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MIDWAY REPORT
ON
INVESTIGATION OF THE OPTICAL PROPERTIES OF
SILICON SOLAR CELL COMPONENT MATERIALS

by **CASE FILE
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K. Vedam

To

California Institute of Technology
Jet Propulsion Laboratory
4800 Oak Grove Drive
Pasadena, California 91103

21 June 1969

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THE MATERIALS RESEARCH LABORATORY

THE PENNSYLVANIA STATE UNIVERSITY
UNIVERSITY PARK, PENNSYLVANIA

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ABSTRACT

A new method using Kramers-Kronig analysis of normal reflectance data for calculation of the maximum and minimum values of the optical constants of silicon has been developed. It does not require any assumptions for the optical properties of the material outside the wavelength interval for which the data are available, and it is also possible to use without standard values inside this interval. The uncertainty in the optical constants arising from this method is compatible in magnitude with typical experimental errors. Correction for the presence of surface film is also considered. Experimental data on Si are analyzed using this method.

1. INTRODUCTION

The primary objectives of this project is (i) to determine both the real and the imaginary parts of the complex refractive index as well as the reflectivity of solar cell quality silicon in the wavelength region 0.4 to 1.1 μ , and (ii) to determine the changes in the above optical properties on irradiation by electrons and protons. Considerable progress has been made in this research project during the first half of the contract period. The first objective mentioned above has been tackled from two aspects. On the experimental side, after considerable time and effort it was found that the cement called "Lens bond" manufactured by Summers Laboratories, Inc., Fort Washington, Pa. can be used to cement the silicon sample to vitreous silica before it is fabricated to the required thickness for optical absorption studies in the spectral region mentioned above. With this arrangement it is possible to carry out the measurements directly with the sample mounted on the vitreous silica. Currently such measurements are in progress with the sample cooled to liquid helium temperatures. As soon as these measurements are completed, efforts will be directed to study the effect of irradiation.

Concurrently with the above experimental studies, a method using the Kramers-Kronig analysis of normal incidence reflectance data has been developed to calculate the maximum and minimum possible values of the optical constants and thus estimate the maximum errors in such analysis. Since these analyses can easily be extended to Ge with minimum effort, these calculations have been performed for both Si and Ge and the results are presented below.

One of the most frequently used methods for obtaining the optical constants of solids in a wide spectral region or outside the visible region is the so-called Kramers-Kronig (K-K) analysis of normal reflectance. The theory and basic formulae are given in Moss'¹ and Stern's² books. As this method requires the knowledge of one optical parameter in the entire spectral region, an impossible condition, some extrapolation to infinity must be used. This means that regardless of experimental

errors this method has limited accuracy. This circumstance is well known and essentially every author using K-K analysis discusses also the influence of errors, e.g. see the recent review by Lavilla and Mendlowitz.³

As the extrapolation procedures are not based on experimental results and are not always justified by good physical arguments, it is reasonable to study the properties of K-K analysis without any extrapolation whatsoever and then estimate the maximum limit of errors. This is the purpose of this paper. We will discuss corrections for the presence of surface film⁴ and also the influence of experimental errors on the optical constants. Sufficient attention has generally not been given to the exact nature of these surface films in the literature. All the results will be discussed for germanium and silicon.

As the experimental data we used our previous results for normal reflectivity⁵ of Si and Ge up to 13 eV. The experimental arrangement and the nature of the samples used are described therein. In the region 13-21 eV we used the results of Philipp and Ehrenreich.⁶ The agreement of both data for energies less than 13 eV is good and any difference between them is smaller than the errors considered below.

2. LIMITS OF ERRORS IN THE METHOD

Let us assume the material can be characterized by complex index of refraction $N = n+ik$. For the normal reflectance R we have

$$R(\omega) = [r(\omega) \exp(i\phi(\omega))]^2 = \left(\frac{N-1}{N+1}\right)^2 \quad (1)$$

where ω is frequency, $r(\omega)$ amplitude and ϕ phase. The equation (1) gives the relation between optical constants n, k and the phase angle ϕ which is given by dispersion relation

$$\phi(\omega) = -\frac{\omega}{\pi} \int_0^{\infty} \frac{\ln R(x)}{x^2 - \omega^2} dx \quad (2)$$

the phase angle ϕ can be written as a sum of ϕ_1 and ϕ_2 ; ϕ_1 corresponds to the contribution from the term in the measured region

$$\phi_1(\omega) = -\frac{\omega}{\pi} \int_0^{\omega_0} \frac{\ln R(x)}{x^2 - \omega^2} dx \quad (3)$$

where $R(x)$ is the normal reflectance in the interval $(0, \omega_0)$, where ω_0 is the frequency limit of available experimental data. Phase ϕ_2 is contribution from the interval $\omega_0 - \infty$ and Velicky⁷ proved that in the interval $(0, \omega_0)$ is ϕ_2 given by the series

$$\phi_2(\omega) = \frac{\omega}{\pi} \int_{\omega_0}^{\infty} \frac{-\ln R(x)}{x^2 - \omega^2} dx = \sum_{m=0}^{\infty} a_m \omega^{2m+1} \quad (4)$$

where $R(x)$ is arbitrary and coefficients a_m are

$$a_m = -\frac{1}{\pi} \int_{\omega_0}^{\infty} x^{-2m-2} \ln R(x) dx \quad (5)$$

Further, we will exploit the following simple properties of equations (1-5)

$$0 \leq \phi(\omega) \leq \pi \quad (6a)$$

$$\phi(\omega) = 0 \quad \text{for} \quad \omega = 0 \quad (6b)$$

$$\frac{d\phi_2}{d\omega} = a_0 \quad \text{for} \quad \omega = 0 \quad (6c)$$

$$a_m \geq 0 \quad (6d)$$

The last condition results from (5) because $0 \leq R \leq 1$.

frequency

The only assumption we will use is that $\phi = 0$ (or $k=0$) in some small interval $(0, \kappa)$. For semiconductors and insulators this assumption is automatically guaranteed by the existence of the absorption edge. For the construction of the minimum and maximum of $\phi_2(\omega)$ we use Fig. 1 which shows the phase angles ϕ_1 and ϕ_2 for silicon plotted as a function of frequency ω . The curve for ϕ_1 was obtained from the experimental results using equ. (3). It is easy to see that the curve for $\phi_{2\min}$ is given by eqs. (6b,c). Further, we have

$$\phi_{2\min}(\omega) = a_0 \omega \quad \text{for } \omega (0 \text{ to } \omega_s) \quad (7a)$$

and from equ. (6a)

$$\phi_{2\min}(\omega) \geq |\phi_1(\omega)| \quad \text{for } \omega (\omega_s \text{ to } \omega_0) \quad (7b)$$

where ω_s is the frequency at the point of intersection of the functions (7a) and (7b).

To eliminate the singularity of the integral (3) for $\omega = \omega_0$ we linearly extrapolated the function $R(\omega)$ in the small interval 21.0-21.5 eV. For ω_0 we used the value 21.5 eV, but we consider only results to 21.0 eV. Thanks to this extrapolation for Ge and also Si in our case ω_s is larger than 21.0 eV.

The broken line for $\omega > 17$ eV in Fig. 1 is the function $(\pi - \phi_1(\omega))$, which is the upper limit for $\phi_2(\omega)$. Now we have for the maximum of ϕ_2 , from eqs. (4) and (6)

$$\phi_{2\max}(\omega) = a_0 \omega + a_1 \omega^3, \quad \omega \text{ from } (0, \omega_t) \quad (8)$$

where

$$a_1 = [\pi - \phi_1(\omega_t) - a_0 \omega_t] / \omega_t^3$$

and

$$\phi_{2\max}(\omega) \leq \pi - \phi_1(\omega), \quad \omega \text{ from } (\omega_t, \omega_0) \quad (9)$$

where ω_t is coordinate of point T where both curves (8), (9) have the same derivative. Without the assumption of the existence of some κ where $\phi = 0$ we can use for the upper limit of ϕ_2 , the linear function $\phi_2 = a_0 \omega$ where

$$a_0 = (\pi - \phi_1(\omega_t)) / \omega_t.$$

Of course the estimation will be less precise.

