

Structure of bulk amorphous GaSb: A temperature-dependent EXAFS study

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(Received 25 April 1997)

We have studied the structure of bulk amorphous GaSb using the extended x-ray-absorption fine-structure (EXAFS) technique over the temperature range from 80 K to 293 K. The possibility of the presence of chemical disorder has been explored throughout the temperature range. The configurational (static) contribution to the Debye-Waller broadening of the distances has been extracted from EXAFS data. The bond-angle distribution for *a*-GaSb was calculated from the results of EXAFS analysis. The mean bond angle has been calculated from Sb *K*-edge data and found to be 108.9°. [S0163-1829(97)02141-3]

The problem of understanding the structure of amorphous materials still attracts a lot of attention in the field of solid state physics both due to the general character of the problem, requiring the development of advanced theoretical, computational, and experimental approaches for studies of disordered matter (see, for example Refs. 1–3), and its technological importance.^{4,5} The unambiguous determination of the structure of materials is also of great importance since this defines their main macroscopic (i.e., electrical and thermal conductivity, elasticity, etc.) and electronic properties. On the other hand, it becomes impossible to build a structure of an amorphous solid in the way that is done for crystals because of the loss of periodicity in amorphous materials, and, as a consequence, the loss of the relationship between structure and symmetry (which allows the building of the structure of a crystalline material from diffraction studies). As a result there are still debates about the structure of well-studied materials such as *a*-Si and *a*-Ge.^{6–8} The question also posed is whether it is possible to obtain a unique structural solution using results of diffraction experiments.⁷

The most widely used methods of direct structural studies of disordered solids are neutron, x-ray diffraction, and extended x-ray-absorption fine structure (EXAFS). The former provides information on long-range correlations, however the procedure of extraction of the information is somewhat complicated for materials with more than one type of atomic species, since diffraction yields the environment of an “averaged” atom. Although the analysis can be done for crystalline materials, it is very complicated for disordered solids. In particular the complications arise from the fact that the disorder in an amorphous solid can be either configurational (spread in bond lengths and bond angles) or chemical (cation-cation or anion-anion bonding) or both. In contrast to amorphous group-IV elements (i.e., *a*-Ge, *a*-Si), which can only have configurational disorder, amorphous III-V compounds, being binary solids, can also contain wrong bonds

(bonds between “like” atoms, i.e., Ga-Ga or Sb-Sb in GaSb) and therefore can be also chemically disordered. Continuous random network models (originally developed by Polk⁹) are usually applied to describe the structure of amorphous covalently bonded materials such as *a*-Si and *a*-Ge. The key feature of such models is the significant extent of chemical disorder.¹⁰ This, in turn, would result in the increase of internal energy, reducing the stability of such materials. Continuous random network models with a high degree of chemical order have been developed by Connell and Temkin,¹¹ and are considered to be most appropriate for III-V compounds. In fact, it has been demonstrated recently¹² that a Connell-Temkin-like structural model can be considered superior, from both structural and energetic points of view, to those calculated using, for example, tight-binding potentials or molecular dynamics. The experimental determination of chemical disorder in amorphous materials is hampered significantly by either the quality of experimental data or difficulties in extraction of such information intrinsic to diffraction. We have used temperature-dependent EXAFS measurements on Sb- and Ga-*K* absorption edges to study the local structure in bulk amorphous GaSb. EXAFS is particularly useful as a probe for short-range structure around a specific type of atom. In this paper we explore the possibility of chemical disorder in bulk amorphous GaSb prepared by solid-state amorphization under high pressure. We will also show how the use of the technique of EXAFS can provide valuable and accurate information on the structure of bulk amorphous GaSb (*a*-GaSb).

