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EFFECTS OF COHERENT SCATTERING ON INFRARED
ABSORPTION IN DOPED SEMICONDUCTORS

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Final Report for Period June 1985 - August 1986

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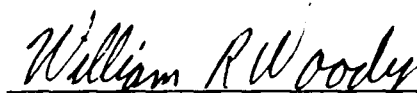
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SECURITY CLASSIFICATION OF THIS PAGE

REPORT DOCUMENTATION PAGE				Form Approved OMB No. 0704-0188	
1a. REPORT SECURITY CLASSIFICATION Unclassified			1b. RESTRICTIVE MARKINGS		
2a. SECURITY CLASSIFICATION AUTHORITY			3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for public release; distribution unlimited		
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE					
4. PERFORMING ORGANIZATION REPORT NUMBER(S) AFWAL-TR-88-4205			5. MONITORING ORGANIZATION REPORT NUMBER(S)		
6a. NAME OF PERFORMING ORGANIZATION Materials Laboratory AFWAL, AFSC		6b. OFFICE SYMBOL (If applicable) AFWAL/MLPO	7a. NAME OF MONITORING ORGANIZATION		
6c. ADDRESS (City, State, and ZIP Code) Wright-Patterson Air Force Base, Ohio 45433-6533			7b. ADDRESS (City, State, and ZIP Code)		
8a. NAME OF FUNDING/SPONSORING ORGANIZATION		8b. OFFICE SYMBOL (If applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER		
8c. ADDRESS (City, State, and ZIP Code)			10. SOURCE OF FUNDING NUMBERS		
PROGRAM ELEMENT NO. 61102F		PROJECT NO. 2306	TASK NO. 2306Q1	WORK UNIT ACCESSION NO. 2306Q106	
11. TITLE (Include Security Classification) Effects of Coherent Scattering on Infrared Absorption in Doped Semiconductors (U)					
12. PERSONAL AUTHOR(S) Grigsby, Peggy J., Universal Energy Sys. and Brown, Gail J.					
13a. TYPE OF REPORT Final		13b. TIME COVERED FROM Jun 85 to Aug 86	14. DATE OF REPORT (Year, Month, Day) 89 April		15. PAGE COUNT 39
16. SUPPLEMENTARY NOTATION					
17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)		
FIELD	GROUP	SUB-GROUP			
20	05		Infrared absorption, absorption spectra, optical channeling, coherent scattering, semiconductors		
19. ABSTRACT (Continue on reverse if necessary and identify by block number)					
An improved theoretical model was developed for interpreting the infrared absorption spectra of doped semiconductors. The model focused on the specific problem of coherent scattering effects or optical channeling. These effects are produced by coherent multiple internal reflections from the polished plane-parallel faces of an optically thin sample. The coherent scattering produces oscillating noise on the infrared absorption spectrum. This noise makes it difficult to determine the correct absorption coefficient from the spectrum. The effect occurs in both silicon and gallium arsenide. The specific expression for the transmittance in the presence of scattering was determined and the inversion of this relation was calculated to obtain the absorption coefficient. In cases where the equation based on coherent scattering did not give results, a combination of coherent and incoherent scattering equations was used to minimize the channeling oscillations. This mixed scattering equation was used to calculate the absorption coefficient versus wavelength from Fourier Transform (cont)					
20. DISTRIBUTION/AVAILABILITY OF ABSTRACT ☒ UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT ☐ DTIC USERS			21. ABSTRACT SECURITY CLASSIFICATION Unclassified		
22a. NAME OF RESPONSIBLE INDIVIDUAL Gail J. Brown			22b. TELEPHONE (Include Area Code) (513) 255-4474		22c. OFFICE SYMBOL AFWAL/MLPO

19. ABSTRACT (Cont)

Infrared (FTIR) transmittance spectra which had shown channeling effects. The results from this calculation were compared to other methods available to eliminate oscillations in spectra.

FOREFORD

This report describes the results of a study to model the effects of optical channeling on infrared absorption in semiconducting materials. The work was performed under the Graduate Student Summer Support Program sponsored by the Air Force Office of Scientific Research. It was conducted in-house with personnel of the Electronic and Optical Materials Branch, Electromagnetic Materials Division, Air Force Wright Aeronautical Laboratories, Wright-Patterson Air Force Base, Ohio 45433-6533 under Project No. 2306, Task 230601, Work Unit 23060106. The report covers work performed during the periods of June 1985 through August 1985 and June 1986 through August 1986.

One of the authors (PJG) would like to thank the Air Force Systems Command, the Air Force Office of Scientific Research and the Laser and Optical Materials Branch of the Air Force Wright Aeronautical Laboratories Materials Laboratory for the opportunity of spending these summers on this research. Special thanks go to Dr. Gust Bambakidis and Mr. David Fischer for their support and guidance throughout this study.

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SECTION I

INTRODUCTION

The Air Force Wright Aeronautical Laboratories Materials Laboratory is currently conducting research to develop semiconductor materials for use in advanced infrared detector systems and improved electronic devices. An important part of this research is the characterization of the electrical and optical properties of various semiconducting materials, in particular silicon and gallium arsenide. One of the optical characterization techniques used is low temperature Fourier Transform Infrared (FTIR) absorption spectroscopy. The low temperature absorption of infrared radiation by impurities or dopants in these semiconducting materials produces a unique excitation spectrum (References 1,2). This excitation spectrum is used to identify what impurities are present in the material and to measure the concentration of these impurities. It is these impurities which ultimately determine the operating limitations of an infrared detector or electronic device.

A typical absorption spectrum resulting from a shallow acceptor impurity in extrinsic silicon is shown in Fig. 1. The series of 10 or more peaks is due to the photoexcitation of the allowed electronic transitions associated with an acceptor atom in silicon (Reference 3). The spectral position of these peaks identifies the particular impurity. To determine the impurity concentration the peak area of one of the strong excitation peaks is used (References 4,5). Complications arise in accurately determining the impurity concentration when the absorption sample measured is less than 1-mm thick. For thin absorption samples optical channeling effects are superimposed on the excitation spectra as shown in Fig. 2. This effect distorts the calculated peak areas. Optical channeling is produced by the coherent (i.e., inphase) multiple internal reflections from the plane-parallel faces of an optically thin, double-side polished wafer.

One method for reducing optical channeling is to have the sample polished to a wedge shape so that the front and back surfaces are no longer parallel. However, since the samples are thin the degree of wedging is limited and therefore does not completely eliminate the channeling effects. An alternative method is to eliminate the channeling from the recorded data through computer modeling. To implement this method a theoretical model for coherent scattering effects, or optical channeling, had to be developed. The theoretical model developed in this report was based on

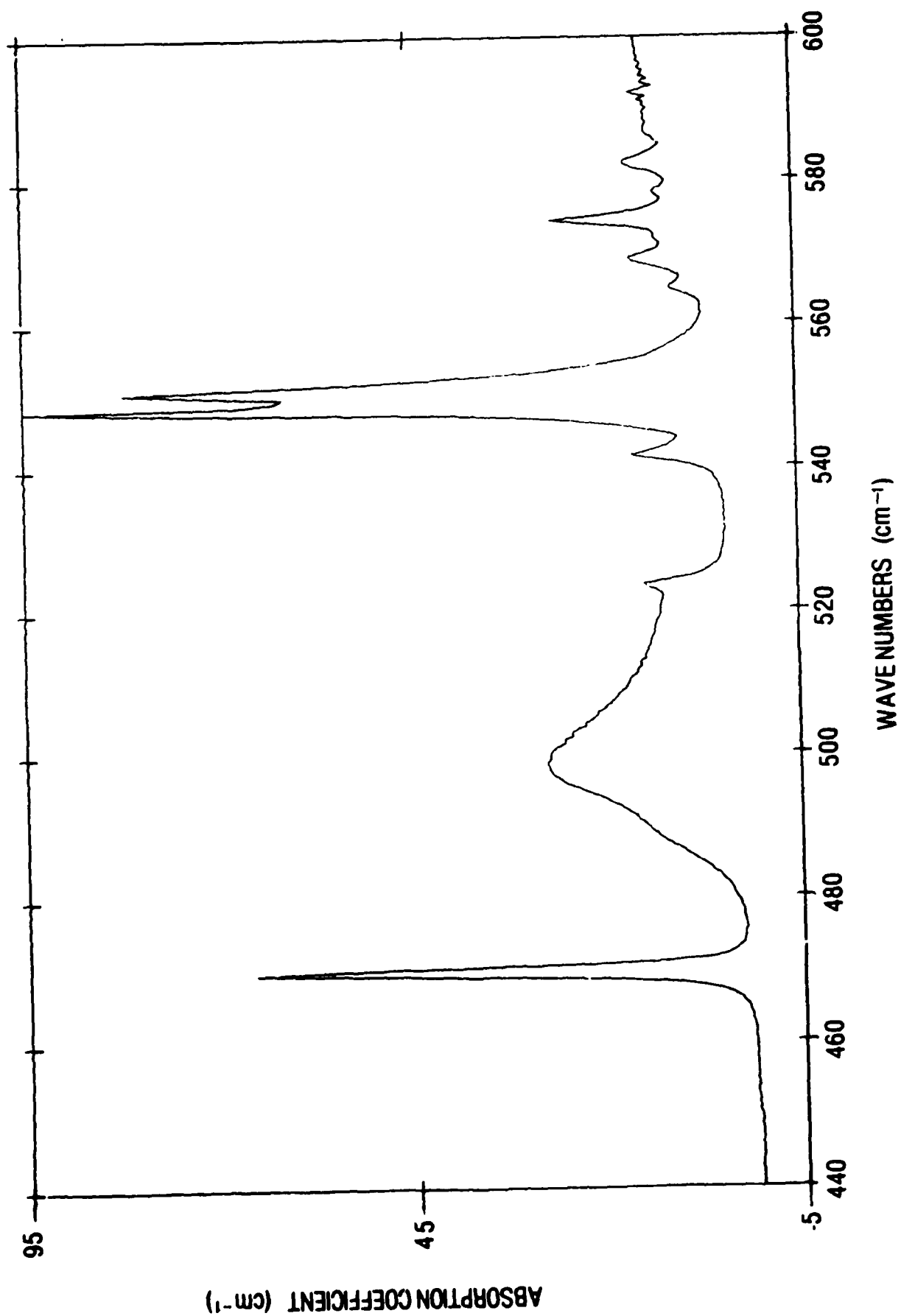


Figure 1. Absorption Spectrum of a Si:Ga Sample at 5 K.

