MASTER

Study of Local Atomic
and
Electronic Structure in Glassy Metallic Alloys
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I. Introduction

This report is a summary of progress made during the period March 1, 1979 to December 1, 1979 under contract DE-AC02-79ER 10382 entitled "Local Atomic and Electronic Structure in Glassy Metallic Alloys" from Department of Energy, Division of Basic Energy Sciences, Materials Science Program. In Section II a brief review of structure in metallic glasses is given as a background. In Section III, the experimental progress from our EXAFS studies during the past year is summarized. In Section IV, the theoretical progress from our molecular orbital cluster studies of electronic structure is discussed.

II. Structure of Metallic Glasses: A Brief Review

To date most of the characterization of atomic arrangements in metallic glasses have been made using conventional techniques of x-ray diffraction^(1,2). These measurements provide a statistically averaged description of the arrangements of atoms which are used for testing three dimensional structural models. The x-ray interference function $i(q)$ of metal-metalloid glasses exhibits a shoulder on the high q side of the second peak. The atomic distribution function $W(r)$ as well as the radial distribution function (RDF) obtained by Fourier transforming the intensity data contain a split double peak beyond the first maximum. The number of neighbors in the first coordination sphere varies from 10-13 depending on the system. The ratio of second to first near neighbor average distance is 1.7. Cohen and Turnbull⁽³⁾ on the basis of their free volume theory⁽⁴⁾ suggested that the random packing of hard spheres proposed by Bernal⁽⁵⁾ for the structure of a monatomic liquid might be a good representation of the atomic arrangements in monatomic glasses. A high resolution RDF for this Bernal type of dense random packing (DRP) has been determined by Finney⁽⁶⁾. Using this DRP as a structural model, Cargill^(6a) suggested that to a first approximation the structure of metal-metalloid glasses could be represented by a random mixture of metal and metalloid in a Bernal DRP of hard spheres (DRPHS) of one size. Good agreement is obtained between the atomic distribution function obtained by Finney for DRP with a sphere diameter of 2.49Å and that obtained experimentally from x-ray data by Cargill for glassy $\text{Ni}_{76}\text{P}_{24}$. In particular both have the split second evident in Figure (1).

The doublet observed in the second peak in the RDF is a characteristic structural feature of glassy metals. A geometrical interpretation of its origin has

been proposed by Finney. In Figure (2) a plot of Finney's $\rho(r)$ to three sphere diameters for DRP is shown. The sphere diameter is taken as 1.00. The first peak which is very sharp is due to spheres in contact. The peak at 1.99 diameter is attributed to the separation x between three collinear spheres shown in Figure (2)a. Slight departure from collinearity shifts the maximum to below 2.00 sphere diameters. This is substantiated by the sharp drop in $\rho(r)$ slightly above $r = 2.00$. The peak at 1.73 is attributed to the characteristic distance y resulting from the arrangement of four atoms into coplanar equilateral triangles sharing an edge shown in Figure (2)b. Thus the split second peak simply arises from the short range structure characteristic of DRP.

Bernal's DRP structure may be described as an assembly of polyhedral holes with atoms at the vertices and with edge lengths that are at most ~15% larger than the hard sphere diameter. Various types of holes were identified^(5,7). These are shown in Figure 3. These holes are surrounded by 4, 5, 6, 7, 8, 9, 10, 11, 12 atoms. Based on Bernal's original findings, Polk⁽⁸⁾ proposed a structural model for transition metal-metalloid glasses having 80 at.% metal. In this model the transition metal would form a Bernal DRPHS and the metalloid would fill in the large 8 and 9 fold coordinated holes inherent in the structure. This simple model postulates (i) that each metalloid is surrounded by 8-9 metal atoms, (ii) that there is no metalloid-metalloid nearest neighbor and (iii) that the metal-metalloid distance will be smaller than the sum of the atomic radii of the atoms.