Amorphous GaSb was prepared by the high-pressure solid state amorphization technique described earlier.^{13,14} Samples were finely ground, and the powder was mixed with boron nitride to ensure the homogeneity of samples for transmission EXAFS experiments. Temperature-dependent EXAFS experiments have been carried out on stations 7.1 (Ga-*K* edge) and 9.2 (Sb-*K* edge) at CCLRC Daresbury Laboratory

synchrotron radiation source, using an Oxford Instruments variable temperature cryostat. The postedge $\chi(k)$ parts of the EXAFS spectra were extracted using SPLINE, the interactive program for background subtraction.¹⁵ The program fits splines to smoothly varying background absorption. It also allows one to check interactively the influence of fitting on the Fourier transform, and thus very effectively minimizes the distortions in the Fourier transform related to the curvature of background absorption. The method of analysis and the quality of the original data are two main standpoints in the treatment of EXAFS data which separate semiquantitative and fully quantitative results. The S/N ratio and therefore maximum k range accessible define the accuracy and amount of information which can be extracted from an EXAFS spectrum. The use of bulk material allowed us to employ the well-established and most accurate EXAFS technique, transmission, and easily maximize the absorption step $\Delta\mu x$ (μ is the absorption coefficient, x is the sample thickness) at both Sb- and Ga-Kedges. The analysis of chemical ordering was also simplified due to the significant difference in scattering amplitudes of Ga and Sb atoms. Analysis of EXAFS spectra has been done by use of the EXCURV92 program.¹⁶ EXAFS analysis using EXCURV92 consists of least-squares fitting of a theoretical model to the experimental data until the best fit is produced. The scattering phase shifts and atomic potentials were calculated within the program by use of the von Barth-Hedin-Hedin-Lundqvist potential set. Crystalline GaSb (99.99+%) was used as a reference material to set amplitude factors.¹⁶ The structural parameters extracted from an EXAFS spectrum are usually the following: \bar{R} (average interatomic distance), \bar{N} (average coordination number), σ^2 (mean square variation (MSD) of bond length or relative Debye-Waller (DW) broadening) and the type of atomic species around the central atom. The error determination is an important part of EXAFS analysis. The procedure ideally has to be done for every spectrum using methods of statistical analysis¹⁷ (included in EXCURV92) to access the correlation between parameters during fitting and, therefore, statistical errors. We always quote the limits of the 95% confidence region, i.e., the $\pm 2\epsilon$ uncertainties, where ϵ is the standard deviation. However there also exists a part of the error which is related to the experimental conditions and the theory used to calculate EXAFS spectra. Here we have used *c*-GaSb to quantify such errors.

The resulting $k^3\chi(k)$ dependencies with their magnitudes of Fourier transforms and theoretical fittings for both Ga- and Sb-K edges for *a*-GaSb at $T=80$ K are presented in Fig.

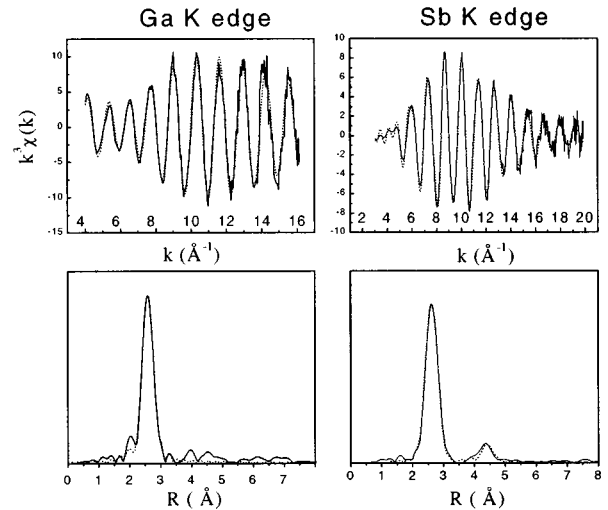


FIG. 1. The $k^3\chi(k)$ functions and magnitudes of their Fourier transforms for *a*-GaSb for Ga- and Sb-K edges ($T=80$ K). Dotted lines are the calculated spectra.

1. The structural parameters mentioned above corresponding to the best fit obtained are listed in Table I. For comparison the results for *c*-GaSb are presented in Fig. 2, and parameters listed in Table II. All calculations were made in the single scattering approximation and the assumption of no chemical disorder. The question of chemical disorder will be discussed later in this paper. We can see from Tables I and II that the number of nearest neighbors and distances in *a*-GaSb are very close to those in the crystal (lower just by ≈ 0.2 in the former). This agrees with the fact that the densities of bulk *a*-GaSb and *c*-GaSb are within $\approx 3\%$. The most important point we would like to stress is that it was possible to obtain the position (\bar{R}) of the second nearest neighbors (see Fig. 1) at $T=80$ K for the Sb-K edge. Another feature of EXAFS is that DW broadening for the first shell is generally lower than that for higher shells. This is due to significant correlation in atomic oscillations for nearest neighbors.

