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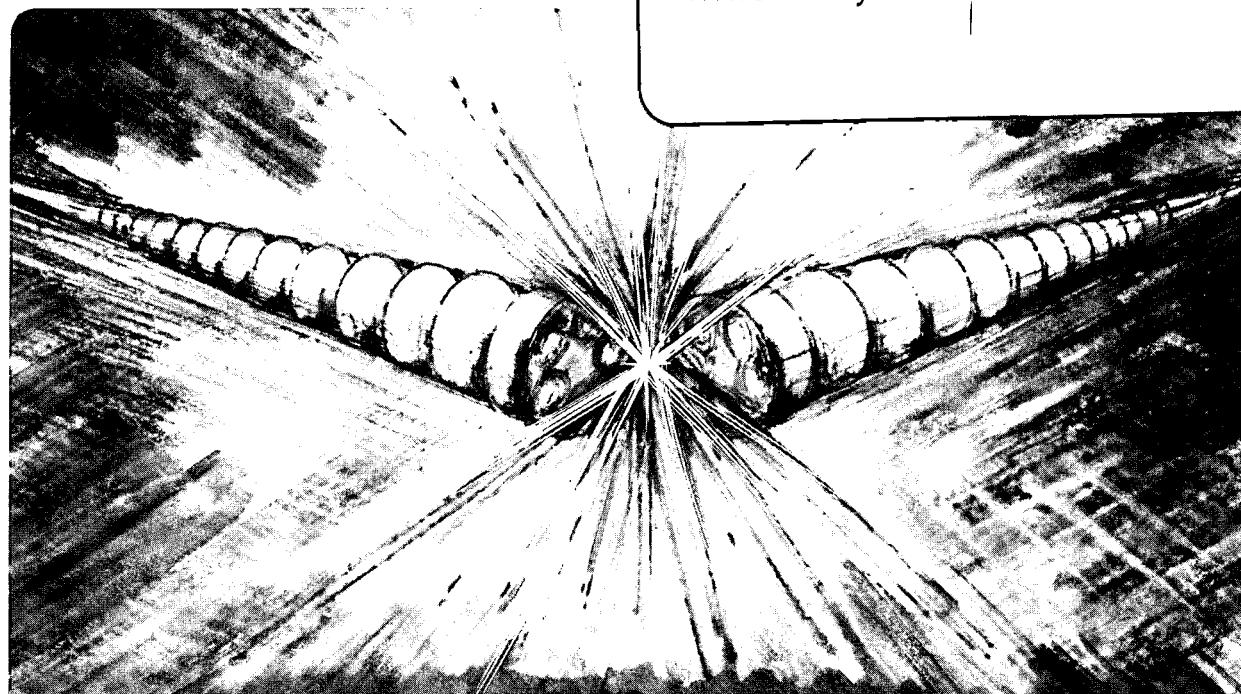
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**Multilayer Optical Elements for
Generation and Analysis of Circularly Polarized X-rays**

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ABSTRACT

Calculations of the relative phase changes of σ and π electric field components on Bragg reflection from and transmission through multilayers are presented. Large relative phase changes can be calculated in certain cases, which may lead to utility of multilayers as quarter-wave plates for generation and analysis of circularly polarized soft x-radiation. Similar behavior may be expected for perfect crystals in the hard x-ray range.

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Introduction

As scientific disciplines utilizing synchrotron radiation mature, interest increases in making use of specific polarization states of the photon beams for a variety of experiments. Circular polarization is of particular interest to many researchers. Radiation from bend magnets has polarization states dependent on the observation angle with respect to the plane of the electron orbit ranging from linear on axis to elliptical off axis [1]. Numerous types of insertion devices have been proposed [2-6], and some implemented [7,8], which would produce beams having predominantly elliptical or circular polarization on axis and, like bend magnets, having polarization states strongly dependent on observation angle. Complete characterization of the polarization of beams produced by such devices in general requires optical elements such as linear polarizers to measure the azimuthal linear polarization dependence, combined with quarter-wave plates to ascertain phase relationships of different components within the beam [9]. Alternatively, quarter-wave plates could be used to convert the predominantly linearly polarized part of a traditional bend or insertion device beam into a circularly polarized beam, thus alleviating the need for sources of circularly polarized beams.

In comparison with insertion device sources for generation of specific polarization states, relatively little attention has been paid to development of x-ray optics for polarization conversion. Some development of optics equivalent to quarter-wave plates for synchrotron radiation applications has occurred. At hard x-ray energies ($h\nu = 10-40$ keV) perfect crystals in the Laue geometry have been used to produce beams with polarization approaching circular from predominantly linearly polarized bend magnet radiation [10,11].

At extreme ultraviolet energies ($h\nu = 12\text{-}21$ eV), a triple-bounce total reflection mirror system having similar polarization behavior has been implemented [12].

This paper reports on calculations of how periodic multilayer x-ray optics might be used as polarization conversion devices in the soft x-ray spectral range, with emphasis on linear to circular conversion. A relative phase difference of 90° of one component of an initially linearly polarized beam with respect to another component is sufficient to achieve this conversion. The ability of multilayers to act as linear polarizers in the extreme ultraviolet and soft x-ray regions, by positioning the multilayer Bragg peak near 45° to give a scattering angle near 90° , has been demonstrated [13]. In this paper calculational procedures are described first, followed by results and discussion.