III. EXAFS Results

A variety of ferromagnetic metallic glasses of general composition $(\text{Fe,Co,-Ni})_{80}(\text{P,C,B,Si,Al})_{20}$ are extremely strong in the as-cast state and deform plastically in bending without fracturing. However, when heated for relatively short times at temperatures well below their glass transition temperature, T_g , these alloys become brittle^(9,10). Auger analysis reveals regions of high phosphorus concentration on the fractured surface, indicative of phosphorus segregation at these low annealing temperatures⁽¹¹⁾. By removing phosphorus from the alloys, the stability towards embrittlement is greatly enhanced as seen in Figure 4. Taking advantage of the atom-selectivity of the EXAFS technique, we initiated a series of EXAFS experiments to study the local structure and dynamics about the ferromagnetic metal atoms in a series of $\text{Fe}_{40}\text{Ni}_{40}\text{P}_{20-x}\text{B}_x$ glasses as a function of phosphorus content and annealing temperature. Spectra were recorded at 77K and 300K and a typical scan is shown in Figure 5(a).

In EXAFS experiments the structural parameters of interest are the distance of separation r_j of the j th shell of atoms from a chosen central atom participating in the photoelectron absorption event, the number N_j of atoms in the j th shell and their relative disorder σ_j which may be static (structural) or dynamic (thermal). The type of j th atom can be identified in favorable cases from the backscattering amplitude $t_j(2k)$ in conjunction with a shell-by-shell back Fourier transform and curve fitting. Since EXAFS is dominated basically by local environment about a central atom, structural information derived for amorphous solids like metallic glasses will be most detailed on the nearest neighbors for which $j = 1$.

The normalized $\chi \cdot k$ vs. k (Figure 5(b)), and its corresponding Fourier transform (Figure 5(c)) are given for the case of Ni in glassy $\text{Fe}_{40}\text{Ni}_{40}\text{B}_{20}$ above its K-absorption edge at 8332.8 eV. The Fourier transform which yields a radial structure function is characterized by a dominant peak at $2.02 \pm 0.02 \text{ \AA}$. The position of this radial peak in all the radial structure functions about both the Fe and Ni atoms in the series of amorphous $\text{Fe}_{40}\text{Ni}_{40}\text{B}_{20-x}\text{P}_x$ where $x = 0, 10, 14, 20$, remains invariant for EXAFS measurements at 77K and 300K. Also annealing for 2 hours below the glass temperature at 197, 250 and 325°C did not alter the position of the first radial peaks of Fe and Ni in the $\text{Fe}_{40}\text{Ni}_{40}\text{B}_{20}$ alloy. For distance determination we obtained empirical phase shift values for Ni-B and Ni-Ni in Ni_3B , Ni-P and Ni-Ni in Ni_2P , and Fe-P and Fe-Fe in Fe_3P by comparing similar EXAFS data in these compounds with available crystallographic data⁽¹²⁾. The average nearest neighbor distances in ternary $\text{Fe}_{40}\text{Ni}_{40}\text{B}_{20}$ and $\text{Fe}_{40}\text{Ni}_{40}\text{P}_{20}$ glassy alloys are given in Table 1. These values are consistent with results in the partial structure factor measurements on binary Fe-P and Ni-P amorphous alloys: Fe-P = $2.38 \text{ \AA}$, Fe-Fe = $2.61 \text{ \AA}$, Ni-P = $2.35 \text{ \AA}$ and Ni-Ni = $2.55 \text{ \AA}$.

From the temperature variation of the magnitude of the first Fourier peak we define a change of disorder $\Delta\sigma^2$ about the nearest neighbor coordination shell: $\Delta\sigma^2 = \sigma_{300\text{K}}^2 - \sigma_{77\text{K}}^2$. This quantity is plotted as a fractional change $\Delta\sigma^2 / \sigma_{77\text{K}}^2$ with respect to a low temperature state at 77K for both the Fe and Ni atoms in $\text{Fe}_{40}\text{Ni}_{40}\text{B}_{20-x}\text{P}_x$ in Figure 6. With increased phosphorus content in the alloy, $\Delta\sigma^2 / \sigma_{77\text{K}}^2$ for Ni increase monotonically. For the Fe atoms, however, $\Delta\sigma^2 / \sigma_{77\text{K}}^2$ decreases initially with phosphorus addition and increases above $x = 10$. This suggests that when $x > 10$ addition of phosphorus enhances dynamics decoupling of both atoms with their nearest neighbor coordination shell. The dynamic disorder data is consistent with Auger spectroscopic observation of phosphorus segregation associated with mechanical embrittlement in phosphorus-containing alloys.