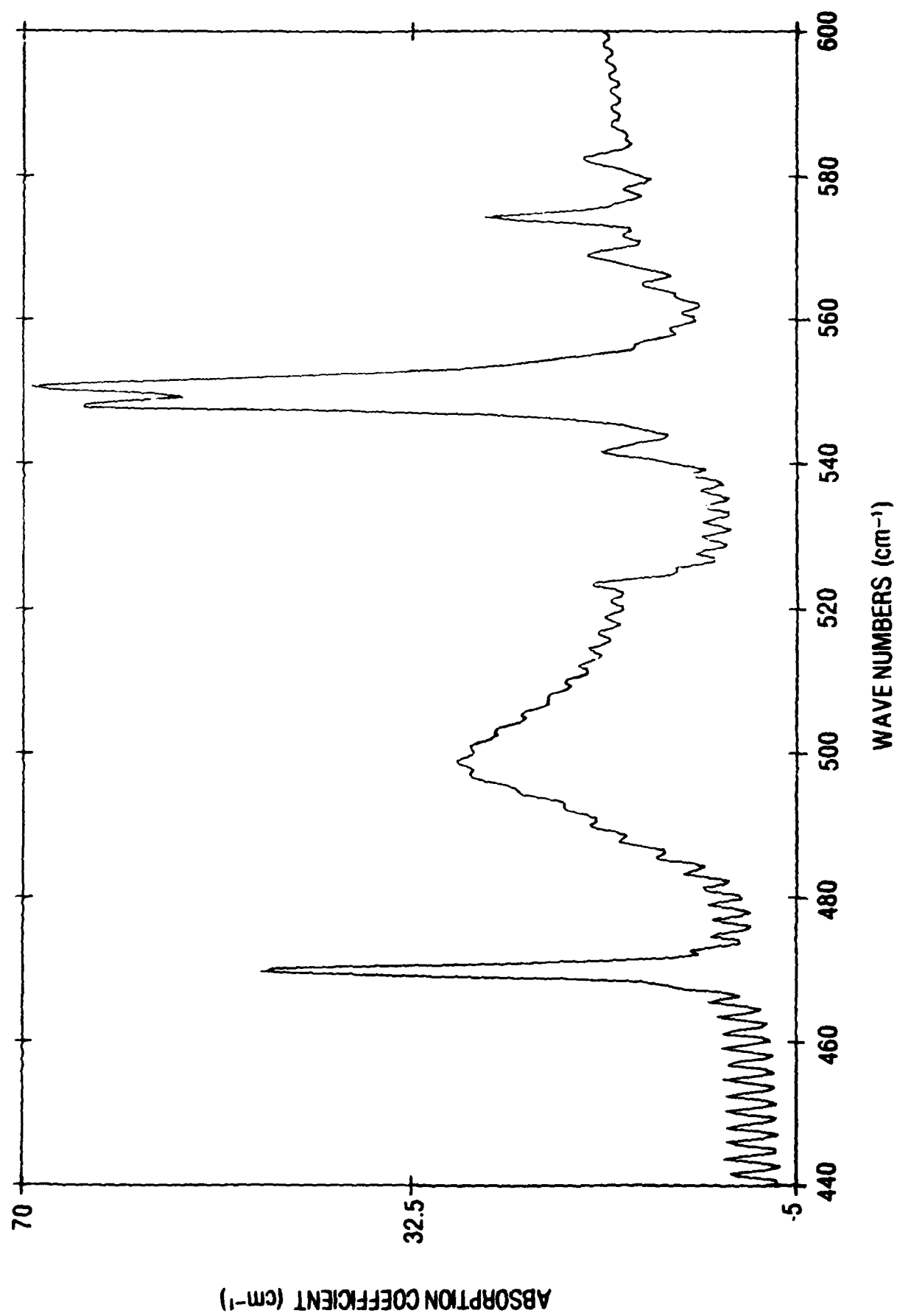


Figure 2. Absorption Spectrum of a Si:Ga Sample that Shows the Effects of Optical Channeling.

finding a mathematical expression for coherent scattering effects and then determining how to combine this formula and the analogous incoherent scattering formula to best transform the actual spectral data.

SECTION II

THEORY

In absorption spectroscopy the intensity of the transmitted radiation (I) is proportional to the intensity of the incident radiation (I_0). For a sample of thickness d , the relationship between the incident and transmitted intensities is given by

$$I = I_0 e^{-ad} \quad (1)$$

where a is the absorption coefficient. The absorption coefficient is defined as the relative rate of decrease in light intensity along its propagation path. Equation 1 does not take into account the multiple internal reflections that can occur in some samples. The equation for transmittance (T) in the presence of these reflections is given by

$$T = \frac{I}{I_0} = \frac{(1-R)^2 e^{-ad}}{1-R^2 e^{-2ad}} \quad (2)$$

where R is the reflectivity of the sample interfaces (Reference 6). This equation assumes that the reflected light was incoherently scattered from the sample interfaces. In practice, this equation is solved for the absorption coefficient since, according to Beer's law, it is proportional to the concentration of absorbing centers in the material. The solution for the absorption coefficient expressed in terms of d , R , and T is

$$a = \frac{1}{d} \ln \left[\frac{2TR^2}{[(1-R)^4 + 4T^2 R^2]^{1/2} - (1-R)^2} \right] \quad (3)$$

To determine the impurity concentration in a semiconducting material the transmittance of the material is measured versus wavelength. The absorption coefficient is calculated using this transmittance data, along with values for the reflectivity and sample thickness. The peak area of a strong impurity excitation line is then calculated from the absorption coefficient spectrum. This peak area multiplied by a calibration factor gives the impurity concentration (Reference 5).

The above procedure works well when no optical channeling occurs. The transmittance equation assumes that the reflected light is incoherently scattered from the sample interfaces. But when the light is coherently scattered, as it is in thin samples with parallel faces, this transmittance equation is no longer accurate. Exact equations for the transmittance in the presence of only coherent scattering can be found in textbooks by both Heavens (Reference 7) and Born and Wolfe (Reference 8). The transmittance equation given by Heavens is

$$T = \frac{16n_0n_1n^2e^{-ad}}{A+Be^{-2ad}+2e^{-ad}[C\cos(4\pi nd/\lambda)+D\sin(4\pi nd/\lambda)]} \quad (4)$$

$$\text{where } A = [(n+n_0)^2+k^2][(n+n_1)^2+k^2]$$

$$B = [(n-n_0)^2+k^2][(n-n_1)^2+k^2]$$

$$C = -(n^2-n_0^2+k^2)(n^2-n_1^2+k^2)+4k^2n_0n_1$$

$$D = 2kn_1(n^2-n_0^2+k^2)+2kn_0(n^2-n_1^2+k^2)$$

and n_0 is the index of refraction of the first medium, n_1 is the index of refraction of the third medium, $n-ik$ is the index of the sample, and λ is the wavelength. Both limiting cases, completely coherent and completely incoherent scattering, can be represented by the simple multiple-scattering ray diagram of Fig. 3. For the completely coherent case (i.e., the sample has perfectly plane-parallel sides and is homogeneous on a scale equal to the incident wavelength) the electric field vector is partially reflected and partially transmitted at each interface. For the completely incoherent case (i.e., the sample has rough or nonparallel sides and internal imperfections on a scale equal to the wavelength) the incident intensity may be considered partially reflected and transmitted at the interfaces. In either case, linear absorption in the sample is included by considering the wavenumber in the sample to be a complex quantity, $2\pi(n-ik)/\lambda$. The absorption coefficient is then given by

$$a = -2 \operatorname{Im} (2\pi(n-ik)/\lambda) = 4\pi k/\lambda = 2\bar{\nu}k \quad (5)$$

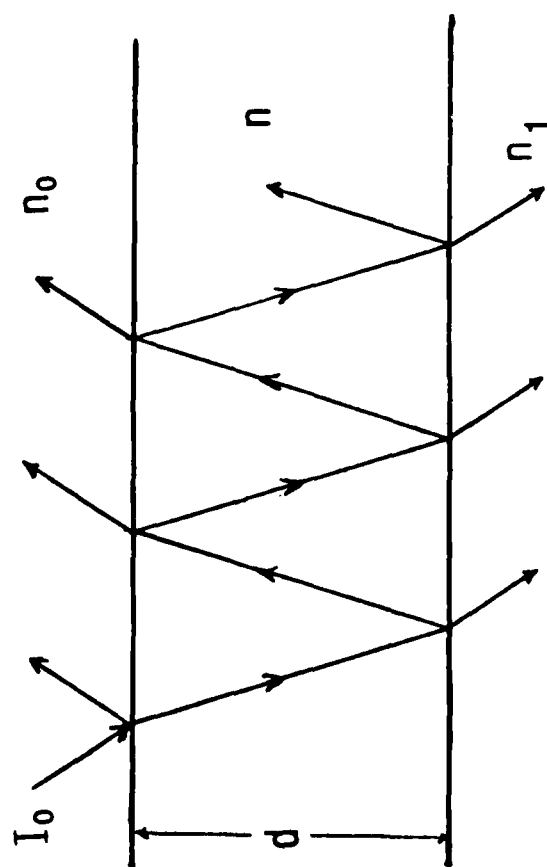


Figure 3. Multiple-scattering Ray Diagram for the Transversal of Light Through a Plane-parallel Homogeneous Slab of Thickness d .

where $\bar{\nu}$ is the wavenumber in air.

An exact inversion of equation 4 to solve for the absorption coefficient, for completely coherent scattering, proves to be impossible since it is a transcendental equation. A paper by Manifacier, Gasiot and Fillard (Reference 9) suggests several approximations which will allow the formula to be inverted. The approximations used are

$$k^2 \ll (n-n_0)^2, \quad (6a)$$

$$k^2 \ll (n-n_1)^2, \quad (6b)$$

$$k^2 \ll (n-n_0)(n-n_1) \quad (6c)$$

$$\text{and } 4k^2 n_0 n_1 \ll (n^2 - n_0^2)(n^2 - n_1^2). \quad (6d)$$

The transmittance equation then simplifies to

$$T = \frac{16n_0 n_1 n^2 e^{-ad}}{C_1^2 + C_2^2 e^{-2ad} + 2C_1 C_2 e^{-ad} \cos(4\pi nd/\lambda)} \quad (7)$$

where $C_1 = (n+n_0)(n+n_1)$

and $C_2 = (n-n_0)(n-n_1)$.

This equation is then inverted to obtain an expression for the absorption coefficient in the presence of coherent scattering. The result is

$$a = \frac{1}{d} \ln \left[\frac{2C_2^2 T}{[(2C_1 C_2 T \cos \theta - 16n_0 n_1 n^2)^2 - 4C_2^2 C_1^2 T^2]^{1/2} - (2C_1 C_2 T \cos \theta - 16n_0 n_1 n^2)} \right] \quad (8)$$

where $\theta = (4\pi nd/\lambda)$. This equation was used for the computer modeling of optical channeling effects.

For Group III acceptors in silicon, conditions (6a)-(6d) are well satisfied for concentrations of the order of 10^{16} atoms/cm³ or less. Taking $n_0 = n_1 = 1$ and $n = 3.4$ (the refractive index of air and silicon respectively), conditions (6a)-(6c) reduce to $k^2/518 \ll 1$, while condition (6d) becomes $k^2/29 \ll 1$. The relevant wavenumber

range is from 200 cm^{-1} to about 1200 cm^{-1} in our case, and the absorption coefficient seldom exceeds 200 cm^{-1} even for the strongest peaks (Reference 10), so $k = a/2\bar{\nu} = 0.50$ and $k^2/518 = 4 \times 10^{-2} \ll 1$.