Calculational Methods

Multilayer structures oriented in symmetric Bragg reflection geometry and transmission geometry are considered here, as shown in Figure 1. Transmission structures considered are assumed to be free-standing for the sake of these calculations, although in reality they would most likely be on thin (≈ 1000 Å), semi-transparent substrates of low-Z materials such as silicon nitride or boron nitride. These semi-transparent substrates would attenuate the beam, but introduce no additional relative phase shifts, which are of primary interest in polarization conversion.

To understand how multilayers can alter the polarization state of an x-ray beam, resolve the incident and reflected (or transmitted) electric fields into orthogonal σ and π components (see Fig. 1), and compare the magnitude and

phase of these input and output field components. To calculate these quantities for the reflected and transmitted fields, an approach based on complex Fresnel reflection coefficients has been used [14,15]. The complex electric field amplitudes, $E_{\sigma,\pi}(h\nu,\theta)$, for σ and π polarization are calculated at the exit surface for the reflected and transmitted beams, and the phases ϕ are calculated by $\phi_{\sigma,\pi} = \tan^{-1}(\text{Im}[E_{\sigma,\pi}]/\text{Re}[E_{\sigma,\pi}])$. The quantities of interest for polarization conversion are the relative phase difference between σ and π components, given by $\Delta\phi = \phi_{\sigma} - \phi_{\pi}$, and the reflected and transmitted intensities, all of which are a function of the photon energy $h\nu$ and incidence angle θ for a given multilayer structure. In all cases considered here, ideal multilayer structures are assumed, which have atomically abrupt, smooth, flat interfaces between homogeneous layers described by published values of optical constants [16]. Some implications of the non-ideal samples obtained in reality will be discussed in the next section.

Results

Results will be presented for a single photon energy, $h\nu = 90.0$ eV, and for a specific pair of materials incorporated into multilayer structures, molybdenum and silicon. Mo/Si multilayers are known to show good reflectance performance for $h\nu$ between the Mo N and Si L_{III} edges, indicating well-formed layered structures. Operation of such devices made of other materials and/or at other photon energies will be discussed later.

To illustrate the quantities calculated, and some general trends, the reflectance and phase change behavior of a semi-infinite slab of Mo at $h\nu = 90.0$ eV are shown in Figure 2. Figure 2a shows the calculated reflectance vs. angle θ from grazing incidence, across the total reflection region, to normal

incidence ($\theta = 90^\circ$). For the π component, the expected fall to almost zero reflectance at $\theta \simeq 45^\circ$ illustrates the standard polarization phenomenon which is often used with crystals and multilayers as a means of producing a linear polarizer in the x-ray range. Figure 2b shows the phase changes of σ and π components on reflection. All phase quantities shown are normalized by 180° . The phase change on reflection of each component changes by 180° across the total reflection region, and the π component shows an additional change by 180° at $\theta \simeq 45^\circ$. These results are very similar to the phase changes on internal reflection from a dielectric/vacuum interface in the visible [17]. Figure 2c shows $\Delta\phi$, the difference in phase change on reflection between σ and π components. In the total reflection region, $\Delta\phi \neq 0$, providing the basis for the triple-bounce total reflection polarization conversion devices used in the extreme ultraviolet [12,18]. Near $\theta = 45^\circ$ and above, very large $\Delta\phi$ values of up to 180° are obtained. Operating at the θ near 45° which gives $\Delta\phi = 90^\circ$ could in principle be used to make a single reflection quarter-wave plate. However the low reflectances, especially for the π component, make this impractical.

If one considers transmission through a thin layer of homogeneous material, one finds that $\Delta\phi$ is essentially zero for the transmitted beam for θ above the critical angle for total reflection.

All phase behaviors shown above for a semi-infinite slab of Mo at $h\nu = 90.0$ eV as a function of angle are general in that they occur for all $h\nu$ in the x-ray regime and that they are expected for multilayers and crystals. The periodic nature of these latter structures give rise to additional reflectance, transmittance, and phase change features.

Additional reflectance and phase change features predicted for a

multilayer are illustrated in Figure 3. This shows results calculated as a function of angle with $h\nu = 90.0$ eV for a Mo/Si multilayer having period $d = 12.0$ nm and thicknesses of the Mo and Si layers of $d/3$ and $2d/3$ respectively. These structural parameters and photon energy yield a multilayer Bragg peak centered at $\theta \approx 39^\circ$. In addition to the $\cos^2(2\theta)$ dependence of the reflectance of the π component, the width of the Bragg peak for this component is roughly proportional to $\cos(2\theta)$. The phase change on reflection of both polarization components undergoes an additional change by 180° as θ varies across the Bragg peak. Because of the difference in widths of the Bragg peaks for σ and π components in the vicinity of $\theta = 45^\circ$ nonzero $\Delta\phi$ values can be obtained (Fig. 3c), which are of potential interest in polarization conversion [19]. For the case calculated, the largest $\Delta\phi$ for this Mo/Si structure corresponds to a phase difference of roughly 45° , which is too small for a single reflection quarter-wave plate. However, $\Delta\phi$ is cumulative in the sense that multiple reflections could be used to add to the $\Delta\phi$ obtained from a single reflection, thus potentially yielding a net relative phase difference of 90° between σ and π components. Because this approach necessarily requires operation near $\theta = 45^\circ$ to obtain significant $\Delta\phi$ values, the efficiency of any quarter-wave plate derived from this phenomenon is expected to be somewhat low.

