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THE STRUCTURE OF NON-CRYSTALLINE MATERIALS. DETERMINATION OF LOCAL STRUCTURE IN AMORPHOUS GeSe, GeSe2, As2, Se3, As2Se3, AND As2Te3 USING EXAFS

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Determination of Local Structure in Amorphous $GeSe$, $GeSe_2$, As_2Se_3, As_2S_3, and As_2Te_3 Using EXAFS

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Determination of Local Structure in Amorphous GeSe, $GeSe_2$, As_2Se_3, As_2S_3 and As_2Te_3 Using EXAFS

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ABSTRACT

Previously, we have shown that Fourier transforms of the extended x-ray absorption fine structure (EXAFS) contains information on the coordination distances and numbers about each constituent in multicomponent amorphous semiconductors. In this paper a method of analysis of the experimentally observed first coordination peak is presented which calculates the absolute number of each kind of atom which contributes to that peak. This analysis depends on 2 factors: (1) normalization of the data to the same scale; and (2) development of 2 sets of equations, one of which represents the first peak amplitudes of the EXAFS data in terms of the number and average scattering power of each kind of atom and the other set which describes the necessary relationships between atoms in a material of a given composition and average coordination. This analysis has been applied to amorphous As_2Se_3, $GeSe_2$ and GeSe. In As_2Se_3 we found the As atom has 3 near neighbors (2Se and 1As) and Se has 2 near neighbors (1As and 1Se). $GeSe_2$ is comparable to the crystalline material with Ge having 4 Se neighbors and Se having 2 Ge's. In GeSe however the

analysis gave nonphysical results which we attribute to assumptions which were made about the average environment of each atom. Nevertheless from our analysis we can show that the random covalent model is not a possible model for amorphous GeSe.

Section 1. Introduction

One of the significant problems in determining the structure of multicomponent amorphous semiconductors is identifying the peaks observed in radial distribution functions with specific interatomic distances which can be identified from postulated structural models; because, the usual scattering experiments measure only a two body correlation function and cannot separate the contributions to the distances from each component in the system. However, Fourier inversion of the extended x-ray absorption fine structure (EXAFS) can measure the distance to and number of atoms surrounding each separate component atom in an amorphous material. Previous application of this technique to several amorphous systems has demonstrated the usefulness of EXAFS for structure determination (Sayers, Lytle and Stern 1971, 1972). Recent improvements in analysis of the data and a reformulation of our theory of EXAFS now permit more accurate determination of distances, distribution of atomic distances and especially of coordination number (Stern and Sayers 1973).

Section 2. Theory

The EXAFS, χ, represents the oscillatory part of the x-ray absorption coefficient on the high energy side of an absorption edge and may be defined by

$$\chi(k) = \mu(k)/\mu_o(k) - 1 \qquad (1)$$

where k is the wave vector of the emitted photoelectron, $\mu(k)$ is the total measured absorption coefficient (i.e. $\ln(I_o/I)$ where I, I_o are the x-ray intensities with the absorber in and out of the x-ray beam, respectively) and $\mu_o(k)$ is the structureless absorption coefficient of the material (see fig. 1c). The experimental determination of $\chi(k)$ is shown in fig. 1 for the EXAFS on the Ge K-edge in amorphous GeSe. In fig. 1a $\ln(I_o/I)$ is plotted versus energy from just below to approximately 1000eV above the K absorption edge. The zero of energy is taken at the Ge K edge. Note that the absorption coefficient not only contains the contribution from the Ge K shell but also contributions from other electrons in Ge, from Se, and from the Al foil and other materials used to form and support the absorber. The contribution of these factors to the absorption was found by fitting a Victoreen formula cross section to the data on the low energy side of the edge and extrapolating through the region of interest as indicated by the dashed line in fig. 1a. This contribution is subtracted from the data leaving only the K shell contribution to the absorption (including EXAFS). This was further decomposed into the oscillatory part of the cross section (fig. 1b) and the smooth and monotonically decreasing ($\mu_o(k)$) cross section (fig. 1c) in the region above the edge using the Fourier filtering technique described previously (Sayers 1971). The curve of fig. 1b is then divided by $\mu_o(k)$ obtained from fig. 1c, which normalizes to unit oscillator strength, to get $\chi(k)$ as defined by equation 1.