The optical constants calculated using $\phi_{2\min}$ and $\phi_{2\max}$ (Figs. 1 and 2) represent also their minimum and maximum values, but only if n and k are monotonic functions of ϕ . This is true in our case for Ge and Si in almost the whole spectral interval considered, with the exception of slight deviation in a narrow region at 4.4 eV and 20 eV. These deviations are small and they are taken into account in Figs. 1 and 2. The difference $\Delta\phi_2 = \phi_{2\max} - \phi_{2\min}$ increases as a third order polynomial up to ω_t (for Si: $\omega_t = 19.5$ eV and Ge: $\omega_t = 19.0$ eV). In the interval (ω_t, ω_0) $\Delta\phi_2$ increases as a higher order polynomial. In the region where n, k are very sensitive to the phase angle ϕ (the region of small ϕ and large R), since the difference $\Delta\phi_2$ is very small, $\Delta n_M = n_{\max} - n_{\min}$ and $\Delta k_M = k_{\max} - k_{\min}$ are also small. For higher

energies where $\Delta\phi_2$ is relatively large the dependence of n , k on ϕ is not so great and Δn_M and Δk_M also have reasonable values ($\Delta n_M, \Delta k_M < 0.4$). For energies less than 5 eV, the region of the most interesting structure, the differences Δn_M and Δk_M are smaller than 0.1 (in steep regions less than 0.2) for both materials. The calculations of the limits of the optical constants does not need any extrapolation of R beyond ω_0 or any other additional assumptions or data in the interval (κ, ω_0) .

Such calculation of the limit of n , k depends strongly on the upper limit of the experimental region ω_0 . To illustrate this we calculated the optical constants of Ge for $\omega_0 = 6$ eV and $\omega_0 = 13$ eV. The former is the limit for conventional experimental arrangement in air, and the latter is the limit for measurement using a vacuum ultraviolet monochromator with a hydrogen light source. Figure 2 shows results for Ge obtained in the same way as described above for silicon. For $\omega_0 = 13$ eV we have reasonable results, especially since the positions and the shapes of the peaks are almost the same as for $\omega_0 = 21$ eV, but the uncertainty in the absolute value is larger. For $\omega_0 = 6$ eV the structure is strongly disturbed but the main features are still evident.

3. EXPERIMENTAL ERRORS

The error in the calculated optical constants n and k caused by the experimental errors ΔR depends on $\Delta R(\omega)$ in the whole interval $(0, \omega_0)$. The function $\Delta R(\omega)$ is different for different experimental arrangements, and varies significantly with frequency. But most of the investigators work with equipment of similar quality from this point of view. The typical absolute error in the normal reflectance in the visible region is 2×10^{-2} (5,8) and this increases with energy. We chose it to be 10×10^{-2} at 21 eV, which represents an error of about 0.2% in the reflectance of Ge and Si. It is possible to estimate the errors $\Delta n_E, \Delta k_E$ by the analysis of equation (2).³

However, once the computer program is written, it is easier to vary only the input data. We multiplied the experimental data R_{ex} by an estimated error factor c , a polynomial of second degree such as by points (0.61; 1.0), (3.0; 1.02), (21.0; 1.1) in the field $(\omega;c)$. Figure 3 shows in the case of Ge the assumed reflectance error $\Delta R_E = R_{ex}(c - 1)$ and the errors introduced by this ΔR_E on the optical constants $\Delta n_E = n_c - n$ and $\Delta k_E = k_c - k$, where n_c and k_c are calculated for $c R_{ex}$. The shapes of the curves $\Delta n_E(\omega)$ and $\Delta k_E(\omega)$ are very close to the curves for the derivatives $dn/d\omega$ and $dk/d\omega$. The absolute value of ΔR , calculated from Δn_E and Δk_E is comparable with ΔR_E . Thus the integral character of the dispersion relation does not contribute too much to the total value of ΔR_E .

4. CORRECTION FOR SURFACE FILM

The fact that the reflectance is influenced by the surface film is well known, but quantitative corrections of experimental data are rarely done. The exact solution of this problem is not simple because we have to know the optical properties of the surface film in the whole region $(0, \omega_0)$. Recently the optical constants of glassy silicon dioxide and germanium oxide were reported⁹ and were used here for the correction.

The reflectance of the sample covered by a thin absorbing film is¹⁰

$$R = \left(\frac{r_{01} + r_{12} \exp(-2i\delta)}{1 + r_{01} r_{12} \exp(-2i\delta)} \right)^2 \quad (10)$$

where r_{01} and r_{12} are the Fresnel reflection coefficients for the air-film: (r_{01}) , and film-substrate: (r_{12}) interfaces, e.g.

$$r_{12} = \frac{N_1 - N_2}{N_1 + N_2}$$

where N_1 and N_2 are the complex indices of refraction of the film and substrate. δ in eq. (10) is given by

$$\delta = \frac{2\pi}{\lambda} N_1 d$$

where d is the thickness of the film and λ is the wavelength.

For small thicknesses we assume linear dependence of R on d

$$R = R_0 + \alpha d \quad (11)$$

where $R_0 = (r_{02})^2$ is the reflectance of a clean sample. Figure 4 shows that this approximation up to 50 \AA for typical values of N_1 and N_2 is reasonable. For the determination of the coefficient α we use an equation similar to (11)

$$R_d = R_{\text{ex}} + \alpha_1 d \quad (12)$$

where R_d is the reflectance calculated from (10) with $N_2 = n + ik$, the index of refraction from (1). In the equation for the calculation of ϕ , we used the directly measured experimental values R_{ex} and $\phi_{2\text{min}}$. Here we assume $\alpha = \alpha_1$, d was evaluated as shown below and from (11), for $R = R_{\text{ex}}$, we obtain R_0 . All the assumptions used here for the corrections are not perfect but are satisfactory for this purpose.

Figure 5 shows a plot of ΔR_F , Δn_F , Δk_F vs ω for Si and Ge. For germanium we estimated $d = 20 \text{ \AA}$ and for silicon $d = 10 \text{ \AA}$. After etching we measured the thickness of the film by the ellipsometric method⁵ to be about 20 \AA . In the case of silicon d was usually found to be smaller, in agreement also with Archer's¹¹ findings. Of course, it is assumed that the experimental results on $R(\omega)$ ⁶ were obtained on samples prepared under similar conditions. The results for both materials show that the correction is large, especially for the refractive index n . The change of reflectance is also surprisingly large. For silicon it is 14% at 10 eV and for Ge, 12% at 11 eV. The shape of the ΔR curves is similar to those of $\epsilon_2(\omega)$.⁹ The larger change of reflectance is connected with the larger optical constants of the film. We must assume that the optical constants of oxides in bulk form⁹ are the same as for thin films. For Si it was proven that the film is amorphous and the index of refraction for $\lambda_{\text{Hg}} = 5461 \text{ \AA}$ agrees well with the bulk value,¹² but for germanium oxide the agreement is not so good, film value $n = 1.639$,¹³

whereas for the bulk material $n = 1.56^9$ or $n = 1.608.^{14}$ In the uv region there are no ellipsometric studies on these films. However, in this region we have no other choice.

Our values of d are probably the lower limit for the surface film thickness of samples exposed to the air. But at the same time the mathematical approximation used above is the upper limit. The limitation of such a procedure is brought out clearly for results above $\omega = 19$ eV where the correction ΔR is higher than the reflectance. For more precise determination of the true optical constants in the uv range it will therefore be necessary to develop better procedures. Experimentally, probably the most promising way will be the measurement on almost clean surfaces or the measurement on several samples with different thicknesses of films.

