Model Calculation for the $Fe_{80}B_{20}$ Alloy Glass

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Three partial radial distribution functions [RDF's] are calculated by means of relaxed dense-random packing models for a $Fe_{80}B_{20}$ glass. The model structures reproduce fairly well recently reported experimental partial RDF's derived from x-ray diffraction and neutron diffraction using isotopic substitutional methods. Most significantly, both the model calculated by means of relaxed dense-random packing models $G_{BB}(r)$, the appearance of a subpeak on the short distance side of the first peak.

Recently, in this journal, Nold, Lamparter, Olbrich, Rainer-Harbach and Steeb [1] reported three partial radial distribution functions (RDF's) for the $Fe_{80}B_{20}$ alloy glass determined by x-ray diffraction and neutron diffraction using the isotopic substitution method. The RDF's, particularly of the B-B pairs, obtained by Nold et al. show very interesting features which were revealed in our previous model calculations on Fe-B alloy glasses of different compositions, e. g. $Fe_{85}B_{15}$, [2] and $Fe_{75}B_{25}$ and $Fe_{60}B_{40}$ [3]. This new result has prompted us to apply the model calculation to the same alloy, $Fe_{80}B_{20}$, for direct comparison.

The model structure for the $Fe_{80}B_{20}$ was constructed by the two-step procedure identical to previous works [2, 3]: production of random packing of hard spheres and structural relaxation using the truncated Mose-type atomic pair potentials. We used the same algorithm employed in the previous work for the Fe-P system [4]. The diameter of B atoms is set to be $0.58\,\sigma$, where σ is the diameter of Fe atoms. The atomic diameter ratio is calculated from the Fe-Fe and B-B potential with an appropriate averaging procedure. We adopt the condition of nonexistence of the B-B pair within interatomic distance of $1.3\,\sigma$. The system size is 1500 spheres with free boundary condition. The starting system was constructed by computer and we monitored the alloy composition in each spherical region with the radius $R = 0.02\,\sigma$, $0.04\,\sigma, \ldots, n \times 0.02\,\sigma$, from the center of the system. After 100 iteration cycles of the structural relaxation process, a reduction of 20% was achieved in the final potential energy. A further iteration step produced only a change of 0.02% in the total energy and $0.0015\,\sigma$ in the averaged displacement. No notable change of the structure was detected by further relaxation.

Figure 1 gives a comparison of the partial RDF's between our model structures and the experimental data of Nold et al. [1]. The first peak profile in model $G_{FeFe}(r)$ agrees quite well with the experimental $G_{FeFe}(r)$. However, the second peak profile for $G_{FeFe}(r)$ in the model structure shows less intensity in the first subpeak than the second one (at larger r), differing slightly from the experimental data. Both model calculations and experimental results show the first peak as well as the second peak splitting more pronounced in the $G_{FeB}(r)$ than in the $G_{FeFe}(r)$. Most significantly, the asymmetrical first

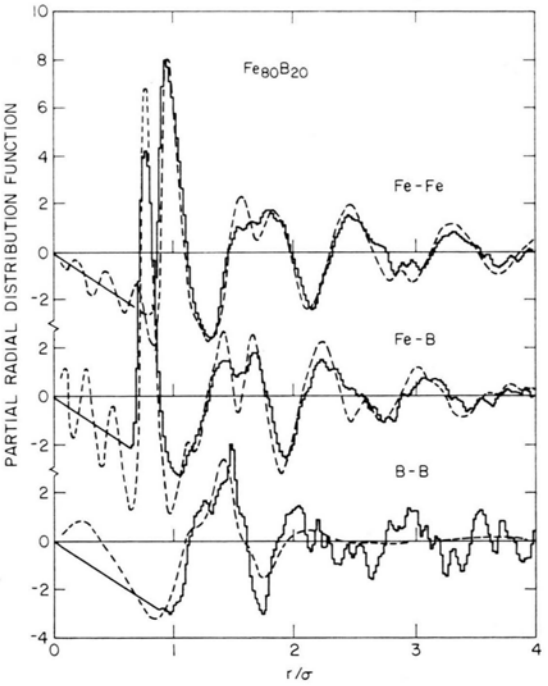

Fig. 1. Comparison of model structure with experimental data in the partial RDF's for the $Fe_{80}B_{20}$ glass. Histogram: relaxed DRP model, dashed line: experimental data [1].