The Polk model for metal-metalloid glass structure is heavily focused on the metalloid environment and specifies its local structure in some detail. A number of diffraction studies have been attempted to determine the metalloid environment in these glasses with special effort at detecting metalloid-metalloid avoidance. The results, though consistent with Polk's postulate, usually are not definitively conclusive. This is due to a variety of experimental reasons such as lack of a complete set of partial distribution functions (e.g. ρ_{MM} , ρ_{MX} and ρ_{XX} in a binary M-X glass), or low signal-to-noise ratio due to low metalloid concentration used. However, the metalloid environment can easily be studied by EXAFS since this technique is atom specific.

In ferromagnetic amorphous alloys the metalloid constituents (B,P,Si) commonly encountered are too light to be studied by EXAFS with the x-ray synchrotron radiation at Stanford due to absorption of the Be windows below 3.5keV. We, therefore, substituted half of the B with Ge in a binary $\text{Fe}_{80}\text{B}_{20}$ glass and used the heavier metalloid to probe the metalloid environment in ferromagnetic glassy alloys for the first time. The Fourier transform of the normalized EXAFS above the Ge K-edge yield predominately a single peak centered at $\sim 2.40\text{\AA}$ after correcting for phase shift. This radial peak in the region 1 to $3\text{\AA}$ is back Fourier transformed to momentum-space and is plotted in Figure 7. Using the values calculated by Teo and Lee⁽¹³⁾, we plotted the theoretical backscatter amplitude function for both Fe and Ge normalized to the maximum of the back transformed envelope. It is seen that the observed first shell envelope coincides quite nicely with the theoretical backscattered amplitude of Fe (open circles) and not at all with that for Ge (crosses), which exhibits a maximum at higher k. This conclusively demonstrates that there is no Ge-Ge nearest neighbor pair in the $\text{Fe}_{80}\text{B}_{10}\text{Ge}_{10}$ glass in accordance with Polk's model.

Another important experimental result is the finding that the metal-metalloid distance is less than the sum of their atomic radii in conformity with Polk's model. Except for the case of Pd-Si glass where high resolution neutron diffraction data exist, determinations of metal-metalloid distance were solely made with EXAFS. Our results for Fe-Ni alloys together with the literature values for Pd-Ge^(14a) and Pd-Si alloys⁽¹⁴⁾ are given in Table 2. Of particular interest is the observation that the measured metal-metalloid distance is more closely approximated by the sum of the covalent radii of the atom pair. The combined results of dynamic disorder and "shortened" distance from its nearest metal neighbors are strongly indicative of chemical ordering about the metalloid atom in the metal-

metalloid glasses. The nature of such chemical interaction has not been investigated until the present theoretical work, which is briefly summarized in the next section.

The 8 to 9-fold coordination of the metalloid by metal in metal-metalloid glasses appears to be a common occurrence in accordance with Polk's model. However, there are exceptions. Suzuki, and coworkers⁽¹⁴⁾ using a high resolution pulsed neutron diffraction technique showed that the coordination of Si and Pd atoms in Pd-Si glasses varies from 6 to 7 with decreasing Si content and extrapolates to 9 at pure (hypothetical) amorphous Pd. Boudreaux⁽¹⁵⁾ also observed in his computer simulation studies that in Fe-B glass the B coordination by Fe atoms is no higher than 7 over the glass composition range of 24-15 at.% B. There is, however, a discrepancy between the neutron data and computer calculation for Pd-Si glass, in that the latter predicts a higher than 8-fold coordination of Si by Pd atoms. The change from 6-fold to 8-9 fold coordination around the metalloid may be rationalized on the basis of size ratio of the metalloid and metal. The larger the r_X/r_M ratio, the more metal atoms can be accommodated as nearest neighbors around the metalloid atom before excess coulombic repulsion sets in. The atom radius ratios for the P-Fe, Ge-Pd, Si-Pd and B-Fe pairs are 1.01, 1.00, 0.96 and 0.77, respectively. Radius ratios below 1.00 give the lower 6-fold coordination as in the case of Pd-Si and Fe-B glasses.