5. CORRECTION OF ϕ_2

For the more precise determination of ϕ_2 we can use any further optical experimental data in the interval $(0, \omega_0)$ if available. We cannot arbitrarily eliminate higher order coefficients in the series given by eq. (4) but as a reasonable approximation we can start with smaller exponents. Using conditions given by eq. (6) we have the following limitation for a_m

$$0 \leq a_m \leq \frac{\pi - \phi_1(\omega) - a_0 \omega}{\omega^{2m+1}} \quad (13)$$

where $\omega = \omega_t$; for $m=1$ in the case of Si, $\omega_t = 19.5$ eV (see Fig. 1), but for $m > 1$, ω_t is also higher. If we know optical constants at ω_i in the interval $(0, \omega_0)$, the coefficients a_m are then solutions of the system of linear equations

$$\phi_{n,k}(\omega_i) - \phi_1(\omega_i) = \sum_{m=0}^{\infty} a_m \omega_i^{2m+1} \quad (14)$$

$\phi_{n,k}$ is calculated from (1), where n, k are known for $\omega = \omega_i$. Condition (13)

enables us to decide which coefficients are important if not too many data are available. Also, it is possible to use analogous procedure for the calculation in the upper and lower limits of ϕ_2 as in the second section for $m=0$ and 1.

Theoretically, the knowledge of both the optical constants in a finite frequency interval allows one to reconstruct the whole function ϕ_2 ,⁷ but in practice this is impossible because experimental data always are subject to some errors and then the error in a_m may be higher than is practical. The usual practice is then to use the condition $\phi=0$ at the energy gap. This condition allows us to calculate a_1 from (14) for $i=1$, but in our case, for both Ge and Si, a_1 was so small that it was comparable with the error of the numerical method. The only useful result is that for lower frequencies ϕ_2 is close to the $\phi_{2\min}$. We tried to calculate the higher order coefficients for $\lambda = 5461\text{\AA}$ where data for Ge¹³ and Si¹² are available. In the case of Si the situation was the same as for data at the absorption edge. For Ge the values were inconsistent with our measurement⁵ - in other words, the coefficient a_1 was negative. It is possible to explain this inconsistency as only being due to an unexpectedly large error in reflectance, or, what is more likely, the data¹² which are for cleaved samples as in the case of Si,¹² may be different from that for the etched samples. There exist also recent experimental data for the optical constants of Ge measured directly in the visible¹⁵ and far uv regions¹⁶ but the errors are comparable to ours, and thus useless for the correction of ϕ_2 .

A further source of information in the uv region is electron energy loss spectra (EELS). As there seem to be some problems about the relationship between optical measurement and EELS (e.g. surface conditions, different samples) and also since the errors in EELS are not clearly known, we cannot use the data directly for the calculation of n, k . If we suppose the position ω_e of the maximum $\text{Im}\epsilon^{-1}$ as a well defined value, we can use that

for the narrowing of $\Delta\phi_2$. From the condition

$$\left(\frac{d \operatorname{Im}\epsilon^{-1}}{d\omega}\right)_{\omega=\omega_0} = 0$$

we have the plot $d\phi/d\omega$ vs ϕ shown on Fig. 6, for the case of Si where $\omega_e = 17$ eV.¹⁷ The point A is the lower limit of ϕ_2 in Fig. 1. The broken line on Fig. 6 represents the maximum value of $d\phi/d\omega$, as is possible to estimate graphically from Fig. 1.

The cross section of both curves gives the upper limit for ϕ (point B), as shown by the dashed line. This correction lowers $\phi_{2\max}$ by about 30% of $\Delta\phi_2$ towards $\phi_{2\min}$ near ω_e for both materials (see Fig. 1). It is possible to utilize the other EELS data in a similar way; but in view of the uncertainties in EELS data mentioned above, we did not use EELS data for corrections to ϕ_2 in the data to be discussed in the next section.

Recently n, k data from reflectance measurements at oblique incidence¹⁸ in the region 22.5 - 40.0 eV was published for Ge. We did not use it for the corrections because the main purpose of this paper is to show an analysis of normal reflectance data. Further, the optical constants data for the surface film are not available and thus the analysis would be incomplete.

6. RESULTS

Even if we do not use any additional information on physical properties inside or outside the frequency interval $(0, \omega_0)$ other than $R(\omega)$, as was supposed in the beginning, we can calculate the optical constants in the following way: using (2) we can evaluate the approximate values of n and k from the experimental data R . Making use of these values for evaluating the correction of R for the surface film we use equation (2) once more and from $\phi_{2\max}$ and $\phi_{2\min}$ we get the limits for n, k ; we chose the average value as the most probable value. The total errors Δn and Δk are the sum of the

difference between the maximum and minimum values and the errors of the experimental data. It may be remarked that this mean value has a limited physical meaning and it was chosen here only for the convenience of discussion. We have almost no physical arguments to prefer any one choice of ϕ_2 inside the interval $(\phi_{2\min}, \phi_{2\max})$ with the exception that for the data at the absorption edge (see discussion above) we prefer $\phi_{2\min}$ at lower frequencies and the shape of ϕ_{\min} (see Fig. 2) at high frequencies is unrealistic because for $\omega_0 = 21$ eV, $d\phi/d\omega$ should be zero. From this point of view this method has the disadvantage that it is practically impossible to use some criteria for the compatibility of data.⁷ We believe that any other method using some extrapolation to infinity will have essentially similar problems on a more detailed analysis. Figures 7 and 8 show data for silicon and germanium calculated in this way, together with the errors of method $(\Delta k_M, \Delta n_M)$, errors of experimental data $(\Delta k_E, \Delta n_E)$ and the results of some other authors.

Silicon: The results up to 6 eV agree in the limit of errors with those of Philipp and Ehrenreich.⁶ At 6.5 eV our spectra show additional structure discussed in a previous paper.⁵ The absolute value⁶ of n is systematically higher because it was not corrected for the presence of a surface film. The directly measured values of Sasaki and Ishiguro¹⁹ are closer to ours, with the exception of near 10 eV where the film correction is slightly large (see Fig. 5). As a result of these corrections there is also a small dip in the n and k spectra. The agreement for k in general is better, since this value is less sensitive to the corrections. Our $\text{Im } \epsilon^{-1}$ curve has a maximum at 16.5 eV, in comparison with 16.4 eV⁶ as calculated from optical data 16.9 eV²⁰ and 17 ± 0.2 eV¹⁷ as calculated from EELS. The corresponding halfwidths are 5.9 eV, 7.3 eV,⁶ 5.2 eV,²⁰ and 3.6 eV.¹⁷ Our values seem to

be closer to that from EELS, but the relatively large errors in $\text{Im } \epsilon^{-1}$ do not allow for a more detailed comparison. In general, Δn_M and Δk_M are smaller than Δn_E , Δk_E for lower energies (0-10 eV), comparable between 10-15 eV and larger (about two times) in the interval 15-21 eV. Both errors are essentially zero from 0 to the absorption edge, because in this region we used⁵ the reflectance calculated from n obtained by the measurement of the angle of minimum deviation.

Germanium: The general remarks just made, concerning the structure up to 6 eV, the character of the errors of the method and of the experimental data, and $\text{Im } \epsilon^{-1}$ are also valid for germanium. The values of n obtained from K-K analysis,⁶ and also from the directly measured experimental data of Sasaki,²¹ are substantially higher than ours between 8 and 19 eV, probably because they were not corrected for the presence of the surface film. There is much better agreement with the recent data of Marton and Toots,¹⁶ who also studied the influence of the exposure of sample to air. Our measurements as well as theirs were not made on clean surfaces but we used the typical value of d as 20\AA . As a result, both measurements when corrected gave results closely corresponding to a clean surface. The k values are less sensitive to the corrections, as in the case of Si, and the agreement with other reported values^{6,21,16} is better. The correction to zero film thickness is important here not only for the absolute value of the optical constants, but also for the structure of spectra. Near 7 eV there is a small peak in the R data^{26,5} which produces some structure also in the optical constants. It coincides with the peak in the R data (Fig. 5) and, after correction to $d=0$, the curves are almost smooth. This circumstance may be important also for other materials, e.g. $\text{A}^{\text{III}}\text{B}^{\text{V}}$, where weak structure exists⁶ in the uv region and almost nothing is known about the surface film. The $\text{Im } \epsilon^{-1}$ data give a maximum at 16.4 eV