Results for the multilayer transmission case are illustrated in Figure 4. Unlike previous transmission x-ray quarter wave plates [10,11] which operate in the Laue geometry, the structures considered here operate in the Bragg geometry with diffracting planes parallel to the surface as in Fig. 1b. In this example the Mo/Si multilayer has a period of 9.0 nm, and 20 periods. For $h\nu = 90$ eV the first order multilayer Bragg peak occurs at roughly 54° , which

corresponds to the minimum in transmitted intensity in Fig. 4a. The phase changes on transmission in the immediate vicinity of the Bragg peak are in Fig 4b. The relative phase difference between σ and π components on transmission is in Fig. 4c, and shows remarkably large values in the regions of the critical angle for total reflection and the multilayer Bragg peak. Near the critical angle transmitted intensities are impractically low for use as a quarter-wave plate. On the low-angle side of the Bragg peak at $\theta = 50.4^\circ$, however, a $\Delta\phi$ of 86° is calculated with transmittances for the σ and π components of 0.39 and 0.16 respectively. By changing parameters of the calculation slightly (e.g., by increasing the number of layer pairs, changing period or relative thicknesses, etc.), a $\Delta\phi \geq 90^\circ$ with similar transmittances can be calculated. Thus transmission through a single multilayer structure can form a quarter-wave plate in suitable conditions. The existence of such large $\Delta\phi$ values in the transmitted beam can be understood by considering the differences in the σ and π component wave fields. In the angular range of a Bragg peak, and in its immediate vicinity, strongly modulated electric fields (standing waves) exist within the diffracting structure with modulation period equal to that of the diffracting structure [20]. On the low-angle side of the peak the modulated intensity is concentrated in the low-absorption regions of the multilayer unit cell, and on the high-angle side of the peak the modulated intensity is concentrated in the high-absorption regions of the unit cell [21]. The σ field is strongly affected by this modulation, with a relative phase advance and a relative phase retardation associated with the low- and high-angle sides of the Bragg peak, respectively, essentially through refractive effects. The π field, on the other hand, is only weakly affected by this modulation because of the proximity to $\theta = 45^\circ$. These behaviors are

seen in Fig. 4b. The net result of strong standing wave induced phase effects for the σ field but not for the π field is the large and changing $\Delta\phi$ near the Bragg peak as in Fig. 4c.

Discussion

From these calculations we see that large relative phase differences between σ and π components can be obtained when operating near a multilayer Bragg peak in both reflection and transmission geometries. Multilayer quarter-wave plates for soft x-rays are thus in principle possible, at least for the cases considered. We have seen that operation with multilayer Bragg peaks near $\theta = 45^\circ$ is important in obtaining these large phase change differences, for slightly different reasons in the reflection and transmission cases. From a practical point of view, a single multilayer in transmission geometry is much simpler to implement than a multiple reflection device, and has an important advantage of providing an undeviated beam. Many issues relating to implementation of such optics require consideration. Some of these are discussed below.

The issues of operable wavelength range and tunability will be considered separately. The range of photon energies over which multilayers can in principle function as quarter-wave plates is an important issue whose resolution is somewhat open. The calculations presented here show large $\Delta\phi$ values for Mo/Si multilayers at $h\nu = 90.0$ eV. All of the phenomena which manifest as phase effects in these calculations are general for multilayers and crystals. However, the magnitude of the phase effects resulting from these phenomena are strongly dependant on specific materials and photon energies through the energy-dependant optical properties in the x-ray regime.

As $h\nu$ increases above 90.0 eV in the soft x-ray, both real and imaginary parts of the optical constants become smaller as the complex refractive index approaches 1. Thus we expect that the refractive mechanisms which lead to large $\Delta\phi$ values for the multilayer transmission case will become smaller as $h\nu$ increases, as is verified by calculation. Similarly, decreasing $\Delta\phi$ values with increasing $h\nu$ are expected for the multilayer reflection case. The ultimate high $h\nu$ limit for which multilayers might be able to function as quarter-wave plates will depend on the ability to produce high quality multilayer structures with decreasing period to allow operation at $\theta \simeq 45^\circ$, an area of much current research. Assuming perfect structures are obtainable, a high $h\nu$ limit will be set by the optical constants of materials, and this has not yet been determined by the authors. It is important to note that the same effects calculated here for multilayers should also be observable for natural crystals in the harder x-ray regime.

The tunability range of a given multilayer quarter-wave plate will be limited. This is primarily because these devices require a Bragg peak near $\theta = 45^\circ$ to obtain significant $\Delta\phi$ values. The range of angles and hence x-ray wavelengths at which a given device may produce an overall $\Delta\phi = 90^\circ$ has not been determined by the authors, and is expected to depend also on the magnitude of the $\Delta\phi$ effects for that specific multilayer as discussed above. Some means of increasing the tunability range may be available, such as using a multilayer with a laterally graded period in conjunction with translation along that gradient to shift the wavelength scale.