The theoretical expression for χ has recently been reformulated to account for data in metallic systems which could not be explained by previous theories. The new theory treats EXAFS as arising from the perturbation of the potential due to the surrounding atoms by the singly ionized hole in the K shell of the absorbing atom. The expression for $\chi(k)$ in a one component system is

$$\chi(k) = 1/k \sum_j N_j \, r_j^{-2} \, E(r_j) g_j(2\underset{\sim}{k}) \exp(-2\sigma_j^2 k^2) \sin(2kr_j + 2\eta(k)) \tag{2}$$

Here $g_j(2\underset{\sim}{k})$ is the backward scattering amplitude from the surrounding atoms in the jth shell of the excited p-state electron of wave number k per unit electric field. $\underset{\sim}{k}$ is directed radially outward from the excited atom to the center of an atom in the jth atomic shell; $E(r_j)$ is the average electric field induced at r_j, the position of the jth shell of atoms, by the ionized atom at $r = 0$; N_j is the total number of atoms in the jth shell; $\eta(k)$ is the phase shift of the photoelectron caused by the potential of the absorbing atom; and σ_j is a measure of the fluctuations of the actual positions of the atoms in the jth shell about their average position r_j. The exponential containing σ_j^2 is a Debye-Waller type factor.

Structural information can be obtained most directly from EXAFS by taking the Fourier transform of $\chi(k)$. From equation 2 this yields a radial structure function

$$\phi(r) = \frac{1}{\sqrt{2\pi}} \int_0^\infty \frac{k\chi(k)}{g(2\underset{\sim}{k})} \sin(2kr+2\eta)\,dk \tag{3a}$$

$$= \sum_j N_j E(r_j)/(8\sigma_j r_j^2) \exp(-2(r-r_j)^2/\sigma_j^2) \tag{3b}$$

The radial structure function is a series of gaussian peaks located at the coordination shell distances r_j whose amplitudes are

$$A_j = N_j E(r_j)/8r_j^2\sigma_j \qquad (4)$$

Thus, it is possible to determine absolute coordination numbers from the measured amplitudes if σ_j and $E(r_j)$ are known. Such a direct approach is complicated by several factors: (1) the actual transforms of the data are convolved with termination effects and uncertainties in the values of η and $g(2k)$; (2) σ_j contains both thermal and disorder contributions and is not well known for amorphous materials (the effects of both (1) and (2) have been discussed previously (Sayers 1971); and (3) $E(r_j)$ is not known although generally it can be thought of as consisting of 2 parts - one being the electric field that is created by the presence of the hole in the K shell of the absorbing atom and the other being the response (polarizability) of the surrounding atoms to this field. While it is possible to estimate the value of $E(r_j)$ the accuracy is insufficient for calculation of absolute coordination numbers. Instead, comparisons of first shell amplitudes between similar materials (such as crystalline and amorphous polymorphs) and between peaks about different species in the same material will be made. The relative coordination numbers obtained by this method are sufficiently reliable to test structural models in amorphous systems.

Section 3. Experimental Results

This section presents experimental EXAFS and radial structure functions for both components in crystalline and amorphous GeSe,

$GeSe_2$, and As_2Se_3 and the As edge in amorphous As_2S_3 and As_2Te_3. These compounds were chosen because of the availability of crystalline and amorphous polymorphs for which structural properties have been measured by other techniques and several models have been proposed.

All EXAFS were measured using an automated X-ray spectrometer (Lytle 1968). Ten experiments were averaged for each sample in order to reduce statistical noise to less than .1%. All data was taken at 77°K. A computer filtering program was used to remove the EXAFS from the monotonic absorption background (as shown in fig. 1) and fourier transforms of the data were made using a fast Fourier transform algorithm.