(halfwidth 4.9 eV) in comparison with 16.0 eV (8.4 eV),⁸ 16.1 eV (3.4 eV),¹⁶ and 16.5 eV (6.4 eV)²¹ from optical data and 16.4 eV,²² 16.3 eV (6.5 eV),²³ and 16.4±0.2 eV (3.4 eV)¹⁷ from EELS. Our value for the position of the maximum is practically identical with the data from EELS and our halfwidth is the average of the recent data.^{23,17}

In the literature it is possible to find some doubts expressed as to the precision of K-K analysis. Figure 9 shows that, in our case, when ω_0 is large the results may be very good. In the visible region of Ge there is fine structure related to the Λ_3 - Λ_1 transition with spin-orbit splitting. The maximum error of the method for the constants n and k is less than ±0.005. The error of the experimental data is much higher (±0.1). Thus the limit of precision depends essentially on ΔR . For comparison Fig. 9 shows the data of Potter,¹⁵ Archer,²⁴ and Knausenberger and Vedam¹³ as measured directly. All these workers have used entirely different techniques for sample preparation. The shape of our spectra is very similar to Potter's and we believe that especially k near 2.3 eV is very good in our measurement. The normal reflectance calculated from Potter's data in this range does not agree very well with experimental values.^{15,25} It is possible to explain this disagreement in the absolute value by different surface preparation techniques and by disagreement in calculated¹⁵ and measured normal reflectance. The absolute values agree quite well with Archer's data.²⁴

7. CONCLUSIONS

It was shown that for a sufficiently high ω_0 it is possible to obtain values for the optical constants using Kramers-Kronig analysis with the same uncertainty as that of published data obtained by direct measurement.^{15,16,19,21,24} This method does not require any extrapolation outside the measured interval and also does not need any further experimental

date inside this interval. However, such data if available may be used for a further improvement in the estimation of the phase angle. For the correct absolute value of n , k in uv region, a correction for the presence of a surface film is necessary, especially in the region where this film is absorbing. Also, some weak structure in the experimental data can be shown to be due to the surface film by this correction. For the total error it is necessary to consider also the error in the experimental data.

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FIGURE CAPTIONS

- Figure 1 - Silicon. Plot of phase angle ϕ_1 , $\phi_{2\max}$, $\phi_{2\min}$ vs frequency. The broken line is the function $(\pi - \phi_1)$. The optical constants n , k are calculate directly from experimental data using $\phi_{2\min}$ (solid line) and $\phi_{2\max}$ ($\text{---}\circ\text{---}\circ\text{---}$).
- 2 - Germanium. The phase angle ϕ , optical constants n , k calculated from $\phi_{2\min}$ for $\omega_0=21$ eV (solid line), $\omega_0=13$ eV (-----), $\omega_0=6$ eV ($\text{---}\cdot\text{---}\cdot\text{---}$) and similarly for $\phi_{2\max}$ ($\text{---}\circ\text{---}\circ\text{---}$), ($\text{---}\circ\text{---}\circ\text{---}$), ($\text{---}\times\text{---}\times\text{---}$).
- 3 - Germanium. Plot of assumed experimental error ΔR_E and the corresponding errors Δk_E and Δn_E vs frequency.
- 4 - Plot of the correction ΔR_F for thickness of surface film for various optical constants ($n; k; n_1; k_1$). (5.0; 2.0; 0.8; 0.5, $\text{---}\circ\text{---}\circ\text{---}$), (5.0; 2.0; 1.5; 0.0, $\text{---}\times\text{---}\times\text{---}$), (2.0; 4.0; 1.5; 0.5, $\text{---}+\text{---}+\text{---}$), (0.5; 1.0; 1.5; 0.0, $\text{---}\circ\text{---}\circ\text{---}$).
- 5 - The correction ΔR_F (solid line), Δn_F ($\text{---}\cdot\text{---}\cdot\text{---}$), Δk_F (-----) for the presence of a surface film with thickness $d=20\text{\AA}$ for germanium and $d=10\text{\AA}$ for silicon.
- 6 - Plot $d\phi/d\omega$ vs ϕ (solid line) for $\omega_e=17.0$ eV for silicon. The broken line is a plot of the maximum value of $dp/d\omega$ evaluated from Fig. 1.
- 7 - Corrected index of refraction n , errors Δn_M and Δn_E vs frequency for silicon and germanium. Results of Philipp, Ehrenreich⁶ ($\circ\circ\circ$); Sasaki, Ishiguro¹⁹ ($\circ\circ\circ$, Si), Sasaki²¹ ($\circ\circ\circ$, Ge); Marton, Toots¹⁶ ($\times\times\times$).
- 8 - Corrected index of absorption k , errors Δk_M and Δk_E vs frequency for silicon and germanium. The results of other authors are marked as in Fig. 7.

Figure 9 - Germanium. Optical constants n , k for $\phi_{2\min}$ (solid line),
 $\phi_{2\max}$ (—○—○—○). Results of Potter¹⁵ (broken line), of
Archer²⁴ (x x x), Knausenberger and Vedam¹³ (Δ).