We have looked for the presence of wrong bonds (Ga-Ga and Sb-Sb) throughout the temperature range at both Ga- and Sb-K edges by direct introduction of such disorder in the fitting parameters. As a result we have found a systematic difference between the amorphous and crystalline EXAFS data. For amorphous GaSb from the Ga-K edge data at $T=78$ K the number of nearest neighbors in the first shell N_{Ga}

TABLE I. The results of EXAFS analysis of *a*-GaSb from Ga- and Sb-K edges at different temperatures.

T , K	Ga-K edge				Sb-K edge				
	Shell	$N(\text{Sb})$	R , Å	$2\sigma^2$, Å ²	T , K	Shell	$N(\text{Ga})$	R , Å	$2\sigma^2$, Å ²
78	1	3.4(3)	2.640(5)	0.0072(7)	80	1	3.8(2)	2.649(5)	0.0084(6)
						2	12(fixed)(Sb)	4.31(1)	0.024(1)
130	1	3.6(2)	2.635(5)	0.0082(6)	100	1	3.9(3)	2.647(5)	0.0088(7)
180	1	3.5(3)	2.637(5)	0.0086(8)	140	1	3.8(3)	2.648(5)	0.0092(8)
240	1	3.5(3)	2.637(5)	0.0098(7)	190	1	4.1(4)	2.651(5)	0.010(4)
293	1	3.7(6)	2.633(5)	0.012(1)	250	1	4.0(6)	2.652(5)	0.011(1)
					290	1	3.9(5)	2.649(5)	0.013(1)

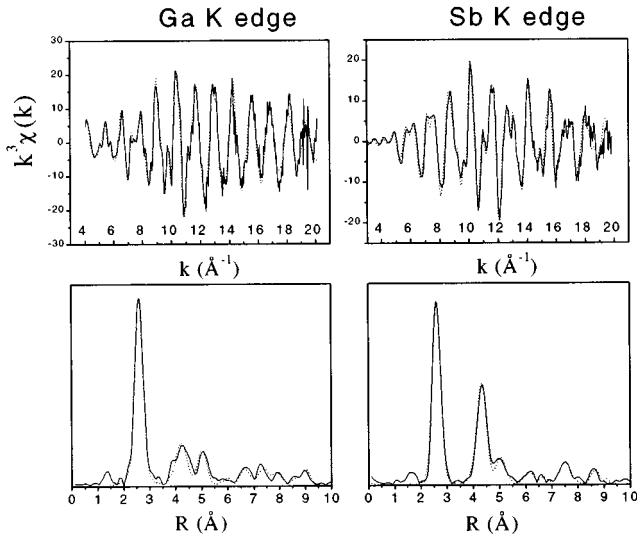


FIG. 2. The $k^3\chi(k)$ functions and magnitudes of their Fourier transforms for c -GaSb for Ga- and Sb-K edges ($T=80$ K). Dotted lines are the calculated spectra.

was found to be 0.7(5) and the MSD of bond length $\sigma_{\text{Ga-Ga}}^2 = 0.009(8)$, while for c -GaSb the N_{Ga} is around zero. It was also found that error in determination of N_{Ga} increases from ± 0.5 to $\pm 0.7-0.8$. Thus it becomes impossible to use both N_{Ga} and $\sigma_{\text{Ga-Ga}}^2$ as free parameters (as has been pointed out in Ref. 18). Although the observation of systematic differences in crystalline and amorphous spectra suggests the presence of wrong bonds it should be noted that uncertainties are relatively large. The fit with N_{Sb} and $\sigma_{\text{Sb-Sb}}^2$ as free parameters at Sb-K edge showed that N_{Sb} remained constant and close to zero. This result puts serious doubts on the presence of Sb-Sb type wrong bonds, though it should be noted that the analysis is complicated due to the similar values of $R_{\text{Sb-Ga}}$ (2.64 Å) (Ref. 19) and the covalent bond length $R_{\text{Sb-Sb}}$ (2.65 Å).¹⁹ From the point of view of EXAFS, chemical disorder can also be detected as a distortion of the shape of the first peak in a Fourier transform of the EXAFS signal. We have used a cumulant²⁰ expansion to study any non-Gaussian character of the first peak in the Fourier transform at $T=80$ K. The results have shown that the third and the fourth cumulants for amorphous (and crystalline) GaSb are close to zero and do not affect the main structural parameters at both Ga- and Sb-K edges. One of the ways of getting information