Crystalline GeSe and $GeSe_2$ were prepared by melting, mixing and quenching appropriate quantities of pure (at least 4 9's) Ge and Se in evacuated quartz tubes. Crystal structures were verified using x-ray diffraction. Amorphous GeSe and $GeSe_2$ were prepared by the evaporation of the crystalline material from a tungsten boat in a vacuum of at least 10^{-5} torr onto substrates of mylar or aluminum foil to a thickness of about 1μm. To reduce non-stoichiometric sublimation of GeSe and $GeSe_2$ various sized pieces were sublimed simultaneously. Measurements of the relative x-ray absorption coefficients proved the composition of the resultant films were within 3% for GeSe and 6% for $GeSe_2$ of the expected composition. As_2Se_3 and As_2S_3 were prepared by melting and mixing the pure elements in evacuated quartz ampoules. The cooled glasses showed only broad x-ray lines. The As_2Te_3 was in the form of a sputtered film. (This film was supplied by John deNeufville of

Energy Conversion Devices).

The radial structure functions obtained from the EXAFS are shown for GeSe, $GeSe_2$ and As_2Se_3, As_2S_3 and As_2Te_3 in fig. 2-4. The compound studied is listed in the figure with parantheses enclosing the element whose EXAFS is being studied; i.e. (Ge)Se-C means the Ge K edge in crystalline GeSe.

In fig. 2-4 the main plots are r^2 times the radial structure function which, according to eq. (4) gives peaks whose amplitudes are proportional to NE/σ. All abscissas are plotted to the same (arbitrary) scale except for fig. 3a and 3c which are 2 times this scale. These plots are roughly comparable to a reduced radial distribution function, much used in x-ray or electron scattering work. Above fig. 2a and 2b and all of the plots in fig. 4 are scales which show the location of atoms around the element being studied as calculated from the crystal structure. Such a scale is not included for $GeSe_2$ since the crystal structure is not well known. Inset in each figure is the EXAFS (plotted vs. $k(\mathring{A}^{-1})$) which has been Fourier transformed to give the accompanying radial structure function.

Comparison of figs. 2a and 2b with the expected positions based on the known crystal structure shows that the EXAFS technique does locate the surrounding atoms with some smearing due to a finite resolution and that the expected differences between the curves due to separate constituent atoms from the third neighbor distance and beyond can be seen. In the amorphous data (fig. 2c and 2d) the first neighbor peak in GeSe-A for both curves shifts from $2.58\mathring{A} \rightarrow 2.38\mathring{A}$. This has been observed previously (Sayers, Lytle and Stern 1972) and is consistent with rdf's of GeSe by

Dove et al. (Dove, Chang, Molnar 1972) and Fawcett et al. (Fawcett, Wagner, Cargill 1972) and GeS, and GeTe by Bienenstock and coworkers (Betts, Bienenstock, Ovshinsky 1970; Rowland, Narashiman, Bienenstock 1972) and by Dove et al. (Dove, Heritage Chopra, Bahl 1970) who found a similar shift. This shift is consistent with the idea that relaxation of the long range order constraint in the crystalline material allows a nearly covalent bond in the amorphous material.

The radial structure functions contain additional structural information beyond the first peak; e.g. the feature at 3.4Å in fig. 2d indicates an Se-Se bond since the (Ge)Se function (fig. 2c) does not contain this peak. Both GeSe-A radial structure functions have a complex of peaks beginning about 3.8Å which has been reported by Fawcett et. al. (1972) as the second peak determined in the radial distribution function. Although much more of this kind of information is conformed in figs. 2-4, this paper is limited primarily to an analysis of the nearest neighbor coordination.

We estimate the error (one standard deviation) in distance determination to be ± 1% and the absolute coordination number to be ± 10%.

The As_2S_3 and As_2Te_3 data could only be analyzed in a qualitative manner because the S and Te absorption edges were beyond the capability of our x-ray spectrometer. A comparison of the As to first neighbor distances gives As to S = 2.21Å, As to Se = 2.42Å, As to Te = 2.75Å where the distances calculated from covalent radii are 2.29Å, 2.42Å and 2.69Å respectively. Previous rdf

measurements have found an As-S distance of 2.30Å (Vaipolin 1963; Petz 1961) which is .1Å longer than the distance we have measured but closer to the expected covalent bond length. Other measurements on As-Se in As_2Se_3 (Vaipolin 1963) and As-Te in As_2Te_3 (Fitzpatrick, 1971; Cornet 1973) found As-Se = 2.4Å and As-Te = 2.7Å which compare favorably with our results. This trend from a tighter bond (more ionic) in As_2S_3 to a more loosely bound As_2Te_3 is to be expected from electronegativity considerations. The $r^2\phi$ amplitudes from figs. 4e and 4f indicate that in all three materials As is approximately 3 coordinated.