Referring back to Figure 5c, which shows a Fourier transform of the normalized k for Ni in a $\text{Fe}_{40}\text{Ni}_{40}\text{B}_{10}$ glass. The Fourier peak at 2.0Å (uncorrected for phase shift) consists of contributions from nearest-neighbor Ni-Ni, Ni-Fe as well as Ni-B pairs which may be sorted out by inverse-Fourier transforming the first radial structure peak back to k -space and carefully curve fitting to evaluate the respective distance of separation and coordination of atom pairs. We have developed computer routines to perform such curve fitting to extract quantitative structural information about the metal constituents in glassy $\text{Fe}_{40}\text{Ni}_{40}\text{B}_{20}$ and $\text{Fe}_{40}\text{Ni}_{40}\text{P}_{20}$ glassy beyond those obtained by the Fourier transform.

Amorphous $\text{Fe}_{75}\text{B}_{25}$ is an excellent experimental system for studying the metal environment in metal-metalloid glasses, since it can be annealed at low temperature to crystallize⁽¹⁶⁾ homogeneously into a single Fe_3B phase, which is isostructural to tetragonal Fe_3P ⁽¹⁷⁾. Thus using the crystal as a model compound, one can hope to gain better quantitative insight into the local structure about the metal in amorphous $\text{Fe}_{75}\text{B}_{25}$ by measuring the Fe EXAFS spectrum. We plan to carry out this study in the coming year.

A natural extension of EXAFS studies of metallic glasses would be to the metal-metal glasses for which there is no adequate structural model⁽¹⁾. By proper choice of systems, the EXAFS of both metal constituents can be measured and their individual local structure determined so that the nearest neighbor environment in the system is completely defined. (This contrasts with the necessary substitution of heavy metalloid atoms for a complete structure analysis in the EXAFS structurally complex ternary systems described above). Furthermore, structural variation with concentration may also be studied systematically since metal-metal glasses are known to have a much larger range of composition of glass formation.

IV. Theoretical Studies of Cluster Models of Amorphous Metal Alloys

Over the last ten years, considerable effort has been devoted to the modelling of amorphous metals and alloys by the dense random packing of hard spheres (DRPHS) and extensions thereof⁽¹⁸⁾. As discussed in Section II, there now appears to be a consensus that a reasonable first order description of the structure for metal-metalloid alloys (for metalloid concentration ~ 20%) is achieved by considering the metal atoms as making up a DRPHS matrix with the larger interstitial sites occupied by the metalloid atoms (at least for metalloids the size of B or P). Figure 3 shows the various interstitial environments to be found in a DRPHS structure; they are the well known Bernal polyhedra first used by Bernal to discuss the local structure of simple liquids⁽⁵⁾.

In spite of the fact that there has been some suspicion that some metalloids may have a strong chemical interaction with the metal atoms surrounding them in the various polyhedra (see Figure 3), there have been no theoretical studies of the electronic structure and bonding in such environments until the present work.

During the first phase of this study we have concentrated on the smallest polyhedron - the tetrahedron (see Figure 3), even though this may not be the most favorable environment for a metalloid atom in an actual amorphous metal. The reason for this initial focus on the tetrahedron is simply that a number of important conceptual and computational questions can be addressed with a minimum of computational time and expense. Among these questions are:

1. to what extent can we expect significant bonding between the metalloid and metal atoms?
2. what is the nature of the orbitals close to the Fermi level - are they pure metallic or do they involve bonding between the metal and metalloids?

3. is it necessary to carry out spin polarized (i.e. magnetic) calculations in order to properly describe metalloid bonding in iron and nickel alloys?
4. can small clusters mimic some of the known magnetic trends observed in Fe-Ni-B-P systems? Which ones? How well?

Obviously the answers to these questions are important to obtain for small systems before embarking upon larger computations.

