phys. stat. sol. (a) **122**, K7 (1990)
Subject classification: 61.40; S1.1

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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, 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/,

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

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\]
the parameters $R_o$ and $\varepsilon$ being determined from experimental data /8/, and

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

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 phases 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 (--.--)]
Fig. 2. Calculated partial radial distribution functions of the Fe$_{85}$B$_{15}$ alloy. (a) $g_{\text{FeFe}}(r)$, (b) $g_{\text{FeB}}(r)$, (c) $g_{\text{BB}}(r)$

$g_{\text{FeFe}}(r)$ 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.

References

/4/ E. SVAB, R. BELLISSENT, and GY. MESZAROS, see /3/ (p. 487).

(Received March 21, 1990; in revised form August 1, 1990)