Section 4. Structural Analysis

The amplitudes of the first neighbor peaks in EXAFS radial structure functions can be used to find the number of each kind of atom around both constituents in a two component system. We develop an analytical method which obtains this information directly from the EXAFS data if the composition is known and the average coordination number in the material is assumed or has been determined from x-ray or electron diffraction measurements.

The amplitudes for the first neighbor peaks in the radial structure function of the A and B atoms in a two component system may be written as

$$(r_1^2\phi)_A = \rho_A N_A(A) + \rho_B N_B(A) \tag{5}$$

$$(r_1^2\phi)_B = \rho_A N_A(B) + \rho_B N_B(B) \tag{6}$$

where $N_B(A), N_A(A), N_A(B), N_B(B)$ is the average number of B atoms around A, the average number of A atoms around A, etc. $(r_1^2\phi)_{A(B)}$ is r_1^2 times the amplitude of the first peak about the A or B atom located at r_1, ρ_A and ρ_B are the effective scattering of the A and B atom respectively. Because of our incomplete knowledge of the factors affecting ρ_A and ρ_B we assumed that the scattering power of each kind of atom in a material is the same in the crystalline and amorphous polymorphs and thus could be determined experimentally. This is equivalent to saying that either the environmental factors which affects ρ are the same in the crystalline and amorphous polymorphs or they do not effect ρ. This assumption also allows the ρ's to be calculated from the crystalline material since the first radial structure function peaks are due to opposite atom types

only (i.e. $N_B(A)=Z_A, N_A(A)=0$, etc. where $Z(A)$ is the coordination number of A atoms). From equations 4-6 the ρ's are

$$\rho_{B(A)} = (r_1^2\phi)^C_{A(B)}/Z^C_{(A(B))} \tag{7}$$

where ϕ^C is the peak amplitude in the crystalline material and $Z^C(A(B))$ is the coordination of A (for B) in the crystalline material and is known from the crystal structure.

The other equations used in this analysis are based on knowledge of the composition and average near-neighbor coordination of the system. A complete derivation and discussion of these equations will be presented elsewhere (Stern, Sayers, Lytle 1973). These relationships are

$$Z(A) + Z(B) = 2\bar{Z} \tag{8}$$

$$C_A N_B(A) = C_B N_A(B) \tag{9}$$

$$C_A N_A(A) + C_B N_A(B) = C_A Z(A) \tag{10}$$

$$C_B N_B(B) + C_A N_B(A) = C_B Z(B) \tag{11}$$

$\bar{Z}$ is the average coordination of both kinds of atoms in a material and may be determined from covalent bonding requirements or radial distribution curves. C_A and C_B are the number of A and B atoms/vol and are determined from the composition. Eqs. 5 and 6 and 8-11 form the set of equations needed to determine $N_A(A), N_A(B)$, $N_B(A), N_B(B), Z(A)$ and $Z(B)$.

Before proceeding with the analysis one other factor must be determined. If the factor σ_j (from eq. 4) in the amorphous

system is different from the crystalline then equations 5 and 6 are not valid. This may be corrected by the following normalization procedure. As long as the average environment remains the same, as we have previously assumed, the total scattering in the two systems (i.e. the total peak areas) must remain the same. We normalize by multiplying the amplitude in the amorphous material by the ratio, R, defined by $(r_1^2\phi)_A^C + (r_1^2\phi)_B^C$ divided by $(r_1^2\phi)_A^A + (r_1^2\phi)_B^A$ where the superscripts C and A denote the crystalline and amorphous values respectively.

The data used in the structural analysis is presented in table I and the results for As_2Se_3, $GeSe_2$ and GeSe are presented in table II. The symbols have been explained previously in the text.