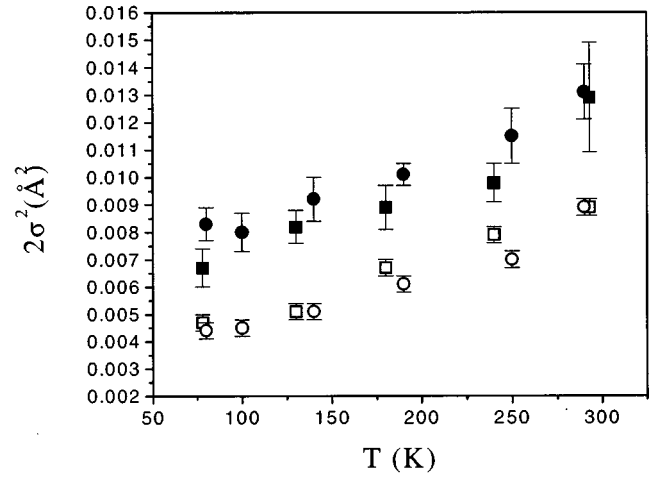


FIG. 3. The Debye-Waller broadening $2\sigma^2$ versus temperature for c -GaSb Ga-K edge (open squares), Sb-K edge (open circles) and a -GaSb Ga-K edge (solid squares) and Sb-K edge (solid circles).

on chemical disorder is the study of Debye-Waller broadening versus temperature. If there is a significant proportion of wrong bonds one expects to observe the nonlinearity of this dependence, due to different temperature dependencies of the MSD of different atomic species. The result of the comparison of temperature dependencies of DW broadening for crystalline and amorphous GaSb are presented in Fig. 3. All dependencies can be considered to be linear versus temperature, as predicted by lattice dynamics (within a Debye model) in this range of temperatures.¹⁰ All the above suggests that the degree of chemical disorder in the material (if there is any) is below the accuracy of the EXAFS technique. This agrees qualitatively with the estimation made using the ordering criteria for binary amorphous alloys developed by Gurman. In his model²¹ the parameter governing the formation of ordered/disordered alloys is $\Delta E/kT$, where ΔE is the *bond ordering energy* as defined in Ref. 21. The bond ordering energy is related to the electronegativities of elements in a Pauling²² representation as

$$\Delta E = C(x_i - x_j)^2,$$

where x_i and x_j are electronegativities of elements i and j which compose the alloy and C is a constant which is almost exactly 1.0 eV.²² It has been shown²¹ that between the lim-

TABLE II. The results of EXAFS analysis of c -GaSb from Ga- and Sb- K edges at different temperatures.

Ga-K edge					Sb-K edge				
T , K	Shell No.	$N(\text{Sb})$	R , Å	$2\sigma^2$, Å ²	T , K	Shell No.	$N(\text{Ga})$	R , Å	$2\sigma^2$, Å ²
78	1	4.1(2)	2.636(5)	0.0036(3)	80	1	4.0(2)	2.626(5)	0.0044(3)
	2	12 (Ga)	4.305(8)	0.0122(6)		2	12(Sb)	4.306(5)	4.306(5)
130	1	4.0(2)	2.634(5)	0.0052(3)	100	1	4.0(2)	2.633(5)	0.0046(3)
180	1	4.0(2)	2.639(5)	0.0068(3)	140	1	4.0(2)	2.631(5)	0.0050(3)
240	1	4.0(2)	2.633(5)	0.0072(3)	190	1	4.0(2)	2.631(5)	0.0062(3)
293	1	4.0(2)	2.628(5)	0.0084(3)	250	1	4.0(2)	2.632(5)	0.0076(3)
					290	1	3.9(2)	2.638(5)	0.0090(3)