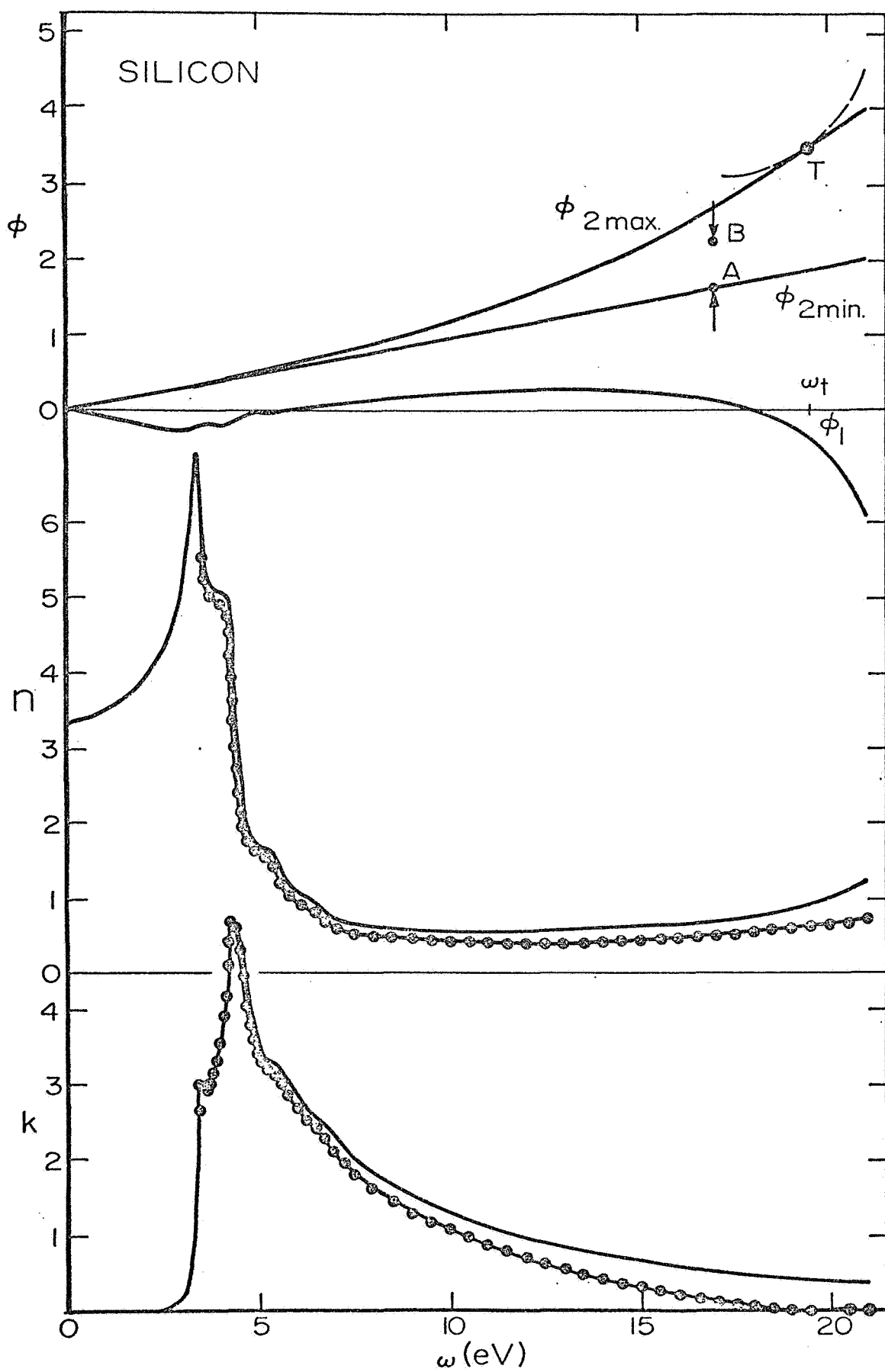


Fig. 1

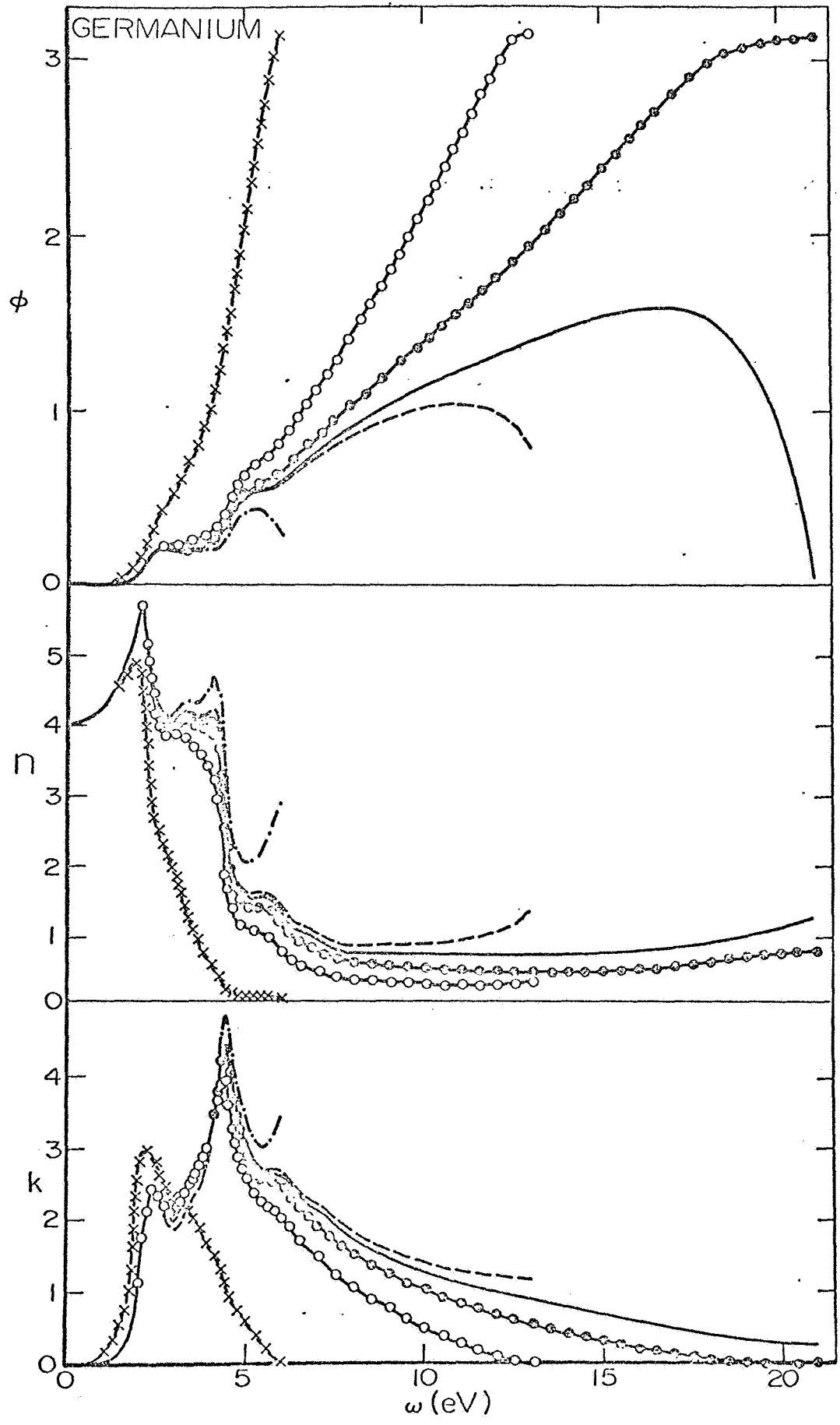


Fig. 2

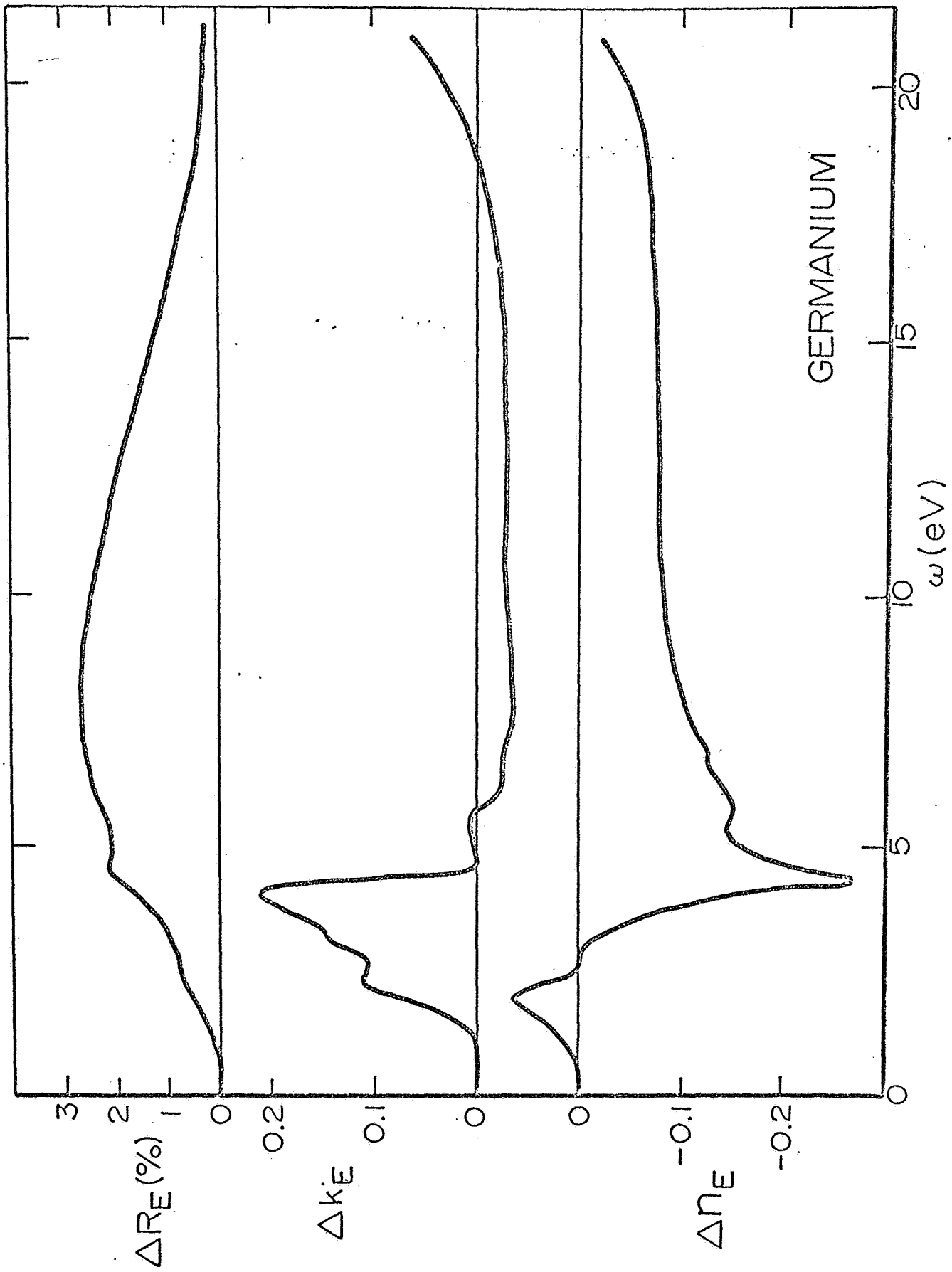


Fig. 3

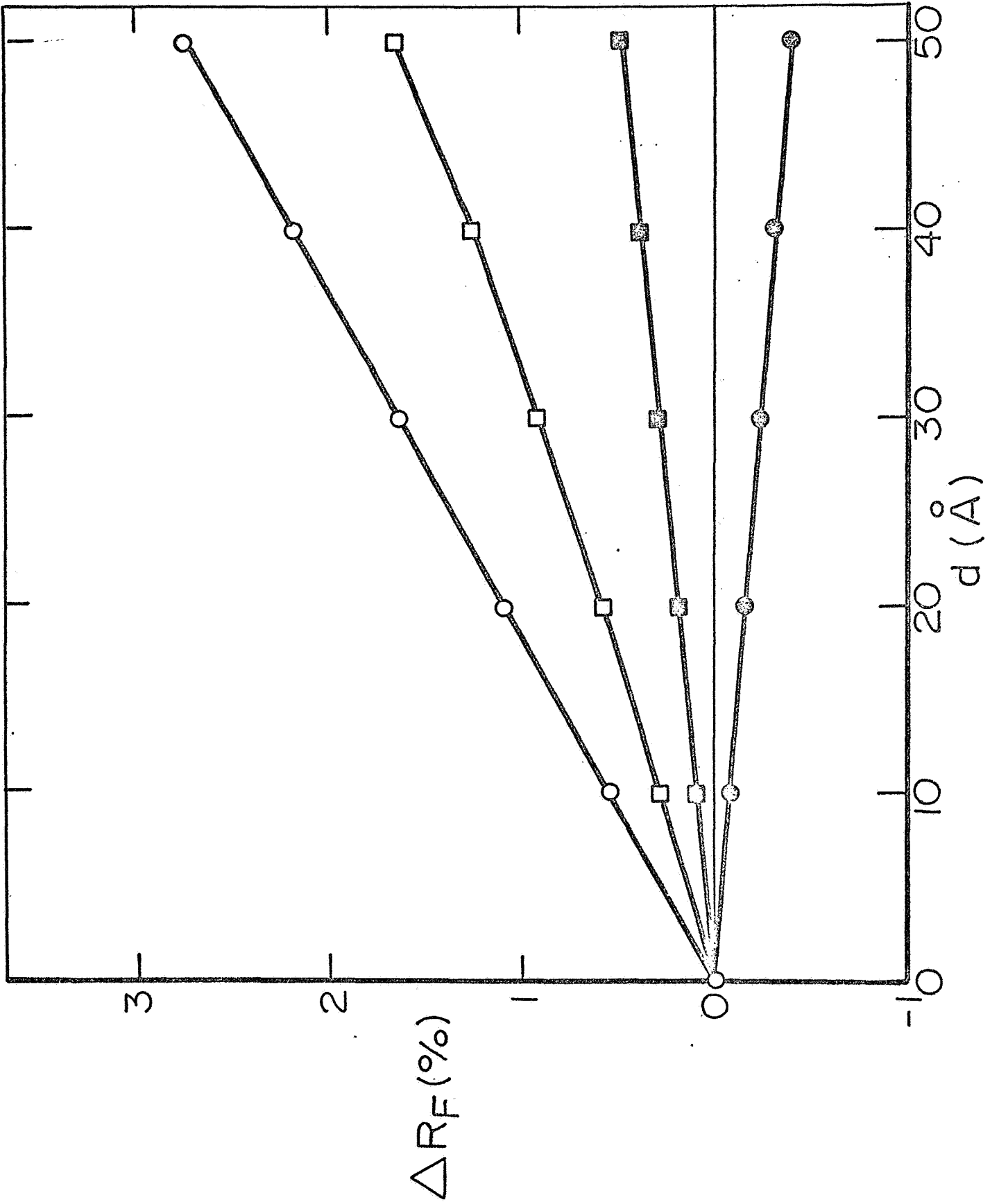