In the case of gallium arsenide, conditions (6a)-(6d) are also well satisfied for the spectral regions considered in this report. Taking $n = 3.62$, the condition to be satisfied is $k^2/6.86 \ll 1$. The maximum absorption occurs at $\bar{\nu} \approx 440\text{ cm}^{-1}$, where $a = 27\text{ cm}^{-1}$ (Figure 15), so $k = 0.0307$ and $k^2/6.86 = 1.4 \times 10^{-4}$.

SECTION III

APPLICATION OF THE MODEL TO IDEALIZED DATA

To test the usefulness of the absorption coefficient equation 8 derived in section II, two sets of idealized transmittance data were developed. Both sets were obtained using equation 4 to calculate transmittance in the presence of coherent scattering for the wavelength range of 370 cm^{-1} to 380 cm^{-1} and a sample thickness of 0.06 cm . In the first data set a constant absorption coefficient of 8 cm^{-1} was used for the calculation. In the second data set a Lorentzian peak was superimposed on the constant absorption coefficient. The Lorentzian peak shape corresponded to line 2 of the excited state spectrum of indium-doped silicon, assuming a concentration of about $7 \times 10^{16}\text{ atoms/cm}^3$.

The first set of idealized transmittance was transformed to absorption coefficient using both equations 3 and 8. Note that equation 3 is the one currently being used in the laboratory to calculate absorption coefficient from the experimentally measured transmittance. Figure 4 shows the absorption coefficients calculated using equation 8 are much more accurate in the presence of coherent scattering than those calculated using equation 3. However, the absorption coefficients determined by equation 8 are not quite the constant value of 8 cm^{-1} that was assumed in generating the ideal transmittance data. When the absorption coefficient scale is expanded, as in Fig. 5, small oscillations about this constant value are apparent. These oscillations evidently arise from the approximations used in obtaining equation 8, but are negligible compared to the noise normally present in experimental data.

To see the effects of these calculations on spectral line shapes, the second set of ideal transmittance data was transformed using both equations. The absorption coefficient calculated for a Lorentzian peak using equation 3 is shown in Fig. 6. The graph shows both the given absorption coefficient and the calculated absorption coefficient. We can see that the calculated values oscillate about the given values and follow the Lorentzian shape only in a general way. Figure 7 shows the absorption coefficient calculated for the second ideal data set using equation 8. Again, this graph shows both the given and calculated values for the absorption coefficient. This time the transformation is so close to the given data that the two curves appear identical. Based on these tests equation 8 appeared to be quite

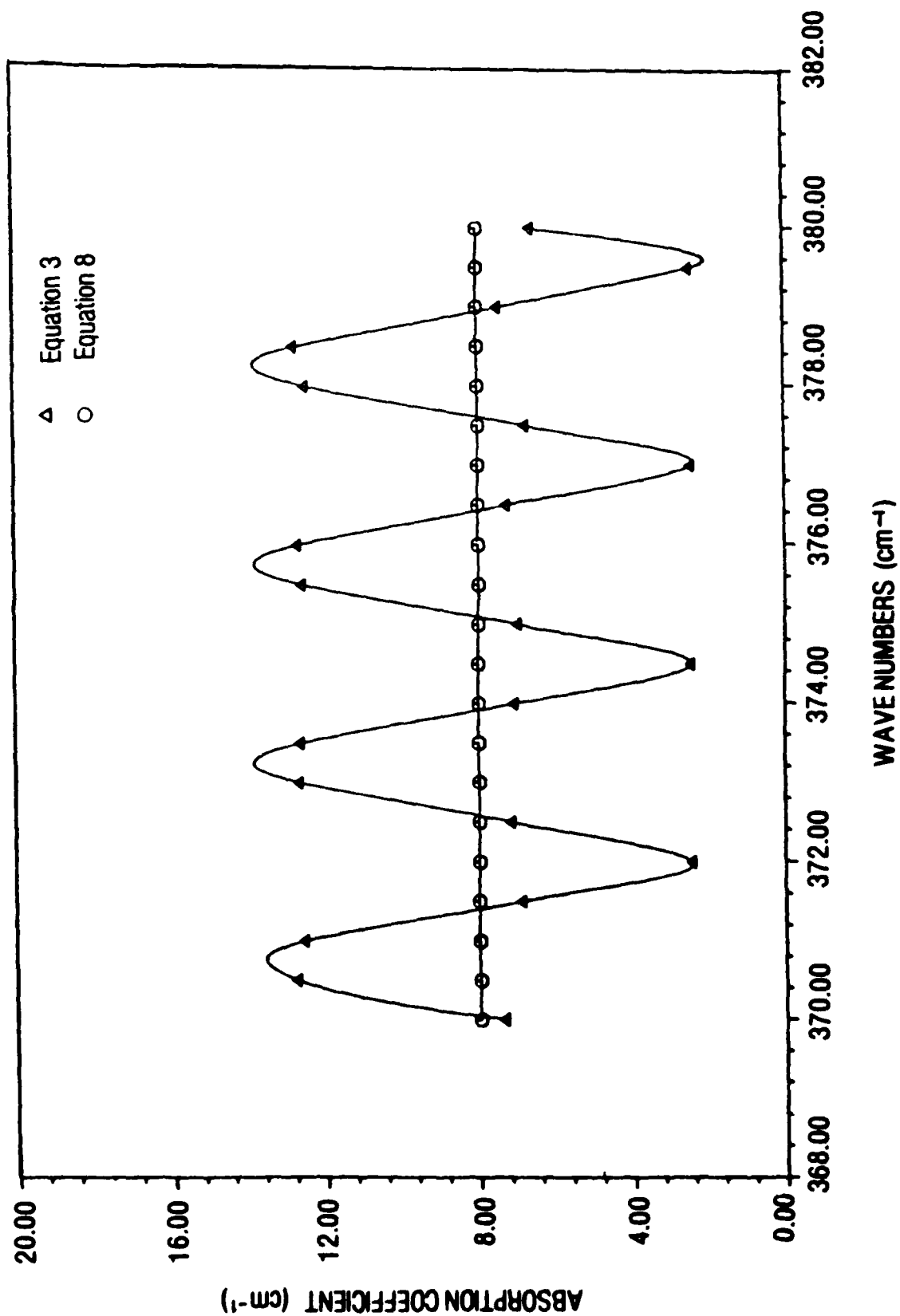


Figure 4. Comparison of the Transformation of Constant Absorption Coefficient Data by Equation 3 (Incoherent Scattering) and by Equation 8 (Coherent Scattering).

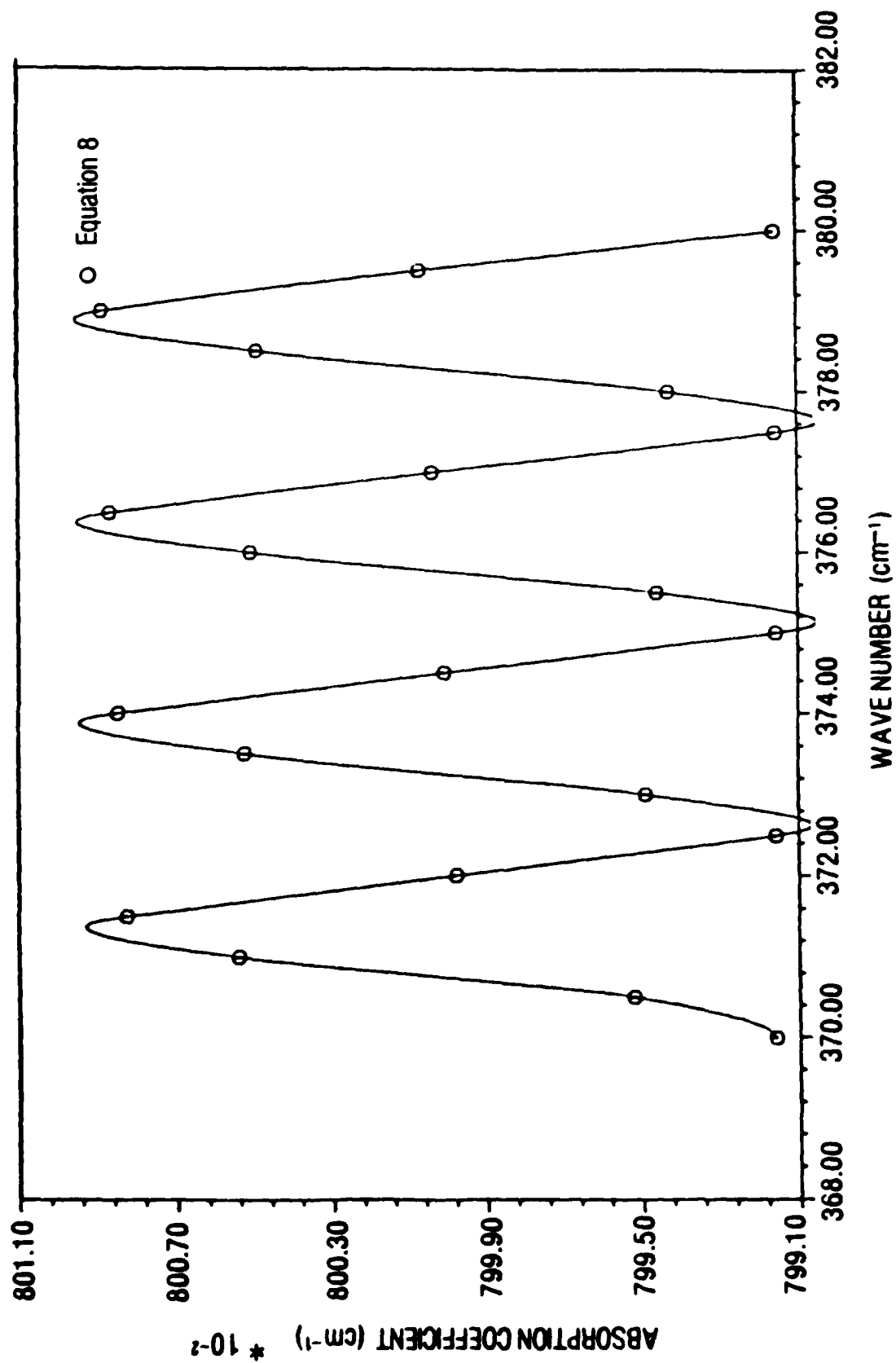


Figure 5. Transformation of Constant Absorption Coefficient Data by Equation 8 (Coherent Scattering) on an Expanded Scale.