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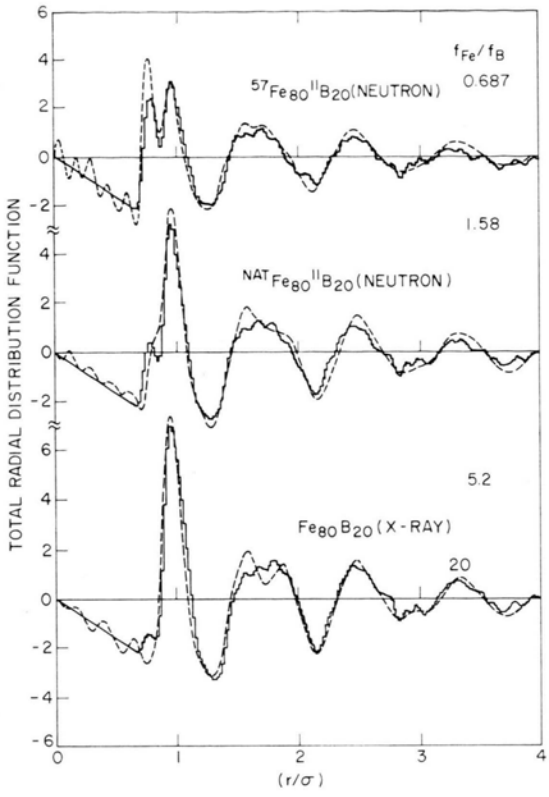

Fig. 2. Comparison of model structure with experimental data in the total RDF for the $Fe_{80}B_{20}$ glass. Histogram: relaxed DRP model, dashed line: experimental data [1].

peak of $G_{BB}(r)$, i. e., the appearance of a shoulder (or a subpeak) on the short distance side of the first peak, is well reproduced by the present model structure. To demonstrate further the agreement between the model and experimental data, in Fig. 2 a comparison is made between calculated and experimental three total RDF's in which the ratio of the scattering factors f_{Fe}/f_B changes widely from 0.69 to 5.2.

The coordination numbers of near neighbour correlations estimated from the partial RDF's by applying the same procedure of Sadoc and Dixmier [5] are summarized in Table 1 together with the

Table 1. The near neighbour correlations in the $Fe_{80}B_{20}$ glass. In the model calculations, the Fe-Fe distance σ (= 2.57 A) is adjusted to the experimental one.

	Origin atom	Fe		B	
		r(A)	n(atom)	r(A)	n(atom)
$Fe_{80}B_{20}$ (model)	Fe	2.57	11.9	2.14	1.9
	B	2.14	7.6	3.44	6.3
$Fe_{80}B_{20}$ (exp. [1])	Fe	2.57	12.4	2.14	2.2
	B	2.14	8.6	3.57	6.5

experimental ones of Nold et al. [1]. The coordination numbers of all possible atomic pairs in the model calculation are smaller than the experimental values by about 10%. This discrepancy, probably, arises from the uncertainties in both experimental data and model calculations, because the coordination numbers in non-crystalline systems are known to be sensitive to the methods of evaluation and the input RDF data.

The main purpose of this note is to demonstrate that our model structures can explain the characteristic structural features of the $Fe_{80}B_{20}$ glass such as the asymmetrical first peak in $G_{BB}(r)$ and the different peak profiles for three total RDF's recently reported by Nold et al. [1]. We conclude that the present calculation by the relaxed DRP model is reasonable, as it reproduces fairly well the experimental data as shown in Figs. 1 and 2. Since the model structures [2, 3] exhibit composition dependent structural features such as a change in the peak profile of the first peak of $G_{BB}(r)$ and a split second peak of $G_{FeB}(r)$, it would be of considerable interest to evaluate the partial RDF's experimentally of Fe-B alloy glasses with different alloy compositions and compare them with the model structures of $Fe_{75}B_{25}$ and $Fe_{60}B_{40}$ [3].

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