Fig. 4

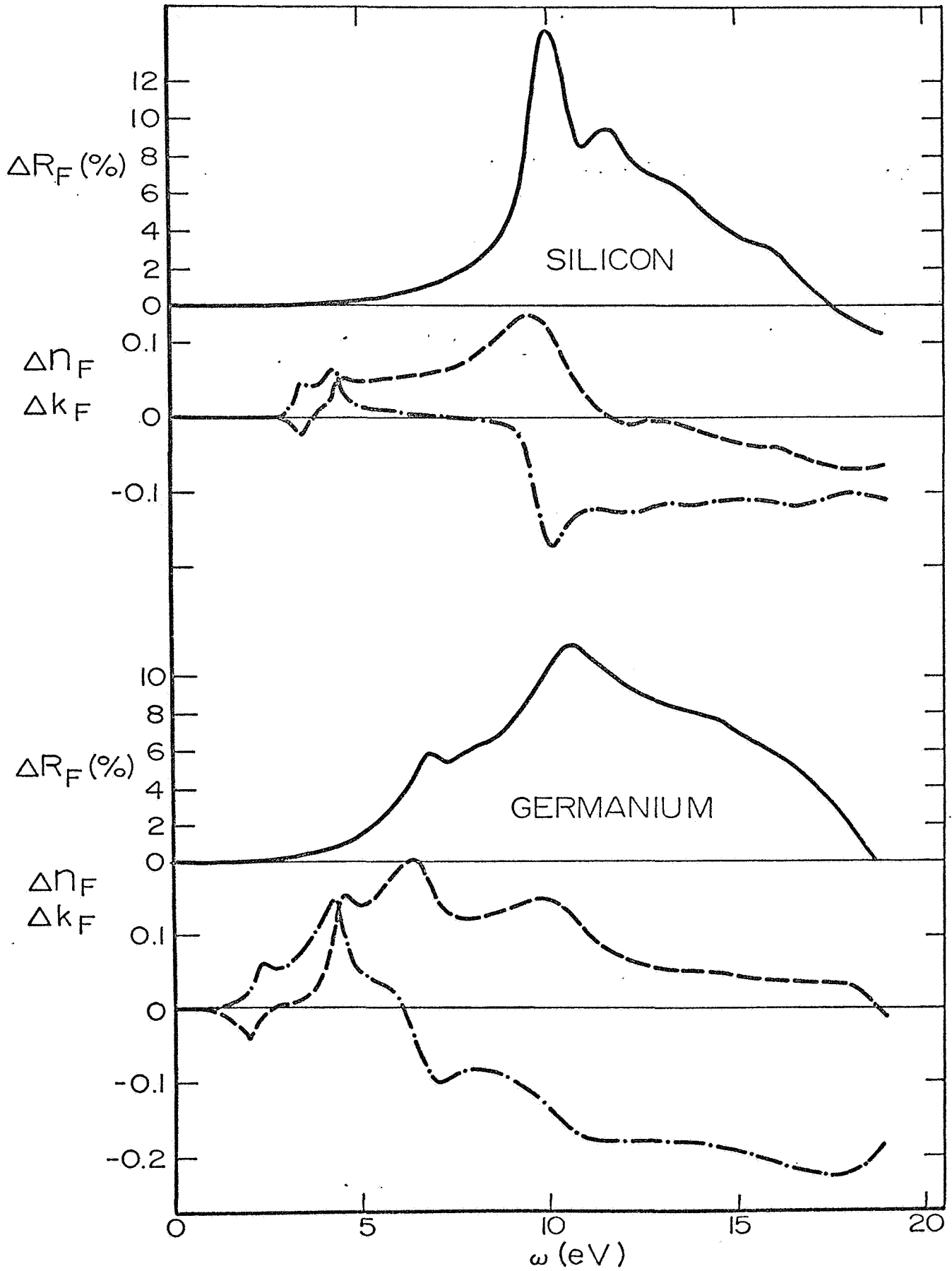


Fig. 5

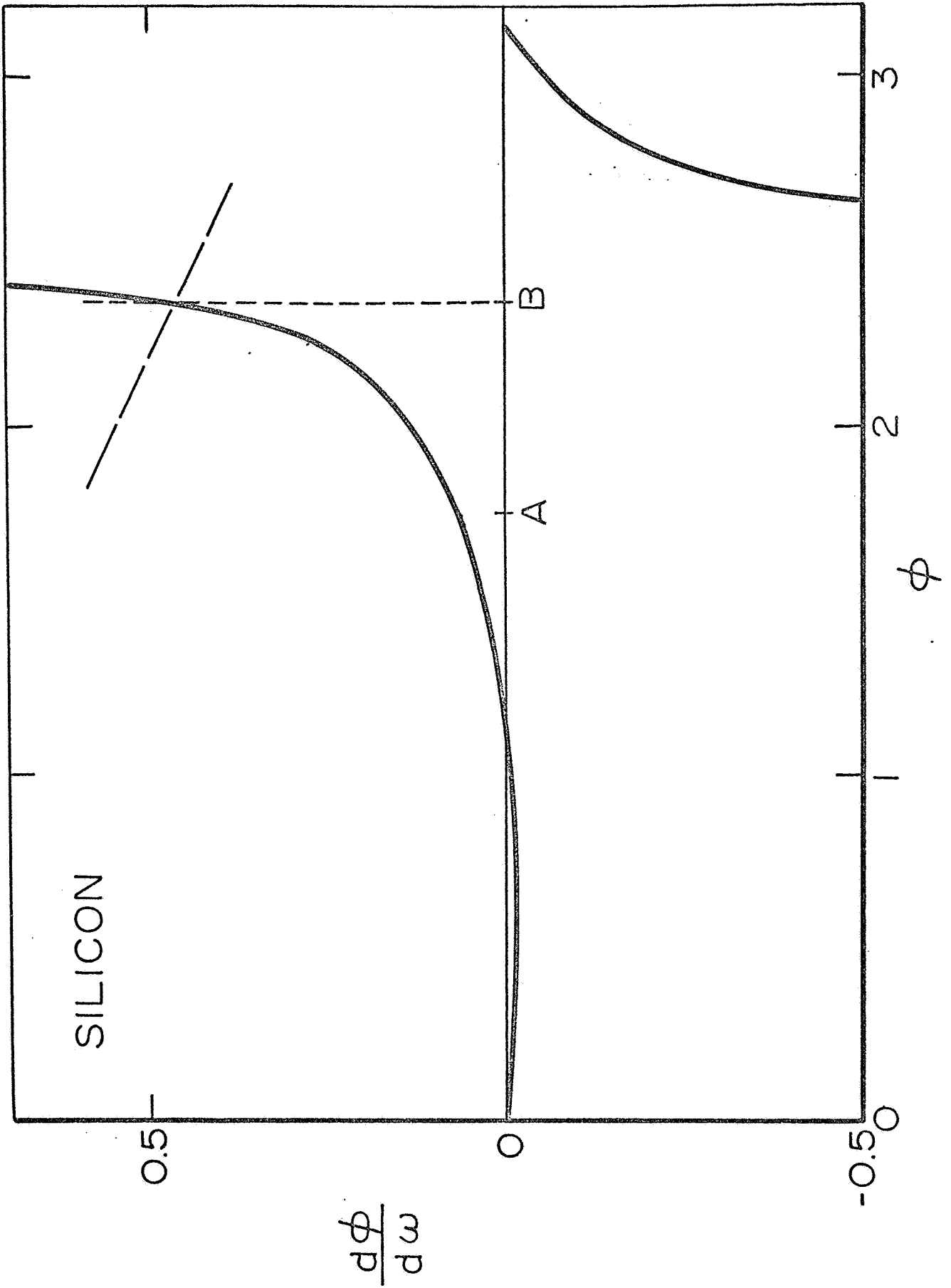


Fig. 6

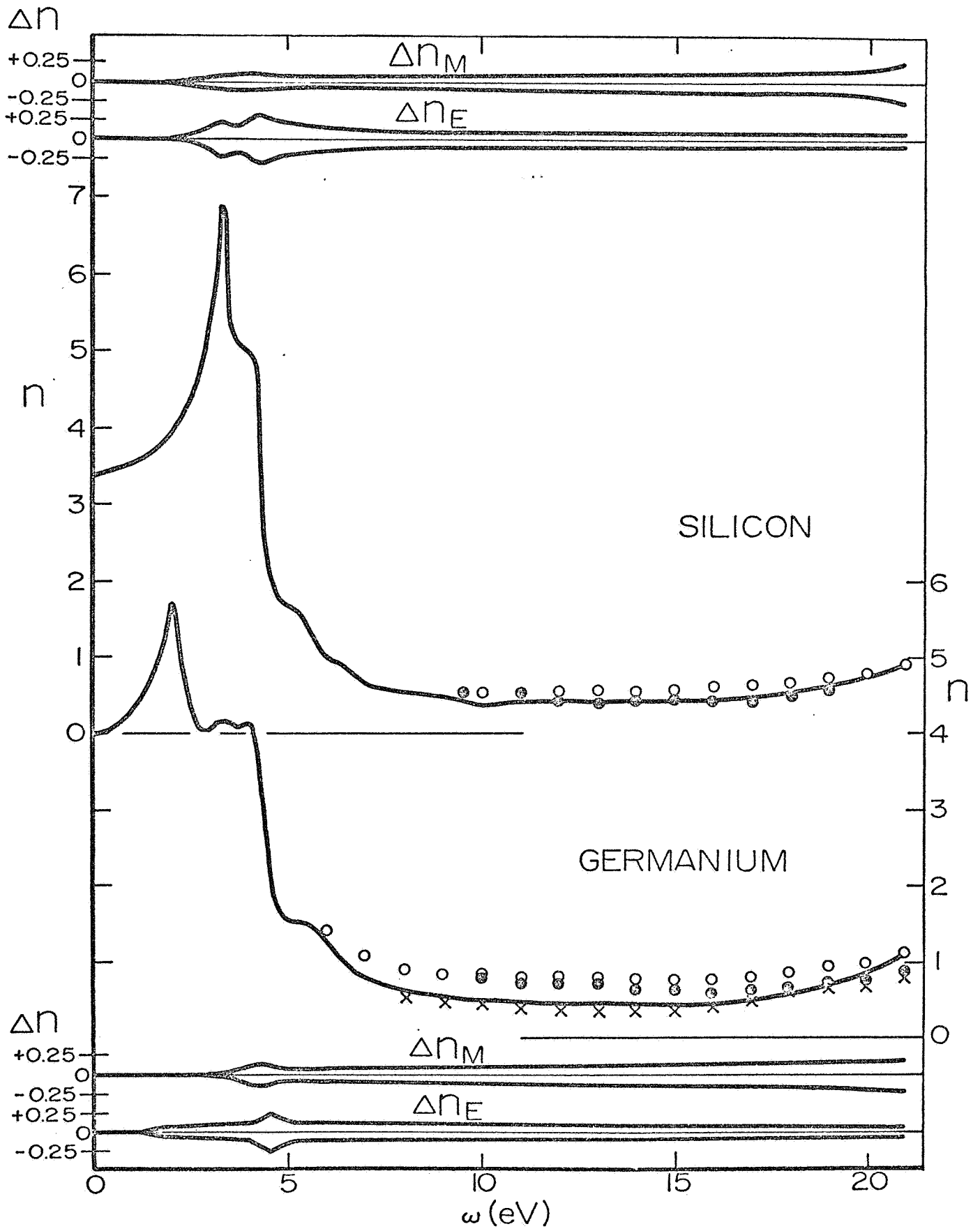