We have carried out calculations for all of the clusters listed in Table 3. Detailed discussions of the results of these calculations will be included in manuscripts presently in preparation and which will be submitted for publication. For the present purposes it is nonetheless worthwhile to summarize a few highlights of the studies thus far and show how they indicate some new directions which we believe should be pursued during the coming year. We will first, however, consider a specific example, Fe_4B with Fe-Fe distance of 2.49 Å, to show how information is extracted from the calculations.

Spin-polarized self-consistent field $X\alpha$ scattered wave calculations for the Fe_4B cluster yield the electronic energy levels shown in Figure 8. The levels labelled $\uparrow$ are the majority spin orbitals and those labelled $\downarrow$ are the minority spin orbitals. The dashed levels are unoccupied and the solid levels are occupied. The highest occupied levels contain arrows representing the occupancy of these levels, and each orbital is labelled according to the irreducible representation of the T_d point group under which its wave function transforms. The diagram in the upper right hand corner shows the geometry of the cluster and the plane in which the orbital wave functions below it are plotted. We find in this case as in the other metalloid-metal clusters studied that there is substantial bonding of the metalloid to the surrounding metal atoms. This bonding occurs in the nondegenerate $1a_1$ level (B 2s interacting with Fe 3d) shown in Figure 8 and in the triply degenerate $1t_2$ level (B 2p interacting with Fe 3d) with one of its orbital components shown in Figure 8. Similar orbital plots (not shown here) demonstrate that the t_2 levels around the highest occupied level do not contain any significant B contributions; the e and t_1 levels do not contain any B contributions by symmetry.

An approximation to the saturation magnetization per metal atom for an $\text{Fe}_{80}\text{B}_{20}$ alloy can be obtained from the simple Fe_4B clusters model by the following:

$$\begin{aligned} \text{Moment (in bohr magnetons/metal atom)} &= \\ &= \text{g-factor} \times (\text{no. of } \uparrow \text{ spins} - \text{no. of } \downarrow \text{ spins}) / \text{no. of metal atoms} \\ &= 1.84 \mu_B / \text{metal atom. This compares with the value of } 1.94 \text{ B for } \text{Fe}_{80}\text{B}_{20} \\ &\text{obtained in our laboratories}^{(19)}. \text{ On increasing Fe-Fe separation of the cluster we} \end{aligned}$$

find that the magnetic moment increases dramatically. Although there is evidence that this increase is qualitatively correct, our calculations over-estimate the magnitude of the magnetic moment for clusters containing a metalloid and only Fe atoms. For the cases of Ni_4 and Ni_2Fe_2 with metalloid atoms the behavior is much more realistic. For example, at the larger metal-metal distance we obtain for the series Ni_2Fe_2 , $\text{Ni}_2\text{Fe}_2\text{B}$, $\text{Ni}_2\text{Fe}_2\text{P}$ the following magnetic moments 1.65, 1.38 and 0.83 respectively. These can be compared to the observed values for $\text{Ni}_{50}\text{Fe}_{50}$ (crystalline alloy) $\text{Ni}_{40}\text{Fe}_{40}\text{B}_{20}$ (amorphous alloy) and $\text{Ni}_{40}\text{Fe}_{40}\text{P}_{20}$ (amorphous alloy) of 1.65, 1.31 and 1.08 respectively. Thus the proper trend is satisfactorily reproduced even with these simple model clusters.

Let us now return to summarize some of the principal findings of the calculations particularly as they regard the questions posed above. We find

1. there are significant metalloid-metal bonding interactions in all clusters studied.
2. for the systems under consideration, the orbitals immediately in the vicinity of the Fermi Level contain little or no interaction between the metal and metalloid atoms, and thus
3. a discussion of the bonding between metalloid and metal atoms for these alloys can be reliably obtained by considering spin-restricted (i.e. non-magnetic) calculations.
4. even with the small clusters considered thus far reasonable trends in magnetic moments can be obtained for system which are not dominated by iron.

