

## Short Notes

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### **B-B Direct Contact in Amorphous Ni<sub>76</sub>B<sub>24</sub> System Based on Molecular Dynamics**

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**Introduction** Recently, the method of molecular dynamics (MD) has become widely popular as a tool for investigating condensed matter. The method requires an adequate description of the interatomic forces, for which two basic ways are favored: the selection of empirical potentials and the quantum mechanical approach on the basis of the pseudo-potential method. The first approach is more simple and realistic, but requires reliable experimental information which is often limited and sometimes contradictory. The second one is more theoretical, no experimental information is needed.

In our present work the amorphous structure of the Ni<sub>76</sub>B<sub>24</sub> metallic alloy is calculated and the results are discussed.

**Calculation** The structure of the Ni-B amorphous system has been investigated widely. There is a discrepancy between the X-ray /1/ and the neutron diffraction experiments /2, 3/. The neutron investigations clearly demonstrate a side-peak near the first big peak of the partial radial distribution function  $g(r)$  at 0.17 to 0.18 nm. Such a side-maximum has not been observed in X-ray diffraction.

In order to resolve this ambiguity we made a MD calculation on the Ni<sub>76</sub>B<sub>24</sub> system. The integration of the equation of motion was carried out by the so-called "leap-frog" method /4/. The equilibrium temperature was obtained by the normal Maxwell distribution of velocities. In the model experiment the system was cooled from 2000 to 100 K at a rate of  $10^{14}$  K/s. The calculation was made in a cube cell with periodic boundary conditions for 195 Ni and 61 B atoms.

In this work the interatomic pair potential is calculated within the framework of the pseudopotential theory /5/. The Animalu form factors /6/ and the dielectric screening function of Vashista and Singwi form /7/ have been used. These potentials were applied within the NVE (constant number of particles (N), constant

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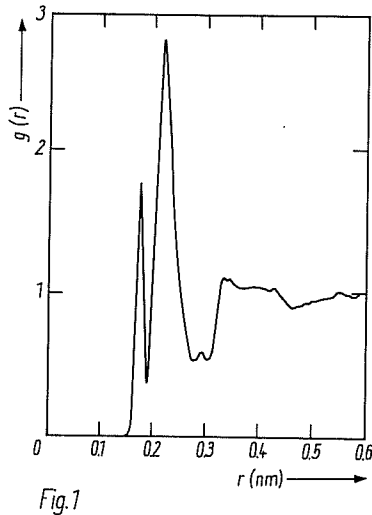


Fig. 1

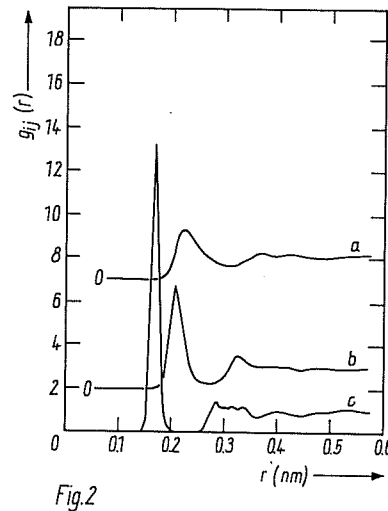


Fig. 2

Fig. 1. Total pair distribution function ( $g(r)$ ) for  $\text{Ni}_{76}\text{B}_{24}$

Fig. 2. (a) Partial pair distribution function  $g_{\text{NiNi}}(r)$ ,  
 (b) partial pair distribution function  $g_{\text{NiB}}(r)$ ,  
 (c) partial pair distribution function  $g_{\text{BB}}(r)$

volume ( $V$ ), and constant energy ( $E$ )) assembly.

One of the central questions in our present work is to know, whether the small number of particles in such a system is sufficient to describe the real properties without using empirical potentials. The total pair-distribution function,  $g(r)$  and partial data ( $g_{\text{NiNi}}$ ,  $g_{\text{NiB}}$ ,  $g_{\text{BB}}$ ) are shown for  $T = 100^\circ\text{C}$  on Fig. 1, 2.

The existence of B-B pairs with a separation of 0.175 nm becomes evident from these results. The calculated partial coordination numbers are given in Table 1 and compared with those from experimental [2, 3] works. The characteristic behavior of the Ni-B structure is presented correctly, but the first peak height of the  $g_{\text{BB}}(r)$  function is overestimated. This effect is caused by the non-correct potential value for B-B interaction at equilibrium position. This just leads to an increased number of connected B-B pairs compared with experimental data.

Obviously our present model is a simplified variant of molecular dynamics. Using a larger number of particles and more realistic empirical potentials more accurate results can be obtained. Our present calculation, however, points to the possibility of using a simple, relatively small, system with an a priori potential to describe the most characteristic features of Ni-B amorphous alloy.

T a b l e 1

Comparison of some calculated and experimental data

peak of the pair-correlation function	r <sub>1</sub> (nm)			coord. No.		note
	calc.	exp. /2/	exp. /3/	calc.	exp. /2/	
g <sub>NiNi</sub>	0.234	0.255	0.253	8.27	9.2	
g <sub>NiB</sub>	0.214	0.212	0.208	4.18	4.9	Ni around B
g <sub>BNi</sub>				7.45	8.7	B around Ni
g <sub>BB</sub>	0.175	0.172	0.187	4.96	1.1	(*)

(\*) The difference is caused by the overestimated B-B interaction calculated by the pseudo-potential method.

Conclusion In accordance with neutron-diffraction experiments we have calculated from a priori conditions a direct evidence for B-B contact using a relatively small number of particles in the amorphous Ni<sub>76</sub>B<sub>24</sub> model system.

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