Modulation of polarization, for example changing from left circular polarization to linear to right circular polarization, can be obtained with multilayer or crystal devices. Such modulation can be obtained by

mechanically changing angular settings of the multilayers with respect to the incident beam, and perhaps by tuning photon energy at fixed angular settings.

Fabrication, stability, and contamination of multilayer structures may also be important issues for implementing multilayer quarter wave plates in the soft x-ray. While technology for production of relatively high-quality multilayers for reflection operation is reasonably well-developed, high optical quality transmission structures are not as easily fabricated. Some work has obtained transmission multilayer structures by chemically etching the back side of a Si wafer whose front surface is coated with a multilayer [22]. Characterization of these structures shows that multilayer optical performance is likely to be degraded by the roughness of the buffer layer between the multilayer and Si wafer which acts as an etch stop [23]. Stability of multilayers in the intense beams of synchrotron radiation is an ongoing area of research, and may be an important issue for transmission structures. If a monochromator is positioned upstream of a transmission multilayer structure to filter out unwanted radiation, this issue should not be limiting. Contamination of multilayers in soft x-ray synchrotron applications, like contamination of total reflection mirrors and gratings, may be a problem if severe. Carbon contamination would not only reduce reflectance or transmittance [24], but if of uneven thickness across the optically active surfaces, could introduce additional phase changes across the beam which would complicate the behavior of a quarter-wave plate.

Summary

The calculations presented here for Mo/Si multilayers in symmetric Bragg geometry at $h\nu = 90.0$ eV predict large phase change differences between σ and

π electric field components on reflection and transmission. Quarter-wave plates based on these results appear feasible. Transmission structures appear especially attractive. Similarly large relative phase changes with multilayers may be anticipated to somewhat higher photon energies in the soft x-ray, and similar behavior with natural crystals is anticipated for photon energies in the hard x-ray region. Work is underway to fabricate and test polarization conversion behavior of the multilayer and crystal optics discussed here.

Acknowledgements

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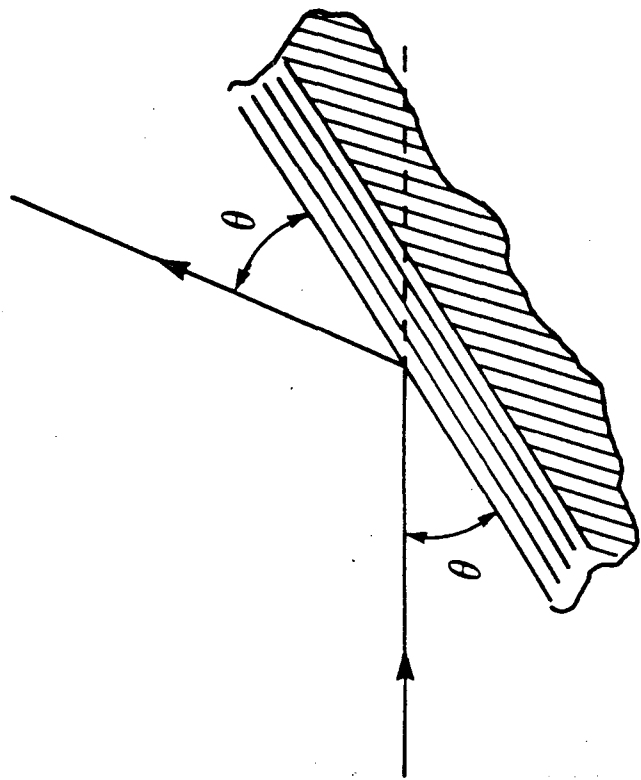
Figure Captions

Figure 1. Geometries considered include symmetric reflection and transmission. Incident and reflected (or transmitted) electric fields are resolved into orthogonal σ and π components, which are perpendicular to and in the plane of the figure, respectively.

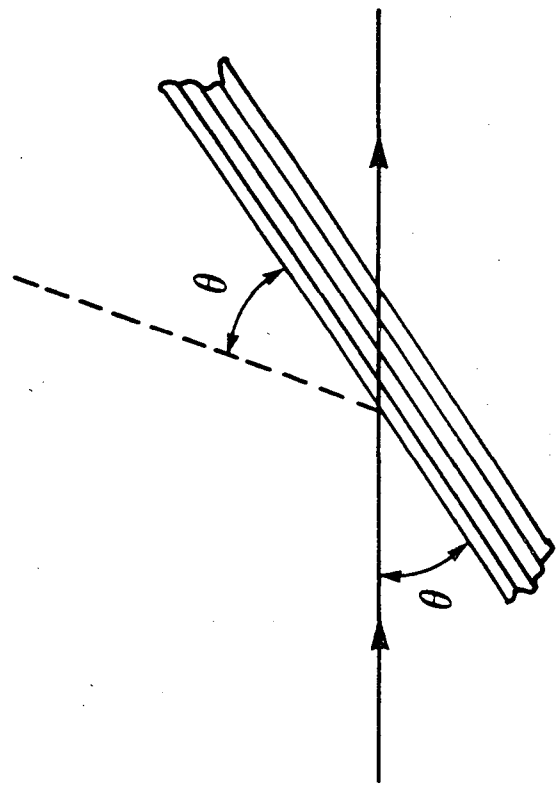
Figure 2. The calculated reflectance vs. angle for σ , π and unpolarized radiation of $h\nu = 90.0$ eV from a molybdenum mirror are shown in (a). Phase changes on reflection are in (b), while the relative phase difference, $\Delta\phi$, between σ and π polarization components is in (c). All phase quantities are normalized by 180° .