The first conclusion is consistent with recent EXAFS measurements⁽²⁰⁾ described in the previous section and neutron diffraction studies⁽¹⁴⁾ which show that the metal-metalloid distances are much closer to the sum of covalent radii than they are to a sum of atomic radii, and in fact one can attribute these observations to the metal-metalloid bonding interactions found from the calculations. Conclusions 2) and 3) allow us to study larger Bernal polyhedra, such as the $N = 8$ polyhedron of Figure 3, without doing the more expensive spin-polarized calculations if we wish to concentrate on chemical bonding effects.

In fact such calculations for larger clusters have now been initiated, in particular for the $N = 8$ cluster of Figure 3 which is shown on an expanded scale in Figure 9. In Figure 10, we show the computed total valence charge density for an

Ni_8 cluster. The plane of the plot is such that it bisects the nuclei of atoms labelled 1, 7, 8, 4, in Figure 9. It can be clearly seen from Figure 10 that the bonding between atoms (1 and 7), (7 and 8) and (4 and 8) is considerably greater than between atoms 1 and 4. However, when a boron atom is inserted into the Ni_8 polyhedron at its center, the computed valence charge density obtained is shown in Figure 11. The contour values are the same as those in Figure 10 and each successive contour moving inward represents a charge density twice as great as the previous contour. Figure 11 shows significant changes in the bonding from Figure 10. The boron atom forms bonds to the four closest Ni atoms (1 and 4 in Figure 11 and 2 and 3 above and below the plane of this figure) but somewhat weakens the bonding between nickel atoms 1, 7 and 4, 8. This effect is found to be even greater for the case of phosphorus in Ni_8 . Such effects will undoubtedly be very important in understanding the radial distribution functions (RDFs) obtained from EXAFS experiments as these bonding considerations will affect the metalloid-metal distances in the first and second coordination shells about the metalloid atom.

We intend to pursue the nature of these bonding effects during the coming year for some of the more relevant polyhedra of Figure 3 (i.e. $N = 8, 9, 10$ clusters). We intend to investigate Fe and Ni clusters as well as mixed Fe-Ni clusters with B and P metalloids. Some of the questions which we believe should be addressed in our studies for the next year are:

1. How does the metalloid's tendency to form bonds with certain metal atoms affect the various metalloid-metal distances, in pure iron environments, in pure nickel environments, in mixed metal environments? What are the systematics for the Ni-Fe-P-B class of alloys? Can this information be used to interpret RDFs more uniquely?
2. Why is it that two metalloid atoms never seem to be nearest neighbors⁽⁸⁾?
3. If properties are calculated for various local environments, how can the information be combined to obtain a description of "bulk" amorphous behavior?

TABLE I

Metal-Metal and Metal-Metalloid Distances (in Å)
in Glassy $\text{Fe}_{40}\text{Ni}_{40}\text{B}_{20}$ and $\text{Fe}_{40}\text{Ni}_{40}\text{P}_{20}$

$\text{Fe}_{40}\text{Ni}_{40}\text{B}_{20}$				$\text{Fe}_{40}\text{Ni}_{40}\text{P}_{20}$			
	r'	Δr	r		r'	Δr	r
Fe-B	1.75	—	—	Fe-P	1.70	.56	2.26
Fe-Fe	2.02	—	—	Fe-Fe	2.02	.61	2.63
Ni-B	1.75	.30	2.00	Ni-P	1.70	.60	2.30
Ni-Ni	2.02	.49	2.51	Ni-Ni	2.02	.45	2.47

r' = position of peak or shoulder in radial structure function; Δr = phase shift values from Ni_3B , Fe_3P and Ni_2P . Actual distance $r = r' + \Delta r$. Errors in the metal-metal and metal-metalloid distances are estimated to be 0.05 Å and 0.10 Å respectively.

TABLE 2

Distance of separation, r_{X-M} , between unlike atoms in metal-metalloid and metal-metal glasses determined by EXAFS and comparison with atomic and covalent radii additivity.

