275 kOe, 235 kOe and 130 kOe, respectively /9/. That is, these iron atoms have nearly the same iron neighbourhood, while their boron environment varies widely and correlated with the variation observed in hyperfine field. Similarly, the
substitution of half of the Fe by Ni (with much smaller magnetic moment) in amorphous Fe$_{40}$Ni$_{40}$B$_{20}$ does not influence the shape of p(H) and the average hyperfine field is decreased only by about 15% suggesting a rather localized type of behaviour /10/. Mössbauer data of amorphous Fe obtained by co-condensation of 10 at.% Ar are in accord with the above argument /11/: the linewidth of this spectrum is 0.4 mm sec$^{-1}$ contrary to that of amorphous Fe$_{80}$B$_{20}$ which is 1.5 mm sec$^{-1}$. Since the evaporated Fe with the non-interacting Ar impurities is the nearest to the assumptions of the DRPHS model, the remarkable difference between the linewidths (i.e. in the widths of the p(H)'s) suggests the dominant role of the metalloid neighbours in determining the p(H) distribution.

In the absence of fixed coordination number the distribution of the metalloid atoms is quite different from that of the transition metal atoms (the metalloid atoms are sitting in the holes of the transition metal framework according to the DRPHS model). As a result p(H) based on the metalloid distribution of a DRP models differs considerably from the measured one /9/.

On the other hand, it has been shown that the short-range order of amorphous Fe$_{75}$B$_{25}$ can be well approximated with that of the metastable crystalline Fe$_2$B compound /12/.

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