Figure 3. The calculated reflectance vs. angle for σ , π and unpolarized radiation of $h\nu = 90.0$ eV from a molybdenum/silicon multilayer are in (a). Phase changes on reflection are in (b), the relative phase difference between σ and π polarization components is in (c).

Figure 4. The calculated transmittance vs. angle for σ and π polarized beams of $h\nu = 90.0$ eV are in (a). The phase change on transmission in the immediate vicinity of the multilayer Bragg peak is in (b). The relative phase difference between σ and π polarization components is in (c).



Symmetric
reflection



Transmission

FIGURE 1

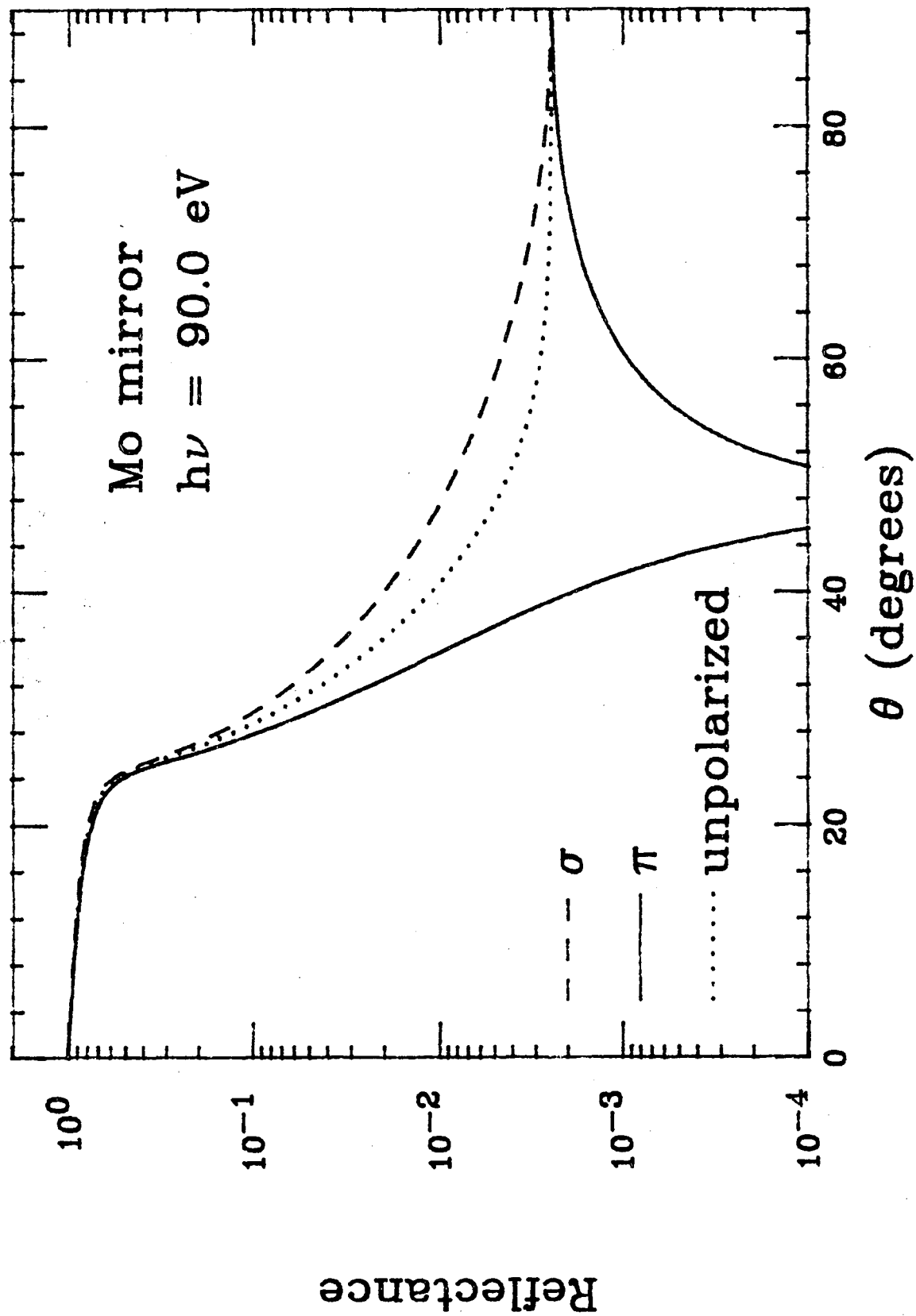


FIGURE 2a