Fig. 7

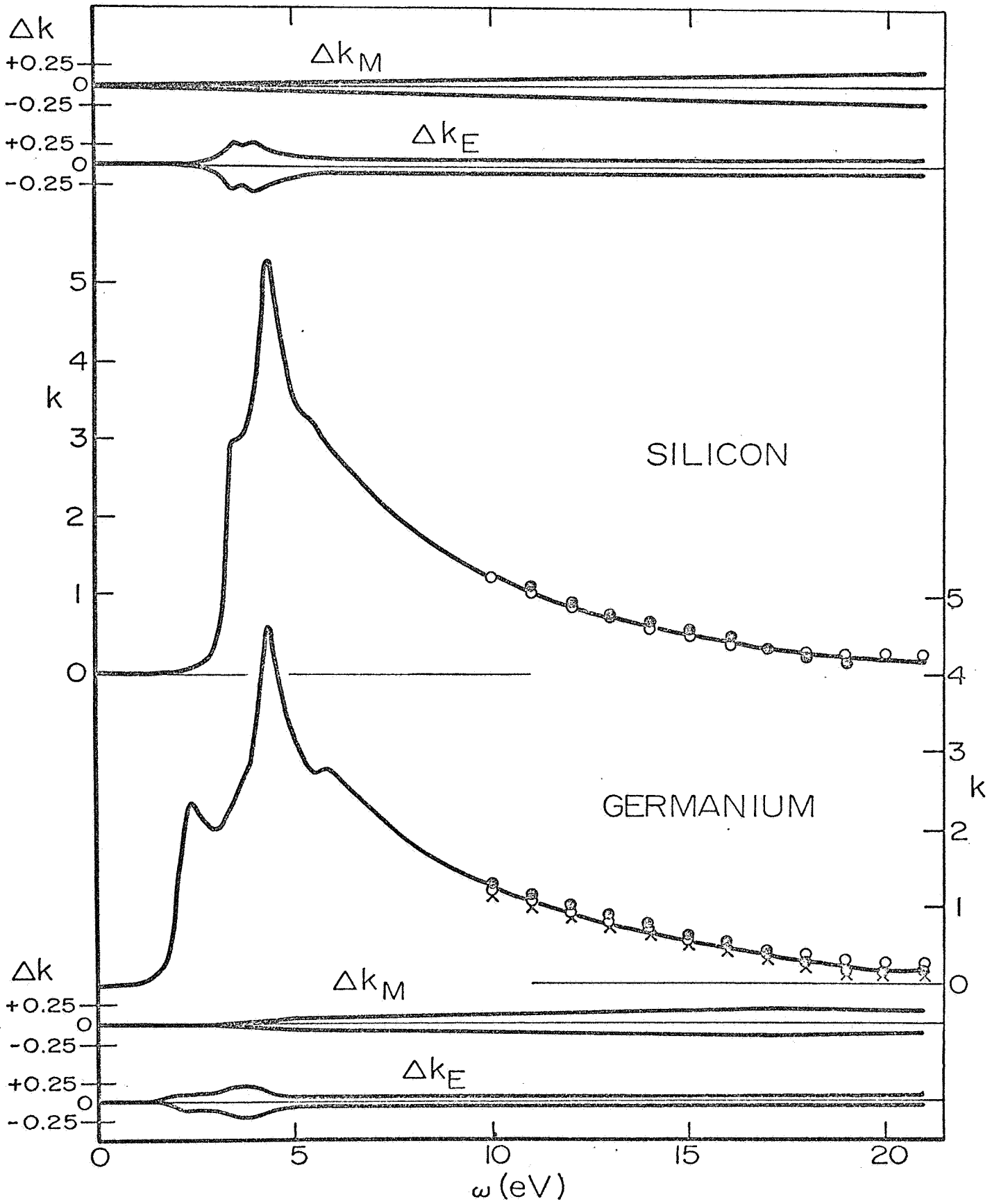


Fig. 8

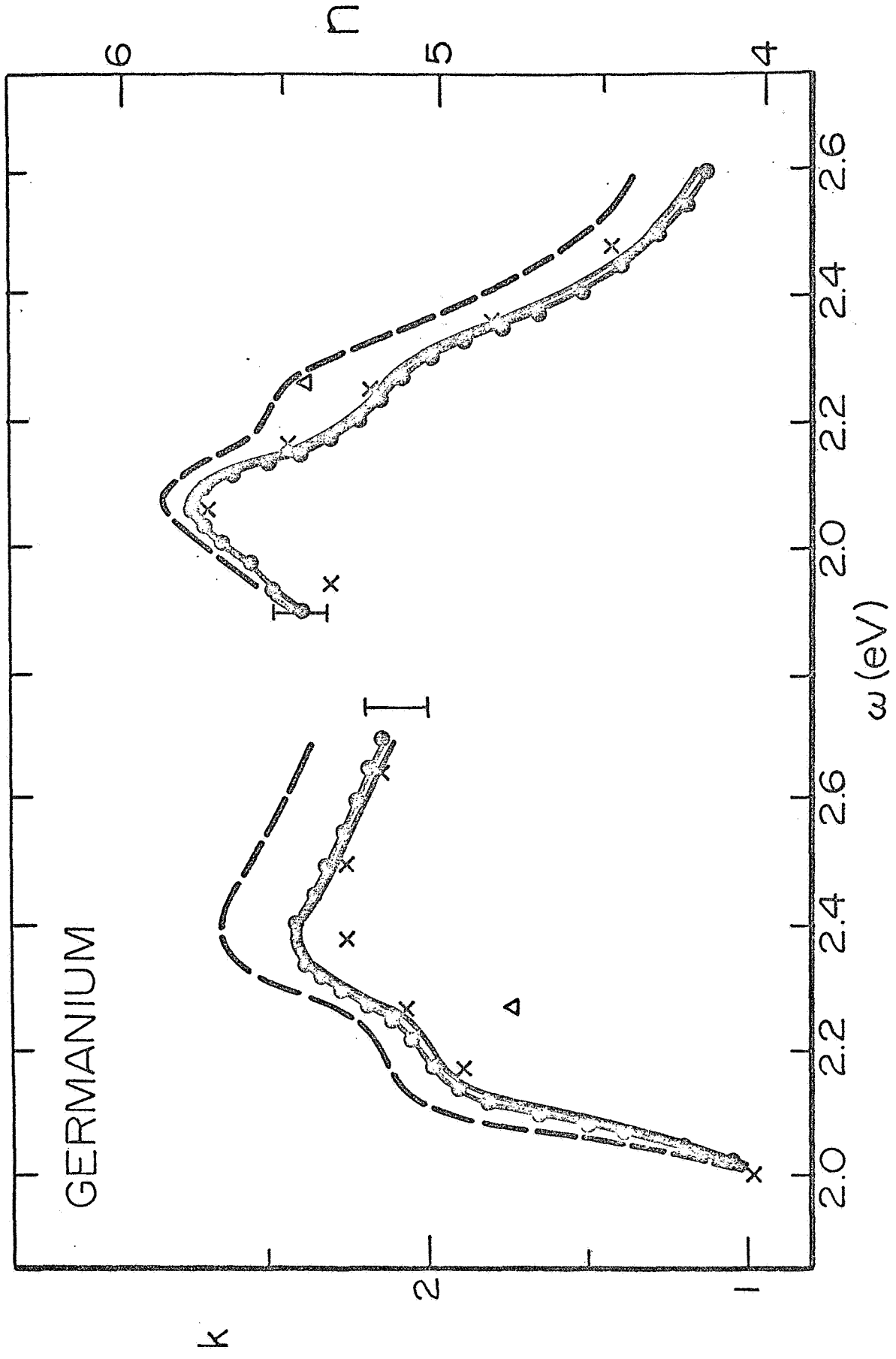


Fig. 9

Recommendations for Research During
the Next Reporting Period

The optical constants of silicon at liquid helium temperature and the changes in these constants on irradiation with electrons and protons should be determined with the new technique.