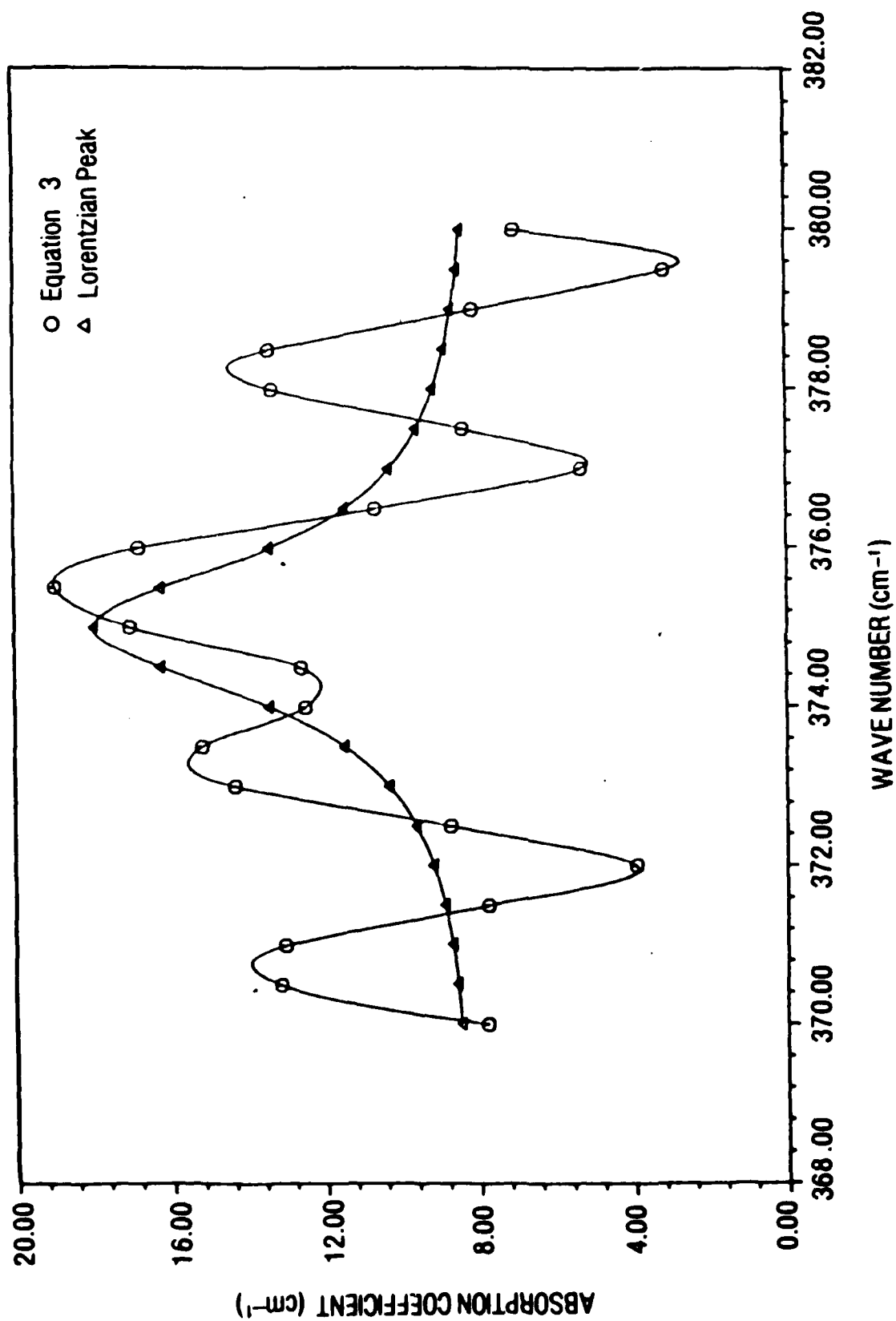


Figure 6. Comparison of the Transformation of a Lorentzian Peak in Absorption Coefficient Data, by Equation 3 to the Original Lorentzian Peak.

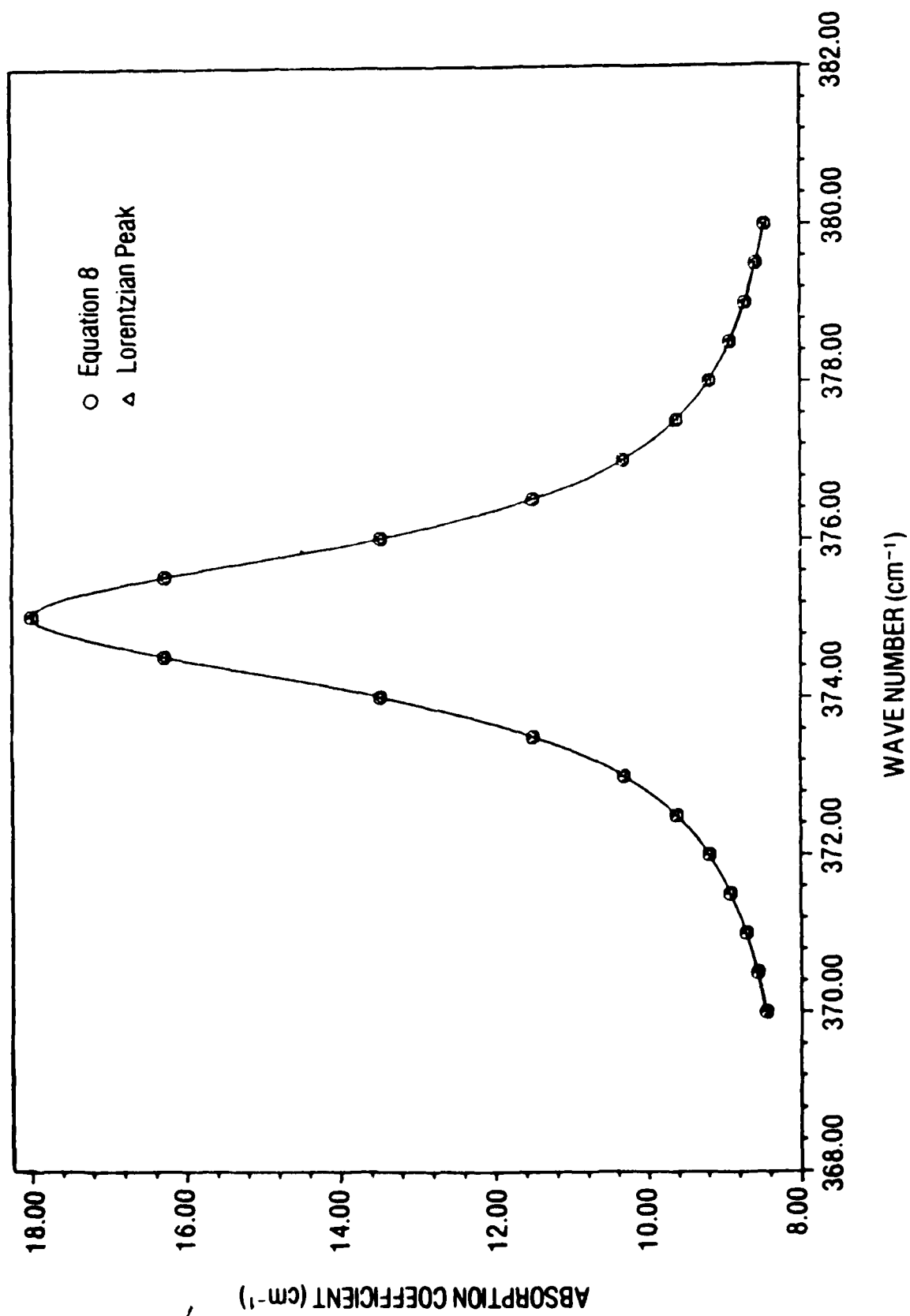


Figure 7. Comparison of the Transformation of a Lorentzian Peak by Equation 8 to the Original Lorentzian Peak.

adequate for calculating accurate absorption coefficients in the presence of optical channeling due to coherent scattering.

SECTION IV

APPLICATION OF THE MODEL TO ACTUAL DATA

The next step was to apply the coherent scattering absorption coefficient calculation to actual transmittance data taken in the laboratory to see if the optical channeling effects could be removed. A transmittance spectrum was digitized and used as data for the absorption coefficient calculations. First the incoherent scattering equation (Eq. 3) was used to calculate a typical absorption coefficient spectrum. This spectrum showed the effects of optical channeling as expected. Next the coherent scattering equation (Eq. 8) was applied to the data. The period and phase of the equation had to be adjusted to fit the period and phase of the transmittance data. The resulting absorption coefficient spectrum was not very good. The spectrum still had oscillations superimposed on the background and there were even some negative values. This poor result for the coherent scattering equation is probably because the sample did not have perfectly parallel, flat sides and thus did not exhibit perfectly coherent scattering.

A comparison of the spectrum obtained from the coherent and incoherent scattering calculations showed that the two spectra oscillate out of phase about a constant value. Since the oscillations were out of phase, it seemed possible that a combination of the two scattering mechanisms would more nearly approximate a constant. The physical justification for this would be that while a sample does not exhibit perfectly coherent scattering it also is not perfectly incoherent scattering either. The sample would probably exhibit both effects depending upon how parallel and flat the faces are. To combine the two scattering mechanisms, a linear combination of the two previous absorption coefficient equations was used. The new equation is given by

$$a(\omega) = x A(\omega) + (1-x) R(\omega) \quad (9)$$

where A is the coherent scattering absorption coefficient, R is the incoherent scattering absorption coefficient and ω is the wavenumber (cm^{-1}). The value of x could be varied to determine what percentage of coherent and incoherent scattering would produce a nearly constant absorption coefficient. Visual inspection of the coherent and incoherent scattering spectra gave an estimate of 33% for x . We see

that in Fig. 8, this value for x results in an absorption coefficient spectrum that shows less oscillation than the two previous calculations.

The new linearized absorption coefficient calculation worked well over a limited range but progressively worsened over an extended range of wavenumbers. We clearly see this in Fig. 9 where the range of data is larger than for Fig. 8. The cause of the deterioration is the change in the period of the channeling oscillations as the wavenumber changes. Theoretically the period of the oscillations should change and these changes can be predicted. However, the theoretical predictions do not match precisely the period on the experimental data. To deal with this problem, the computer program for absorption coefficient was revised. The revised program continually determined the period in the transmittance data by comparing data points to find successive maxima. The program then used this period in the equation to transform the transmittance data to absorption coefficient. Comparing Fig. 10 to Fig. 11 shows that continually readjusting the period results in an absorption coefficient that is more constant. Figure 12 shows how this revised program works well over a larger range.

The next improvement to the program was to eliminate the need to determine the weighting factor (x) by visual inspection. The program was revised to compare the magnitude of the oscillations in the absorption coefficient calculated by the coherent scattering equation to those calculated by the incoherent scattering equation. The weighting factor was determined by averaging over all such oscillations. To minimize the chance that the program would interpret a spectral peak as one of these spurious oscillations, the standard deviation of the average was determined. Then a new average was computed using only those magnitudes within one standard deviation. The weighting factor determined by this method was surprisingly close to the one determined by visual inspection. For example, for the sample shown in Fig. 8 through 12 the visual estimate was 33%. The weighting factor determined by computer averaging the size of the oscillations was 35% and by using only those values within one standard deviation was 36%. The results were similarly close for other samples. Figure 12 shows that the general shape and location of spectral peaks remains unchanged by this method. While the weighting factor did not vary significantly over the range of wavenumbers investigated, it did vary considerably from sample to sample. The minimum value was 8% and the maximum was 71%.