In As_2Se_3 -A the coordination is approximately 3 about As and 2 about Se as in the crystalline material but there is a significant change from total opposite neighbor coordination in the crystalline material to both As and Se in the amorphous material having about 1 similar atom in the first shell.

$GeSe_2$, on the other hand, is very similar to the crystalline material with the Ge being 4 fold coordinated by Se atoms and Se being 2 fold coordinated by Ge. This indicates that the layered structure of the crystalline material is retained in the amorphous material except that the layers are no longer regularly stacked.

For GeSe the results of the analysis are nonphysical. Since GeSe is the only one of the three systems which showed a significant change in the near neighbor environment between the crystalline and amorphous systems, this probably means that our assumption of

similar scattering of Ge and Se atoms in the crystalline and amorphous systems is not valid. A better understanding of the factors affecting the scattering power of each atom is necessary before systems such as GeSe can be analyzed by our technique. There are, however, some statements which can be made about this system on the basis of our analysis. First, the random covalent model proposed by Betts, et al. (Betts, Bienenstock, Ovshinsky 1970) is not a possible model for GeSe since it is inconsistent with the requirements of eq. (9) that an equiatomic compound have the same number of opposite neighbors about each kind of atom. In fact eq. (9) represents a stringent constraint on any model in a two component amorphous material. Second, qualitatively it seems that in the amorphous material the coordination of Ge increases while that of Se decreases with respect to the crystalline polymorph as can be seen by comparing $r^2\phi$ from both edges as seen in table I. This suggests that in GeSe is 4 fold coordinated and Se, 2 fold coordinated, although the distribution of atoms can't be determined. This result casts some doubt on the 3 fold coordination model recently proposed by Bienenstock (Bienenstock 1973).

Section 5. Conclusions

We have shown that Fourier transforms of EXAFS can be analyzed in detail to produce complete enumeration and identification of nearest neighbor atoms in multicomponent amorphous materials when the EXAFS of each different atom may be measured (in As_2S_3 and As_2Te_3 the S and Te atoms were beyond the capability of our x-ray

spectrometer). The analysis presented here was limited by the need to normalize the data to the case of the crystalline polymorph because σ, was not known. However, this is not a fundamental limitation and work in progress will determine the EXAFS at 2 temperatures and determine σ, thus eliminating the need for normalization. These initial studies have shown that the calculated results are very sensitive to the values of $r^2\phi$, thus indicating that the analysis has the potential of giving very accurate results when data of sufficient accuracy is available.

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Table I Summary of 1st Peak Data for As_2Se_3, GeSe, $GeSe_2$

Sample	N	Crystalline r_1 (Å)	Crystalline $\phi(r_1)$	Crystalline $r_1^2\phi$	Crystalline $r_1^2\phi/N$	Amorphous r_1 (A)	Amorphous $\phi(r_1)$	Amorphous $r_1^2\phi$	Amorphous $Rr_1^2\phi$
						(C_{As}/C_{Se} = 2/3, $\bar{Z}$=2.5, R = .9)			
$(As_2)Se_3$	3	2.41	2.06	12.0	4.0	2.41	2.04	11.8	10.6
$As_2(Se_3)$	2	2.42	1.11	6.2	3.1	2.43	1.39	8.2	7.4
						(C_{Ge}/C_{Se} = .5, $\bar{Z}$=3, R=1.2)			
$(Ge)Se_2$	4	2.35	4.87	26.8	6.7	2.38	3.82	21.6	25.9
$Ge(Se_2)$	2	2.34	1.66	9.4	4.7	2.38	1.51	8.6	10.3
						(C_{Ge}/C_{Se} = 1, $\bar{Z}$=3, R=1.16)			
(Ge)Se	3	2.59	2.01	13.5	4.5	2.38	2.40	13.6	15.8
Ge(Se)	3	2.59	1.34	9.0	3.0	2.38	1.10	5.7	6.7

