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Structure of the Amorphous Fe-B Alloy Modeled by Molecular Dynamics

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The Fe-B alloy structures have been widely investigated. Earlier studies /1, 2/ gave a traditional picture of the radial distribution function (RDF): the first maximum is a single one, the second being slightly split. Recently high resolution neutron diffraction measurements /3, 4/ made it clear that the first maximum has a small sub-peak on its left side. A pseudo-crystalline model of the amorphous Fe-B alloy was proposed /3/ and from this model the RDF (g(r)) was calculated. A comparison of the calculated and experimental g(r) for $Fe_{81}B_{19}$ /3/ shows practically coinciding curves near the first maximum. Nevertheless, the shape of the second maximum does not agree well with the calculated curve above 0.5 nm /3/.

A calculation by molecular dynamics (MD) was previously performed /5/. A weak sub-peak on the left side of the first maximum has been observed, and has been compared with a limited number of experimental results /1, 2/. The deviations of the calculated data from the experiments were explained, and it was concluded that the observed sub-peak is related to the correlation of Fe-B pairs. Furthermore, a an a priori calculation based on the pseudopotential method has been provided /6/, overestimating the boron-boron interaction.

To clarify these problems we carried out a new MD investigation on these alloys. In our present short note we report on a MD calculation for 256 atoms with Morse pair potential, based on the integration of the equations of motion in the frame of a microcanonical (NVE) assembly, in which N (the number of particles), V (the volume of the system), and E (the energy of the system) are kept constant. The calculation is done for the atoms in a rigid box with periodic boundary conditions imposed. The interaction between atoms is given by the Morse potential /7/,

$$V(r) = \varepsilon \left[\exp(-2A(r/R_o - 1)) - 2 \exp(-A(r/R_o - 1)) \right] f(r/R_o) \, , \qquad (1)$$

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the parameters R_o and ε being determined from experimental data /8/, and

$$f(y) = \begin{cases} 1 & , & y \leq 1 , \\ 3z^4 - 8z^3 + 6z^2 & , & 1 < y < R_c/R_o , \\ 0 & , & y > R_c/R_o , \end{cases} \qquad (2)$$

where

$$z = (y - R_c/R_o)(1 - R_c/R_o) , \quad A = 3.76, \quad R_c/R_o = 1.4 .$$

The equations of motion were integrated by the "leap-frog" method /9/ with a time-step of 10^{-15} s.

In the initial state the atoms are arranged in the nodes of an f.c.c. lattice and their velocities assumed were in accordance with a Maxwell distribution for 2000 K temperature. After a thermal stabilization at this temperature the system was cooled at a constant volume with an average rate of 10^{14} K/s until getting an amorphous state. A rescaling of particle velocities by multiplying with a constant factor after every 10 steps was introduced. The entire process contained cooling and thermal stabilization stages at several intermediate (every 3000 steps) temperatures adjusting the distribution of atoms to a Maxwellian at the given temperature.

For amorphous $Fe_{85}B_{15}$ the total $g(r)$ function and the partial $g_{FeFe}(r)$, $g_{FeB}(r)$, and $g_{BB}(r)$ functions are illustrated in Fig. 1 and 2. The total $g(r)$ has two main maxima. On the left side of the first peak a weak sub-peak is observed and the second maximum is slightly split and almost symmetrical. It should be noted that in the $g(r)$ curve both the positions of all the maxima (up to $r \approx$ 0.6 nm) and the minima are lying very close to the experimental data, /3/. This means that the molecular dynamic modeling yields a $g(r)$ which agrees with the experimental $g(r)$ better than that obtained on the basis of the pseudo-crystalline model.
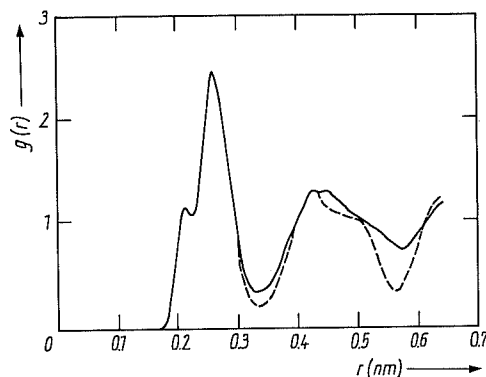
The weak sub-peak of the first maximum (Fig. 2) is caused by the high probability of finding Fe and B atoms at a distance of approximately 0.22 nm. Moreover the second maximum of the $g_{FeB}(r)$ curve coincides with the minima of the

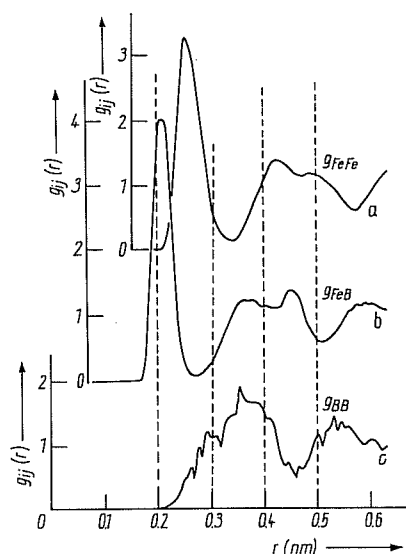Fig. 1. The total radial distribution function of the $Fe_{85}B_{15}$ alloy, calculated (———) and experiment (– – –)

(2)

Fig. 2. Calculated partial radial distribution functions of the $Fe_{85}B_{15}$ alloy. (a) $g_{FeFe}(r)$, (b) $g_{FeB}(r)$, (c) $g_{BB}(r)$

$g_{FeFe}(r)$ curve and vice versa, which confers a relatively high stability to the amorphous phase the $Fe_{85}B_{15}$ alloy.

Our present investigation proves the applicability of a molecular dynamics approach for obtaining the correct radial distribution function of this alloy.

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