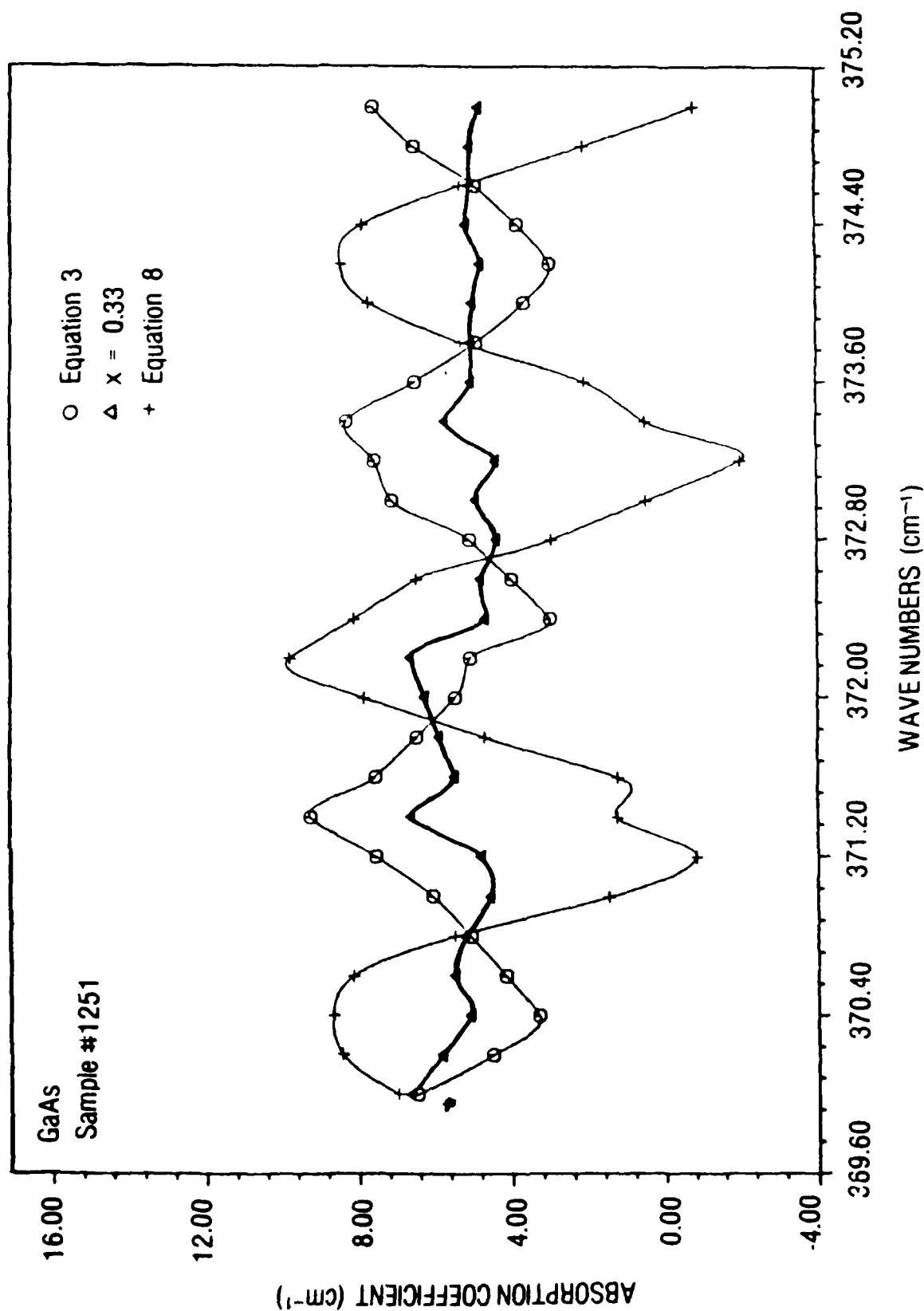


Figure 8. The Transformation of Actual Spectral Data by Equation 3 (Incoherent Scattering), Equation 8 (Coherent Scattering) and a Weighted Average of the Two Equations.

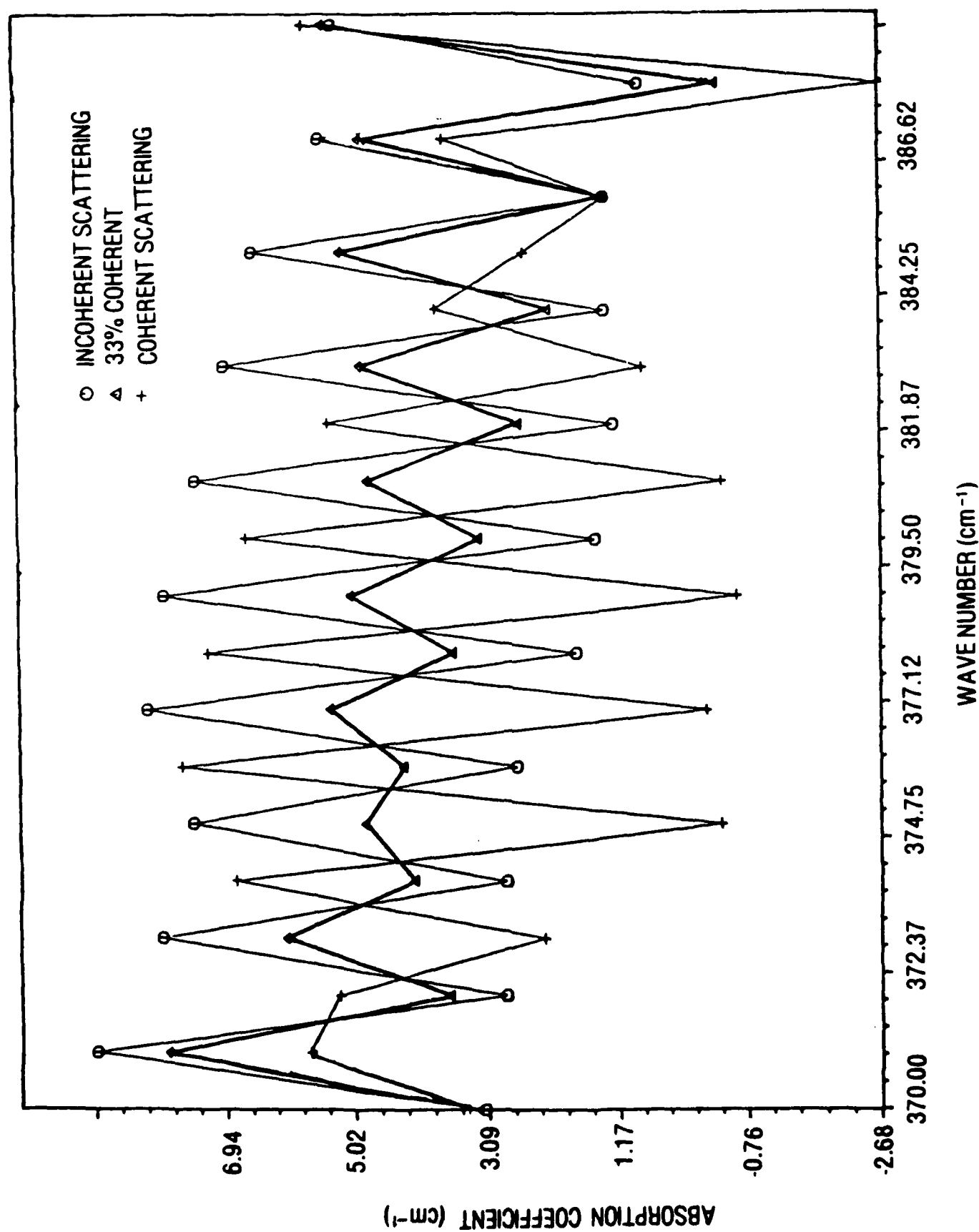


Figure 9. Deterioration of the Mixed Scattering Calculation of the Absorption Coefficient Over an Expanded Range of Wavenumbers.

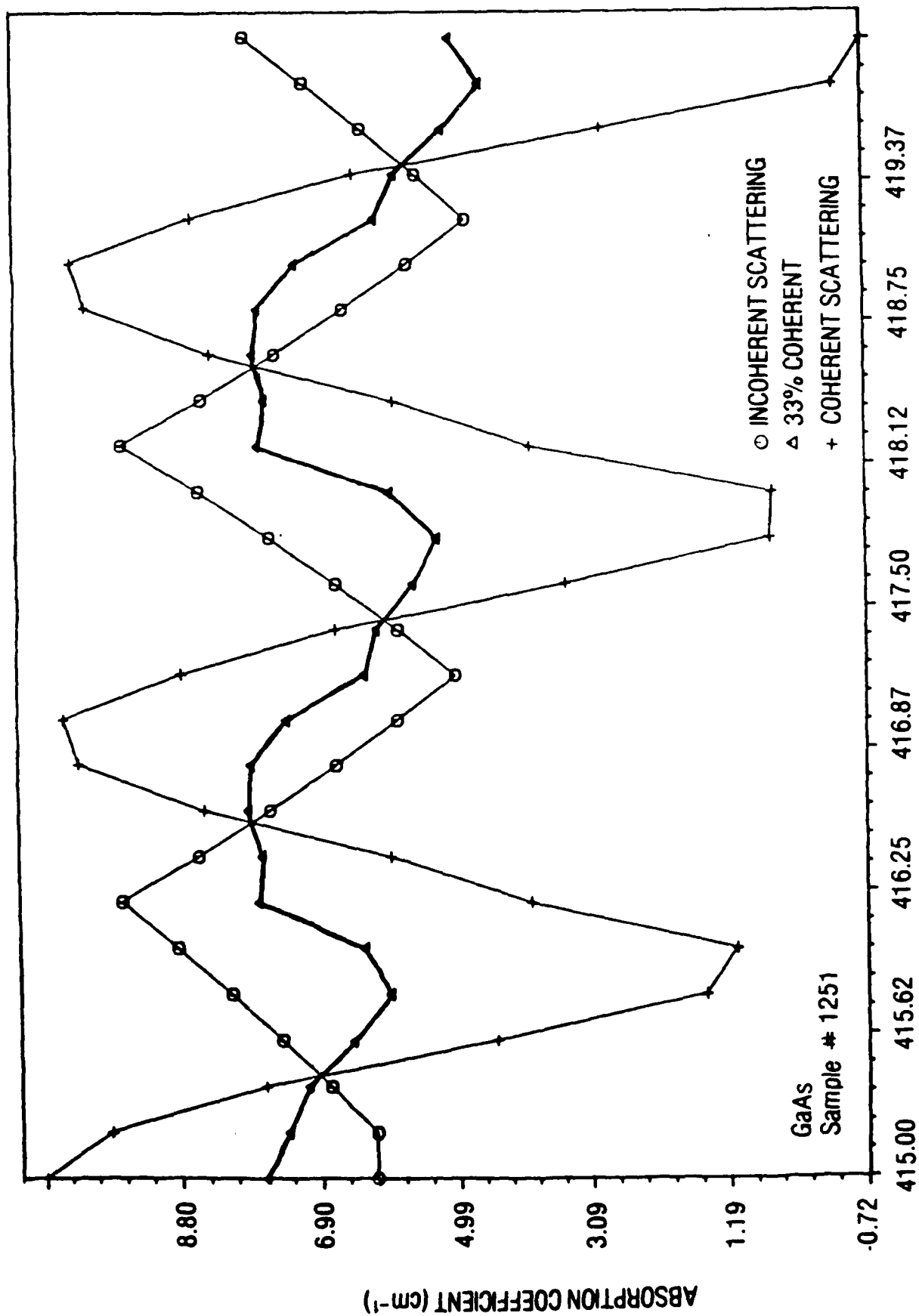


Figure 10. Absorption Coefficient Calculation Over a Specified Range of Wave-Numbers Without Adjusting the Period.