Table II. Structural Results for As_2Se_3, $GeSe_2$, GeSe

$(As_2)Se_3$	$Z(As) = 2.8$	$N_{As}(As) = .9$	$N_{Se}(As) = 1.9$
$As_2(Se_3)$	$Z(Se) = 2.2$	$N_{Se}(Se) = .9$	$N_{As}(Se) = 1.3$
$(Ge)Se_2$	$Z(Ge) = 3.9$	$N_{Ge}(Ge) = .1$	$N_{Se}(Ge) = 3.8$
$Ge(Se_2)$	$Z(Se) = 2.1$	$N_{Se}(Se) = .2$	$N_{Ge}(Se) = 1.9$
(Ge)Se	$Z(Ge) = 3.0$	$N_{Ge}(Ge) = -1.5$	$N_{Se}(Ge) = 4.5$
Ge(Se)	$Z(Se) = 3.0$	$N_{Se}(Se) = -1.5$	$N_{Ge}(Se) = 4.5$

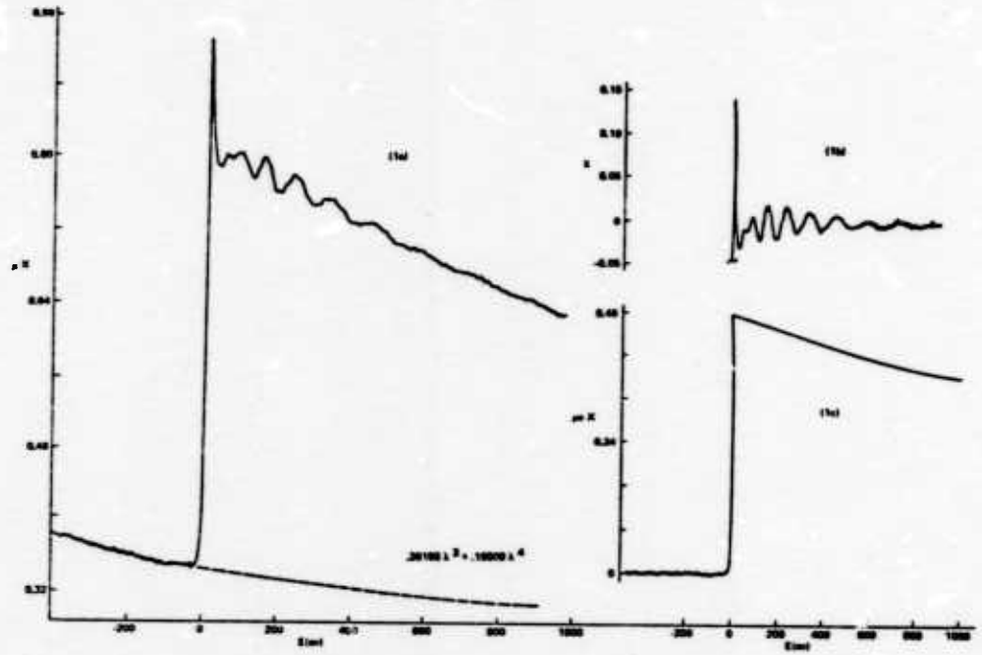
Figure Captions

Fig. 1a) The measured K x-ray absorption edge of Ge in amorphous GeSe plotted x-ray absorption coefficient times thickness (μX) vs. the photoelectron kinetic energy, E. 1b) χ vs E normalized and extracted from fig. 1a) as explained in the text. 1c) $\mu_o X$ vs E, which is the function used to normalize χ and is obtained by subtracting the Victoreen extrapolation (dashed line on 1a) from μX and then Fourier filtering to remove the oscillatory part of the absorption coefficient.

Fig. 2a)-d) Radial structure functions for crystalline (C) and amorphous (A) GeSe plotted $r^2\phi$ vs radial distance, Å. The notation (Ge)Se-C indicates that the function is a plot of atomic distribution around an average Ge atom in crystalline GeSe, etc. Near the top of each crystalline case is a horizontal line plotting the respective positions of Ge sites and Se sites radially from the origin atom. The inset plots χ vs k ($k= (.263E)^{1/2}$) for each of the respective K absorption edges. In each case this function was Fourier transformed to obtain the radial structure function.

Fig. 3a)-d) Radial structure functions for crystalline and amorphous $GeSe_2$. See fig. 2 for general description.