iting cases of $\Delta E/kT \rightarrow 0$ (random order) and $\Delta E/kT \rightarrow \infty$ (total order), the special value $\Delta E/kT \approx 2.0$ can be distinguished such that only alloys with $\Delta E/kT < 2.0$ can be separated from the totally ordered case. Taking electronegativity values for Ga and Sb from Ref. 22 (1.6 and 1.9, respectively) we obtain $\Delta E/kT \approx 1.7$ for the sample under question (preparation temperature $T_{\text{syn}} = 700$ K). This shows that the determination of chemical disorder can indeed be ambiguous, though the tendency for chemical disorder can be expected in this case.

The presence of a second peak in the Fourier transform of the Sb- K edge EXAFS signal from a -GaSb means that we can extract the value of partial mean bond angle which is $\theta_{\text{Sb-Ga-Sb}} = 108.9(9)^\circ$ ($\theta = 109.47^\circ$ for c -GaSb and $\bar{\theta} = 108.6^\circ$ for bulk a -GaSb from neutron studies²³). However, due to strong correlation between N and σ^2 for this shell, it appeared to be difficult to obtain unambiguous information on values of these parameters. Fitting with all parameters set free resulted in the best fit produced, but gave too low a value for $N_2 = 2.3(1.2)$, while $\sigma_{\text{Sb-Sb}}^2 = 0.006(3) \text{ \AA}^2$ [whereas $N_2 = 12$ and $\sigma_{\text{Sb-Sb}}^2 = 0.006(1)$ in crystal]. Therefore we decided to fix the number of the Sb neighbors $N_2 = 12$ since it was found that the number of nearest neighbors in amorphous material is close to that for the crystal (Table I). This procedure is also acceptable because the error in the determination of the numbers of nearest neighbors is usually $> 10\%$ for second shell. With the number of neighbors being fixed the fitting resulted in $\sigma_2^2 = 0.012(1) \text{ \AA}^2$. The value of second shell distance was found to be independent of the fitting process used (within error) and can be found in Table I.

Having obtained this information we can also calculate the angle distribution function in a -GaSb (considering the distributions of two distances being of Gaussian form) related to amorphous nature of samples. Unfortunately EXAFS can only provide the relative values of MSD of atoms from their positions (expressed as bond length variation) and to calculate angle distribution we, of course, require the absolute values. However we can obtain the necessary information if we consider that $\sigma_{\text{am}}^2 = \sigma_{\text{cr}}^2 + \sigma_{\text{con}}^2$ (where σ_{cr}^2 is solely due to the finite temperature, and σ_{con}^2 is the configurational part related to bond angle and bond length variations). This implies the similarity of the temperature-dependent contributions for the first shell in both amorphous and crystalline materials, and is valid because of the similarity of local structure. Then from the results for the first shell at the Sb- K edge in a -GaSb and c -GaSb we obtain $\sigma_{\text{con}}^2 = 0.0020(6)$ [$0.0036(10)$ at Ga- K edge], and for the second peak at Sb- K edge $\sigma_{\text{con}}^2 = 0.0075(4)$. The above values are necessary parameters for the two distributions of distances ($R_{\text{Ga-Sb}}$ and $R_{\text{Sb-Sb}}$), and these in turn allow the calculation of angle distribution. A gaussian distribution of bond lengths and their statistical independence were assumed for calculations. These initial conditions result in a unique solution.