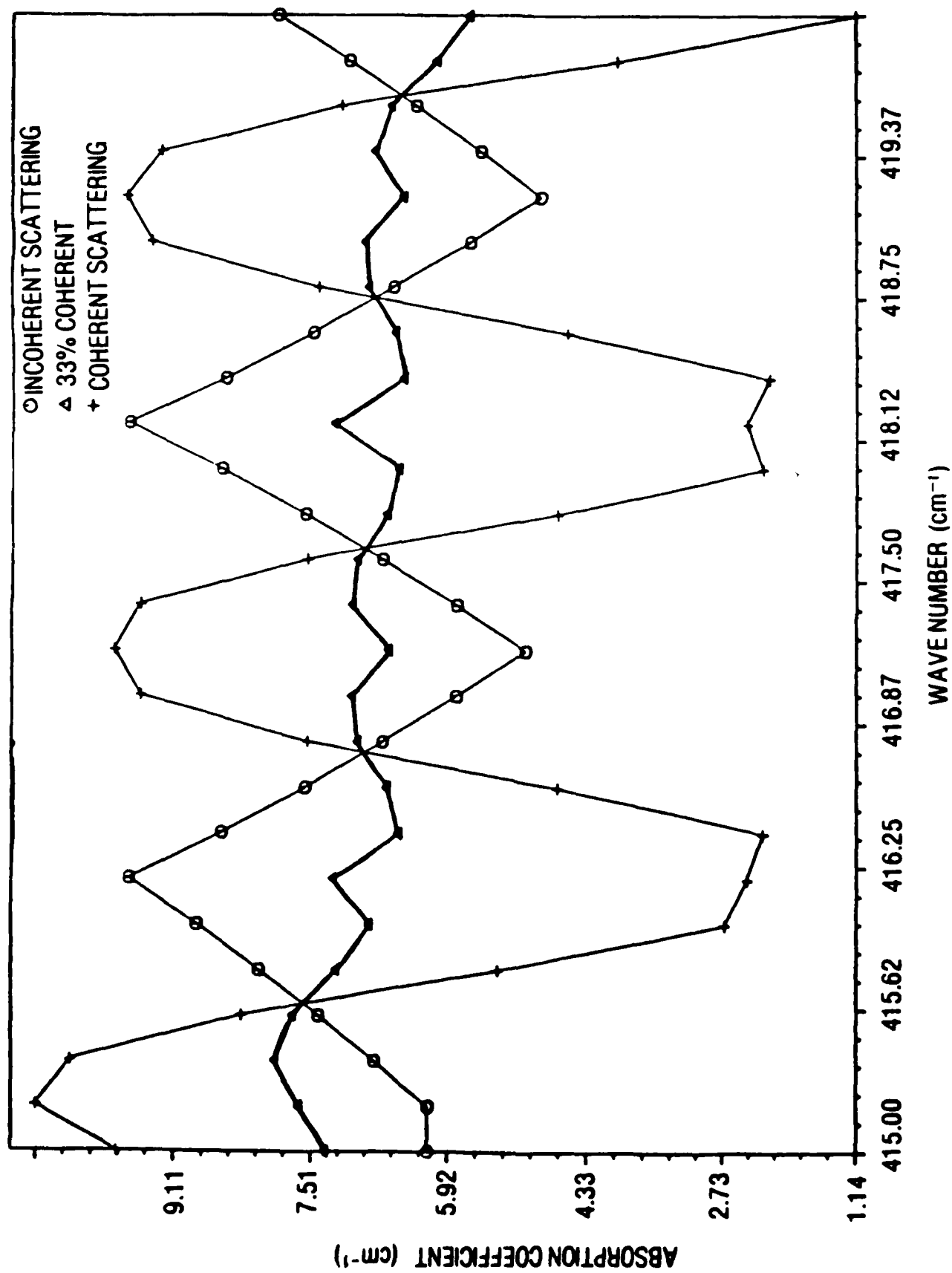


Figure 11. Absorption Coefficient Calculation Over the Same Range of Wave-numbers as Figure 10 but with an Adjustable Oscillation Period.

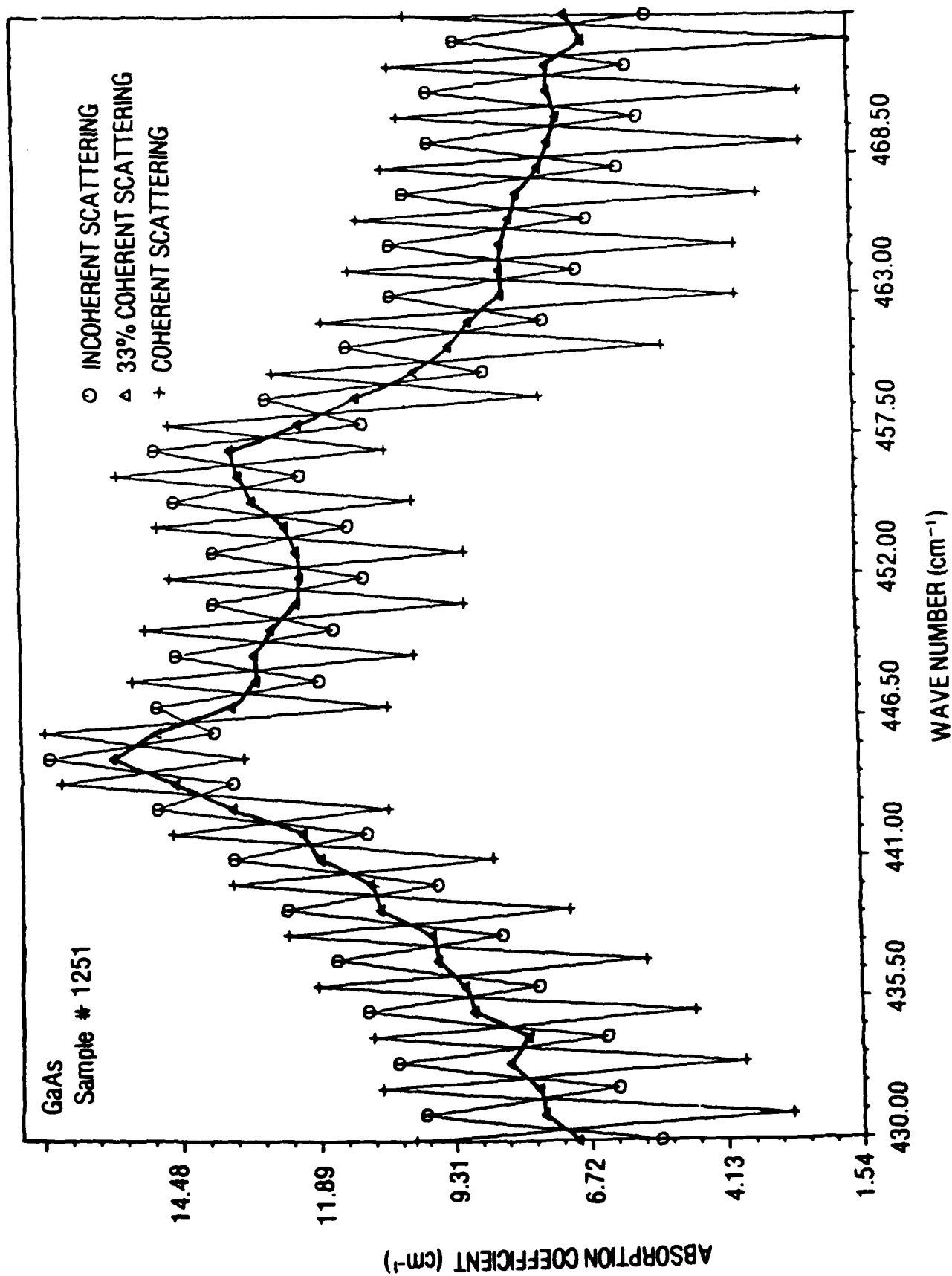


Figure 12. Absorption Coefficient Calculation with an Adjusting Oscillation Period Over an Expanded Range of Wavenumbers.

SECTION V

COMPARISON OF THE MODEL TO OTHER METHODS

In addition to the computer program developed in this report, there are two Fortran programs (Reference 11) included in the spectrometer's software that are designed to eliminate channeling from the spectral data. Unlike our program, these programs modify the interferogram, before it is Fourier transformed into a spectrum, to eliminate channeling. These programs are based on the assumption that channeling will appear in the wings of the interferogram as a glitch and therefore can be easily edited from the data. (See Figs. 13 and 14.) To compare these different methods, one particularly strong channeling sample was analyzed by all three programs.

First the transmittance data was analyzed with the computer program developed in this report. The results are shown in Fig. 15. The absorption coefficient spectra obtained by using both the incoherent and the coherent scattering equations are shown as well as the result obtained by using a linear combination of 71% coherent and 29% incoherent scattering. The linear combination method provides a significant improvement in the spectrum. Next a program called FRINGELIM was tested. This program has three ways to edit a glitch, due to channeling, in the interferogram. The glitch may be

1. replaced by a straight line connecting the end points of the remaining interferogram,
2. replaced by another section of the same interferogram, or
3. replaced by the same section of a reference interferogram.