Fig. 4a)-f) Radial structure functions for crystalline and amorphous As_2Se_3 and amorphous As_2S_3 and As_2Te_3. See Fig. 2 for general description.


(1a)
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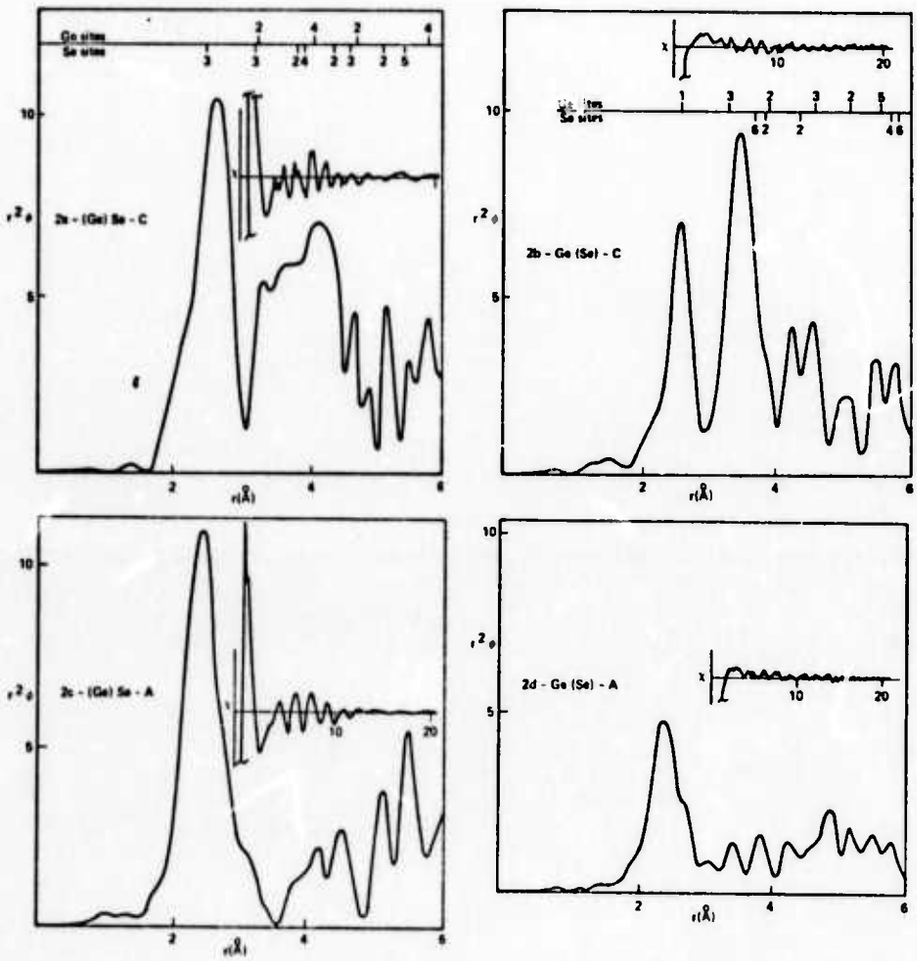
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Se sites