The analytical derivation of the angle distribution in question is a rather difficult task but computer calculations can be done in a straightforward manner. The resulting angle distribution for 5×10^4 atoms (iterations) is centered at $\theta_{\text{Sb-Ga-Sb}} = 108.9^\circ$ and has a standard deviation of 3.8° . We can also estimate the total spread in bond angle related to both con-

figurational and thermal disorder. The contribution of temperature to the Debye-Waller factor can be calculated using, for example, a Debye approximation. The calculated values of Debye-Waller broadening at $T = 80$ K are then the following: $\sigma_{\text{Ga-Sb}}^2 \approx 0.012 \text{ \AA}^2$, $\sigma_{\text{Ga-Ga}}^2 \approx 0.007 \text{ \AA}^2$, and $\sigma_{\text{Sb-Sb}}^2 \approx 0.005 \text{ \AA}^2$. Therefore the total absolute mean square deviation of atoms from their positions is 0.014 \AA^2 for the Ga-Sb bonds in a -GaSb. We obtain in a similar way the value of 0.013 \AA^2 for Sb-Sb distance. This results in a standard deviation of 6.9° for the Sb-Ga-Sb bond angle in a -GaSb. The above values are the lower limits for bond angle distortions in a -GaSb. The absence of a second shell at the Ga- K edge implies a higher degree of disorder in the Ga-Ga distance. We can estimate this disorder by introducing a second shell in the fitting of the Ga- K edge data. The fit with $N_{\text{Ga}} = 12$ and $R_{\text{Ga-Ga}} = 4.31 \text{ \AA}$ resulted in $\sigma_{\text{Ga-Ga}} \approx 0.025 \text{ \AA}^2$ which can serve as a lowest possible value of broadening. Using this value and those from Tables I and II in the procedure described above we obtain the values of standard deviations 5.8° and 8.5° for configurational and total angle distortions, respectively, of the Ga-Sb-Ga bond angle. The value of mean bond angle is 109.7° .

The result for the values of θ agrees with those reported on the value of bond angle in thin film GaP, GaAs, and InP,²⁴⁻²⁶ a -Si, a -Ge, a -C,⁶⁻⁸ and bulk a -GaSb,²³ where it was suggested that the mean angle is most likely to be close to its tetrahedral value.

We have thus shown how the EXAFS technique can provide access to very important structural information (bond length and angle distributions, chemical disorder) for an amorphous material. A harmonic approximation and single scattering approach can be used to adequately describe the local structure (first shell) in a -GaSb. We conclude that chemical disorder can hardly contribute significantly in the topology of the amorphous network of bulk a -GaSb. The temperature dependence of the MSD for bond lengths and values of standard deviations both due to the amorphous nature of samples and finite temperatures have been presented. The results suggest that the degree of angle disorder is higher for Ga-Sb-Ga bond angle than that for Sb-Ga-Sb, although at $T = 80$ K we still have not reached the lower limit saturation for DW broadening predicted by the Debye model [$\sigma^2(T) = \text{const}$]. This leaves an opportunity to obtain accurate information on second shell structural parameters from Ga- K edge EXAFS at $T < 80$ K. We have also shown that calculations of partial bond angle distributions (θ_{i-j-i} and/or θ_{j-i-j}) can be done as a result of low temperature EXAFS experiments in an amorphous material. The averaging of information obtained by diffraction experiment makes possible coexistence of nonunique structural solutions. The information on partial correlations (distance, angle, and DW broadening) in EXAFS allows one to obtain more constraints for subsequent modeling without involving the complex, and not always possible, procedure of isotopic substitution. The question is still unresolved however of what kind of information we require to describe fully the structure of a disordered material. The ultimate representation of an amorphous material will be of course the coordinates of every particular atom in the material. However, until this information is accessible one has to use computer modeling for calculations of, e.g., EDOS, elastic properties, etc. An essential feature of all

such calculations is the number of constraints one can obtain prior to simulation. Using all the experimental information we have obtained to date on α -GaSb such modeling can be very promising indeed.

We gratefully acknowledge DMU and CCLRC Daresbury Laboratory for financial support (for A.V.S.), and CCLRC

Daresbury Laboratory for beam time and computer facilities, and the Royal Society for the award of FSU-UK joint project grant. A.G.L., V.V.B. and A.V.S. are grateful to Dr. S. J. Gurman and to Professor S. V. Popova for many useful discussions. A.G.L. and V.V.B. also thank the Russian Fund for Fundamental Research for financial support (Grant No. 95-02-03677).

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