All three of the above operations were performed for each glitch identified in the interferogram. The most significant glitch occurred between wavepoints 3350 and 3600, as seen in Figs. 13 and 14. The absorption coefficient spectra obtained from these modified interferograms were compared to a spectrum obtained without using FRINGELIM at all. The results are seen in Fig. 16. For the glitch between wavepoints 3350 and 3600, that was edited from the interferogram, no improvement is seen. In fact the channeling, or fringing, is worse. The program called SIDEBURST

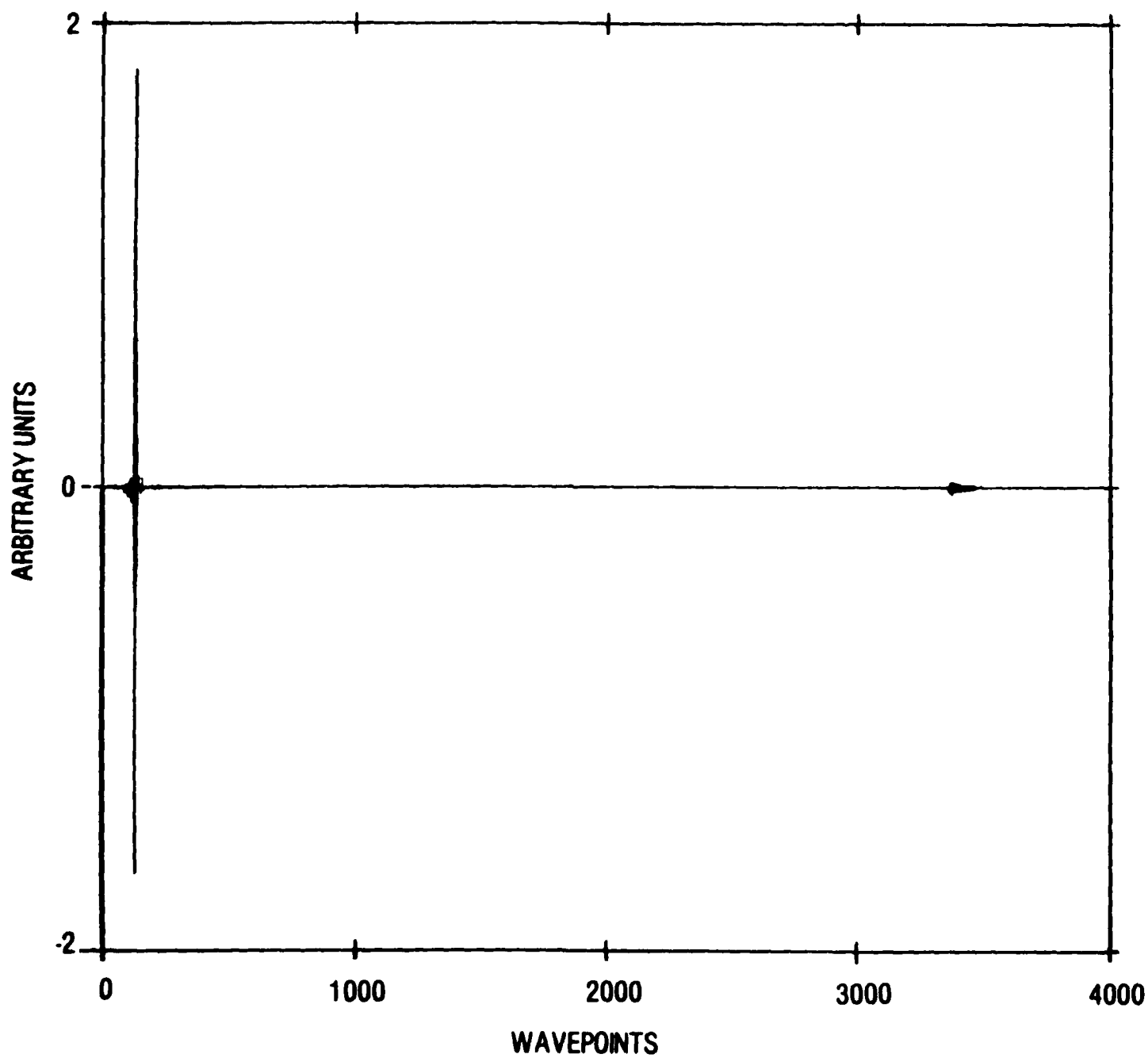


Figure 13. A Plot of a Complete Interferogram Showing the Glitch that Occurred Out in the Wings of the Data.

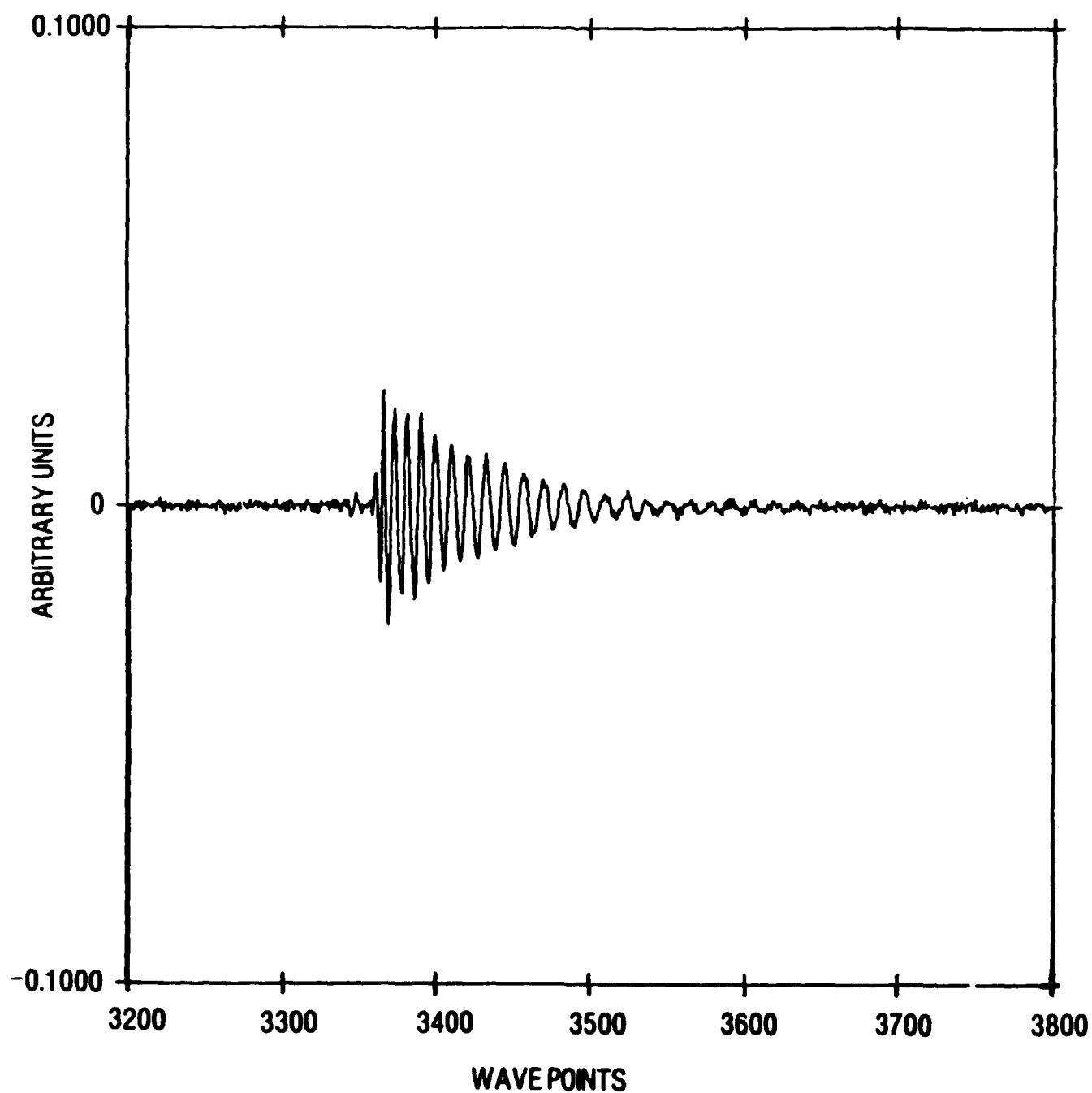


Figure 14. A Magnified Plot of the Glitch that Occurred in the Interferogram of Samples with Optical Channeling.

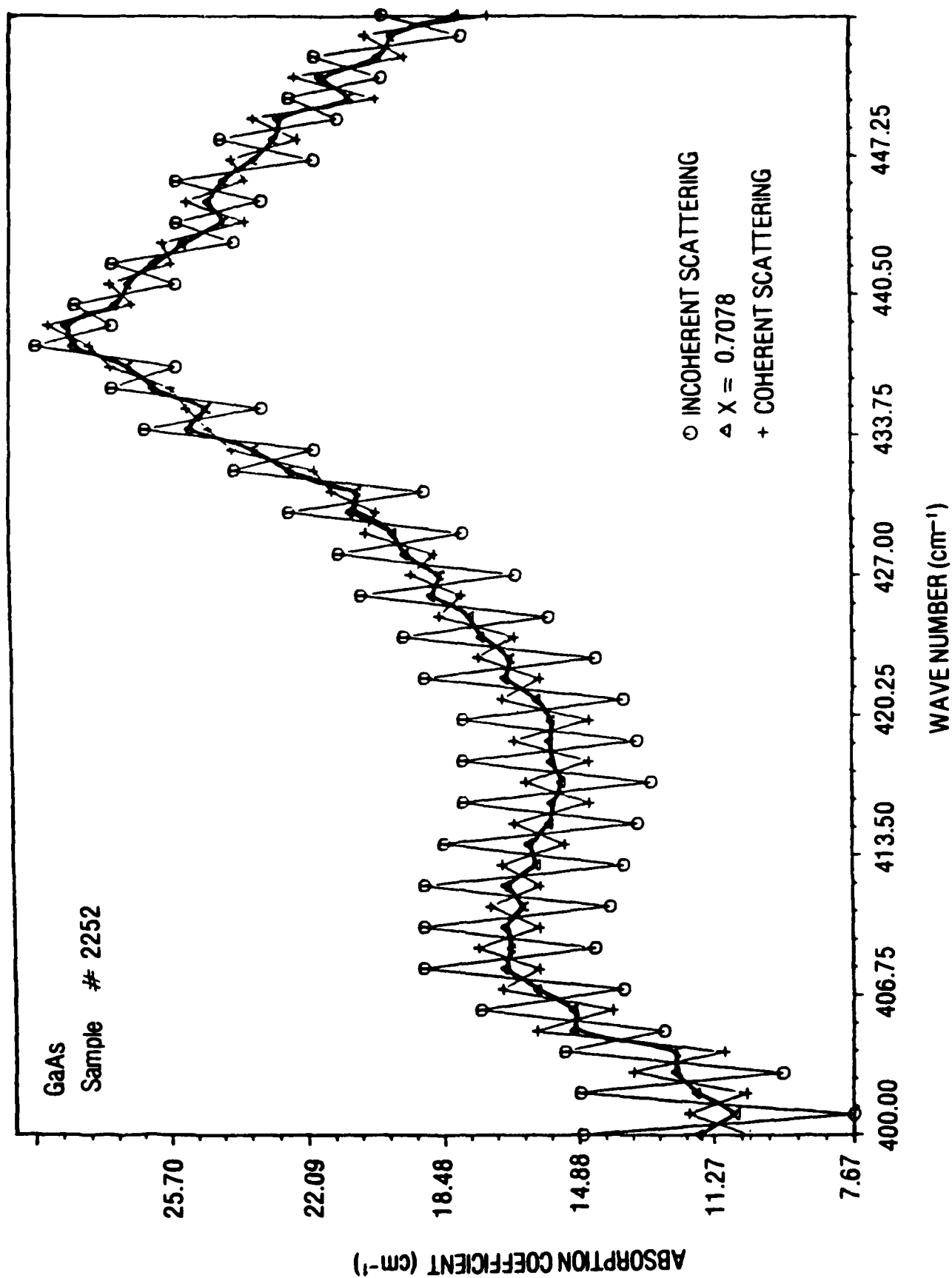


Figure 15. Absorption Coefficient Spectrum Calculated with Mixed Scattering, and with a Weighting Factor and a Period Adjustment Determined by the Computer Program.