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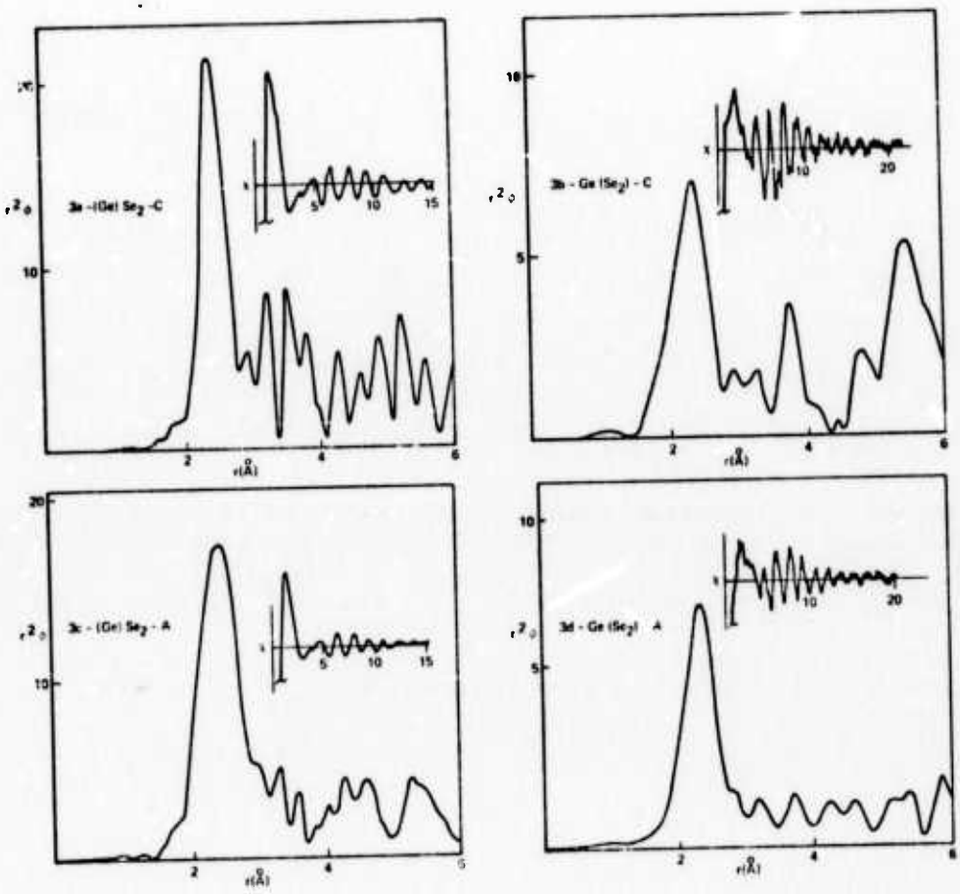
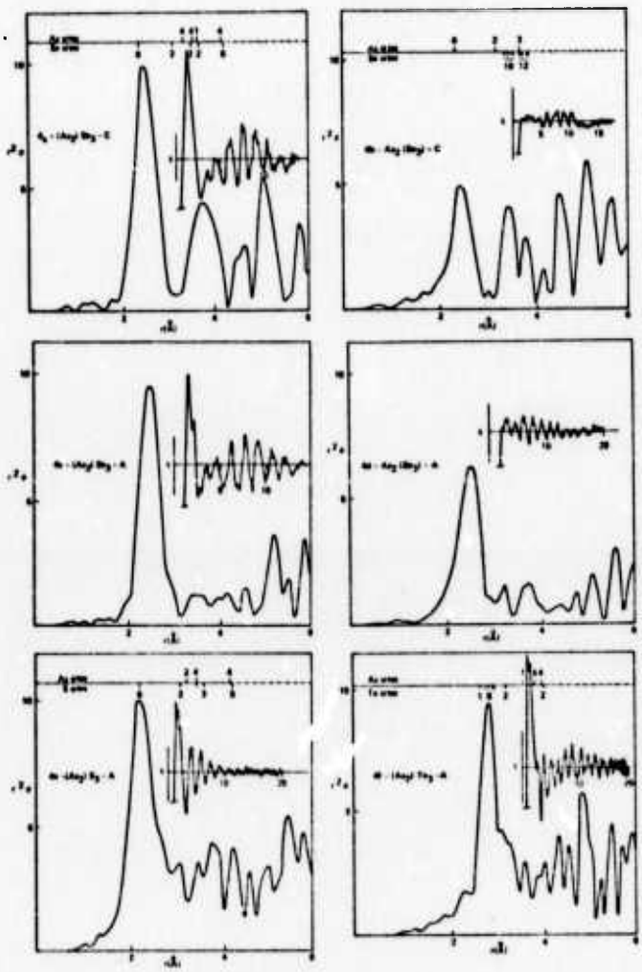
2b - Ge (Se) - C
2c - (Ge) Se - A
2d - Ge (Se) - A
r(Å)


3a - (Ge) Se2 - C
3b - Ge (Se2) - C
3c - (Ge) Se2 - A
3d - Ge (Se2) A
r(Å)