Glass System	Atom Type	Atomic	Covalent	$r_{X-M}(\text{\AA})$ (exptal)	Expt Type
$\text{Fe}_{40}\text{Ni}_{40}\text{P}_{20}$	Fe P	1.26	1.17	2.26	EXAFS
		<u>1.28</u>	<u>1.06</u>		
		2.54	2.23		
$\text{Fe}_{40}\text{Ni}_{40}\text{P}_{20}$	Ni P	1.24	1.15	2.21	EXAFS
		<u>1.28</u>	<u>1.06</u>		
		2.52	2.21		
$\text{Fe}_{40}\text{Ni}_{40}\text{B}_{20}$	Ni B	1.24	1.15	2.00	EXAFS
		<u>.98</u>	<u>.82</u>		
		2.22	1.97		
$\text{Pd}_{80}\text{Ge}_{20}$	Pd Ge	1.37	1.28	2.49 $\pm$ 0.1	EXAFS
		<u>1.37</u>	<u>1.22</u>		
		2.74	2.50		
$\text{Pd}_{80}\text{Si}_{20}$	Pd Si	1.37	1.28	2.40	Neutron
		<u>1.32</u>	<u>1.11</u>		
		2.69	2.39		

TABLE 3

CLUSTERS FOR WHICH CALCULATIONS ARE COMPLETED⁺

Ni_4	Ni_4B	Ni_4P
Fe_4	Fe_4B	Fe_4P
Ni_2Fe_2	$\text{Ni}_2\text{Fe}_2\text{B}$	$\text{Ni}_2\text{Fe}_2\text{P}$

⁺For each cluster, calculations have been carried out for at least two metal-metal distances 2.49Å and 3.47Å. Spin-polarized (i.e. magnetic) calculations have been carried out for all clusters.

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PUBLICATIONS

J. Wong "EXAFS: A Novel Probe for Local Structure of Glassy Solids",
Proc. of the 23rd International Symposium of SPIE, San Diego,
(1979).

J. Wong "EXAFS Studies of Metallic Glasses", Chapter in "Metallic
Glasses" edited by H. J. Guntherodt, Springer-Verlag Publisher,
Berlin (1980).

R. P. Messmer &
J. Wong "Short-Range Order in Amorphous Solids" (manuscript in prep-
aration).

J. Wong "Metalloid Environment in Metal-Metalloid Glasses" (manuscript
in preparation).

R. P. Messmer Local Electronic Structure of Some Cluster Models of Amor-
phous Metal Alloys (manuscript in preparation).

Invited Lectures (R. P. Messmer)

1. "Theoretical Studies of Chemisorption Using Clusters: Accomplishments and Challenges", Colloquium on "The Structure of Small Molecules Adsorbed on Surfaces", Gargnano del Garda, Italy, June 13, 1979.
2. "Recent Progress in Theoretical and Experimental Surface Science and Its Implications for Ceramics", American Ceramic Society National Meeting, New Orleans, October 16, 1979.
3. "Recent Theoretical Studies of Metal Clusters", Exxon Corporate Pioneering Research Seminar, Linden, New Jersey, November 5, 1979.

PRESENTATIONS (J. Wong)

1. "EXAFS: A New Structural Probe for Matter"
MIT Chemistry Department Seminar April/79
2. "Local Structure Probe for Matter Using EXAFS"
State University of New York, Albany
Phys. Department Seminar May/79
3. "Dynamic Disorder in Glassy Solids"
Invited paper give at the 5th University Conference on Glass Science
RPI Aug/79
4. "A Novel Technique for Studying Glassy Solids by EXAFS"
Invited paper given at SPIE's 23rd Annual International Symposium,
San Diego Aug/79
5. "Introduction to EXAFS and Its Applications to Chemical and Bio-
logical Problems"
State University of New York, Albany
Biology Department Seminar Sept/79
6. "EXAFS Studies of Glassy Solids"
Invited paper at the annual Materials Research Soc. Meeting
Boston, MA Nov/79

Figure 1

Figure 2

Figure 3

Figure 4

(a)

(b)

(c)

Figure 5

Figure 6

Figure 7

Figure 8

Figure 9

TOTAL CHARGE DENSITY FOR N18 IN YZ PLANE

Figure 10

TOTAL CHARGE DENSITY IN THE YZ PLANE OF NIBB

GENERAL ELECTRIC

Figure 11

Figure 12

(a)

(b)