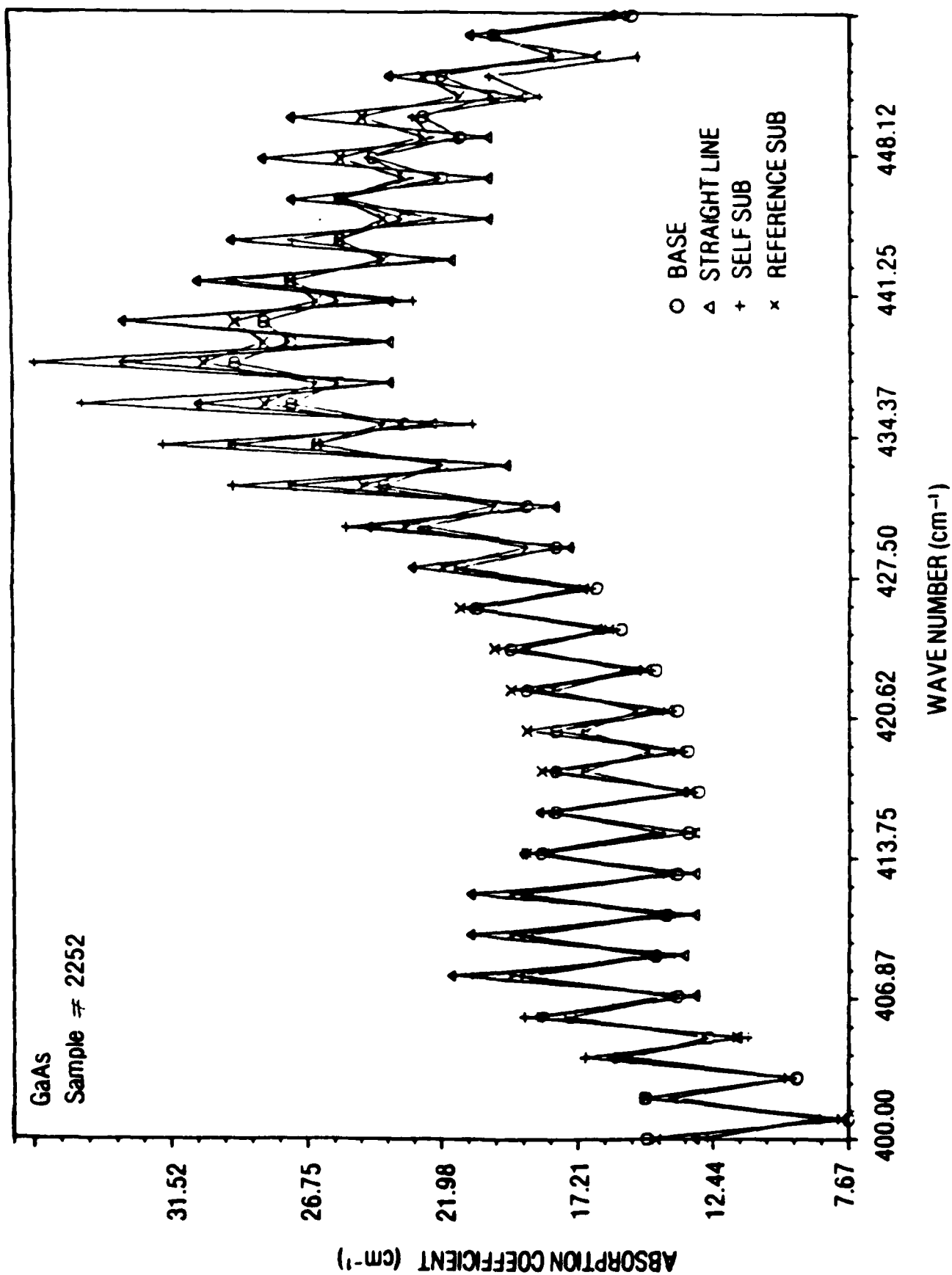


Figure 16. The Effect of the FPINGELIM Program on the Optical Channeling.

was also tested to see if it could remove channeling. In this program, similar to FRINGELIM, there are two options for editing glitches in the interferogram. The options are

1. replace the section with the glitch by data points all equal to zero, or
2. replace the section by another section of the same interferogram.

For comparison, the same glitch that was edited by FRINGELIM was chosen for editing by SIDERHST. The results for SIDERHST are shown in Fig. 17. Once again there is no improvement in the spectrum. This procedure was repeated for other glitches and other sections of the interferogram but the results were substantially the same. It is still possible that the SIDERHST and FRINGELIM programs can be used to improve spectra, but it requires knowing exactly which glitch to edit. Determining which glitch is significant will take a lot of practice and experimentation.

A

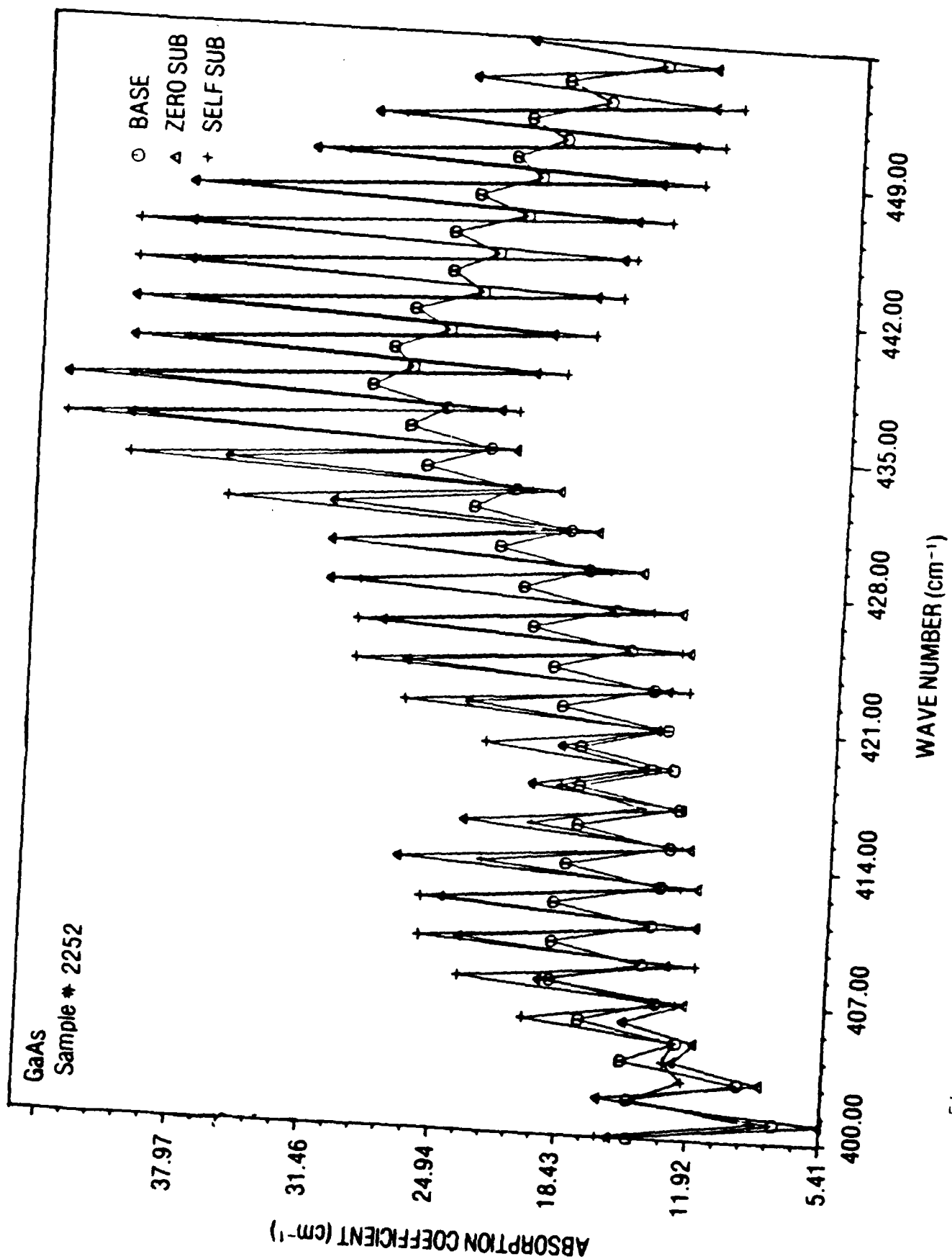


Figure 17. The effect of the SINGRIST program on the Optical Channeling.

SECTION VI

CONCLUSIONS AND RECOMMENDATIONS

Of the methods tested to eliminate optical channeling, the computer program developed based on coherent scattering in the sample was the most successful. As Fig. 15 showed, this computer program did significantly reduce the channeling effects on the absorption coefficient spectrum. The mixed scattering program reduced the magnitude of the oscillations by about a factor of 5. However, this program was only used over small wavenumber regions so its usefulness for an entire spectrum (4,000 to 200 cm^{-1}) still needs to be tested. Small wavenumber regions were used because the transmittance data was digitized by hand from recorded spectra. In order to handle large spectral regions the transmittance data should be directly accessed from the laboratory computer data file. This capability did not exist at the time of this work.

The scattering program should also be tested for a larger variety of samples. As noted above the coherent weighting factor varied considerably for the few samples that were used in this study. The relationship between the weighting factor and physical properties of the samples should be investigated. A weighting factor study could reveal which sample properties, besides thickness, are the most critical to control in order to reduce coherent scattering.

But perhaps the most significant step to make at this point is to add the mixed coherent/incoherent scattering program to the data acquisition system's analysis routine. At present the absorption coefficient calculation used takes into account only incoherent scattering within the sample. This calculation is insufficient for thin samples with parallel faces that exhibit optical channeling. For these samples, there should be the option of calculating the absorption coefficient spectrum with the mixed coherent/incoherent scattering equation. As this report has demonstrated, most of the channeling effects can be eliminated from the spectrum with the use of this equation. This step would not be difficult to implement since a new fortran applications program can easily be added to the data acquisition system software.

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