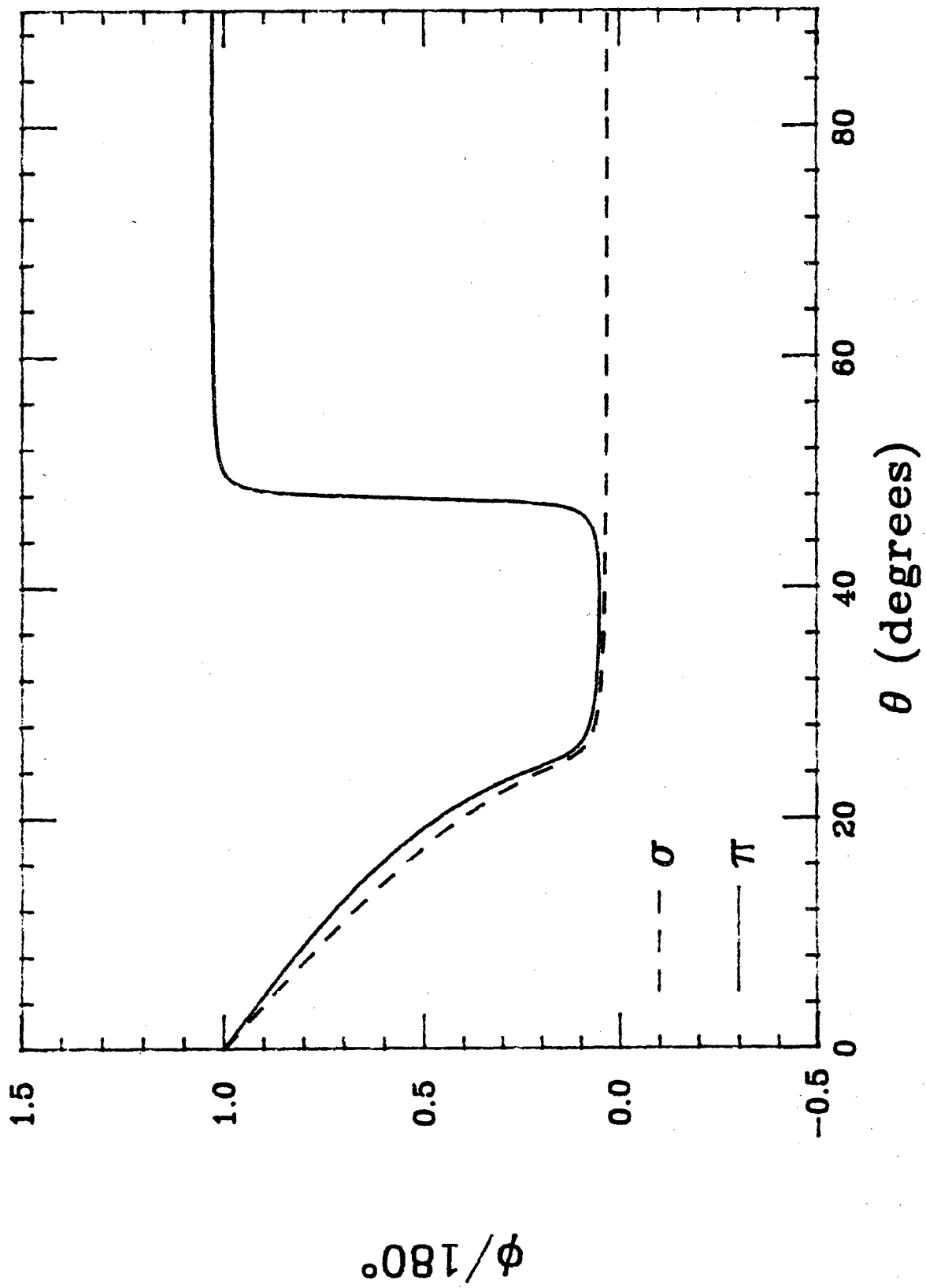


FIGURE 2b

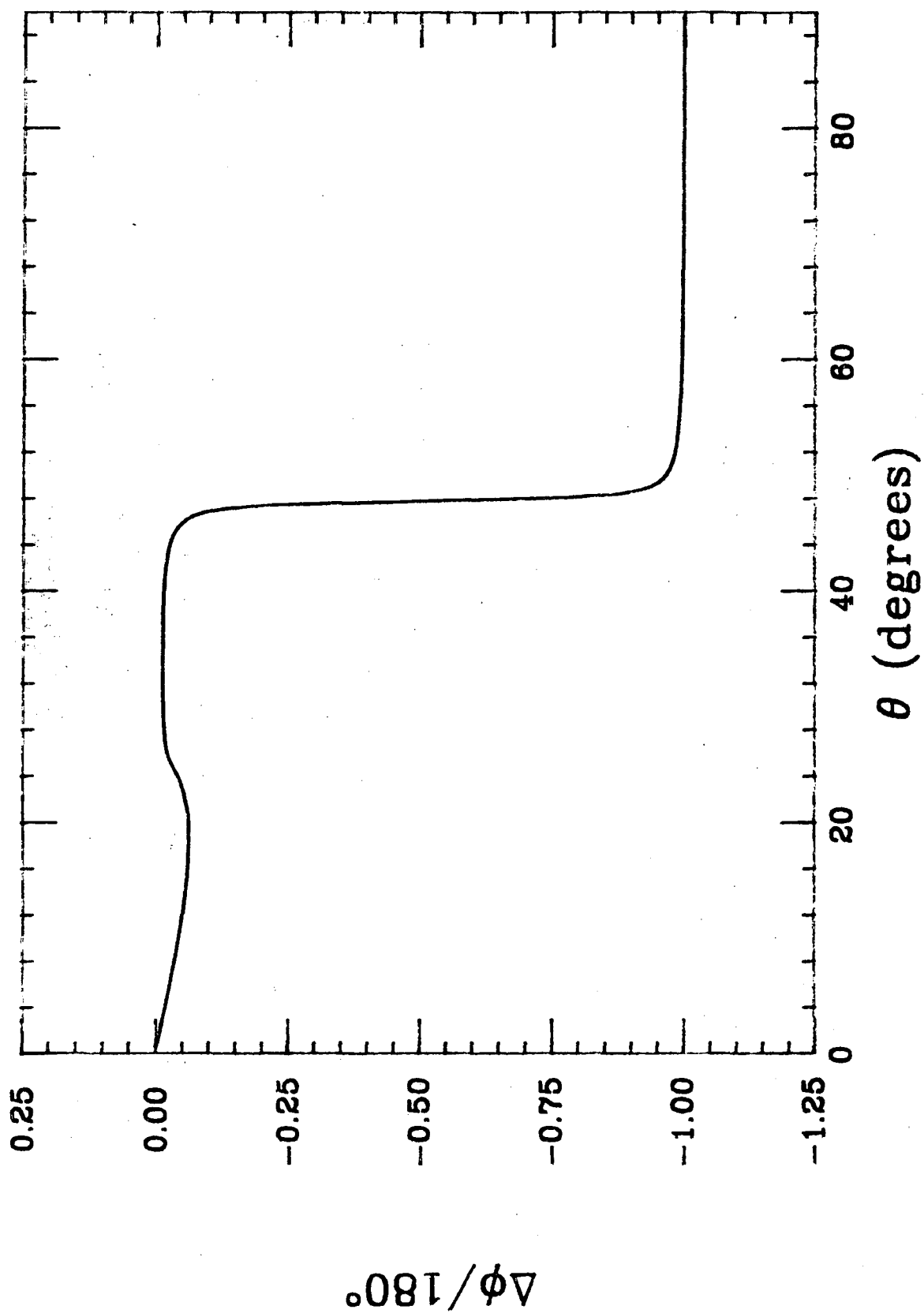


FIGURE 2c

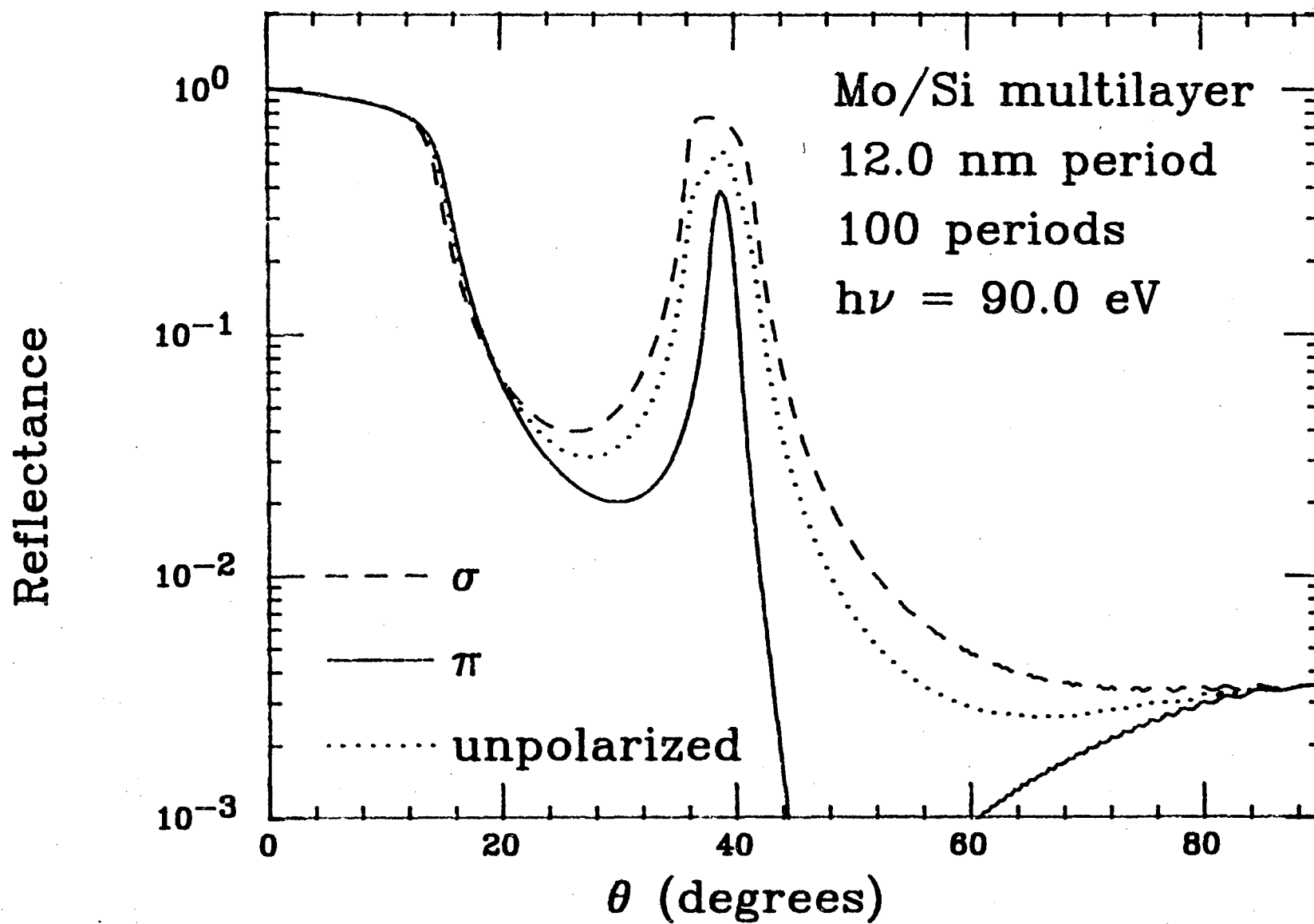


FIGURE 3a

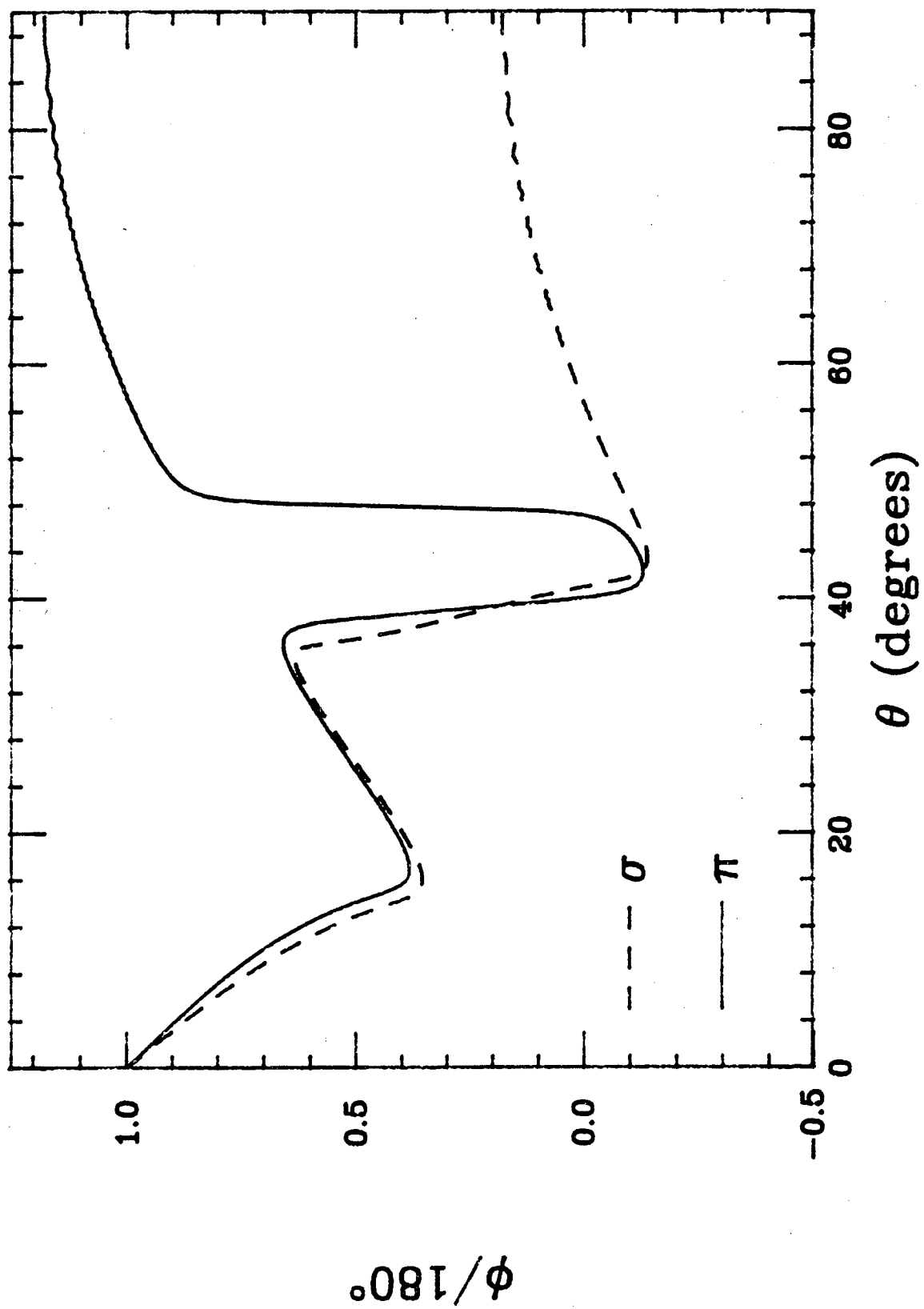


FIGURE 3b

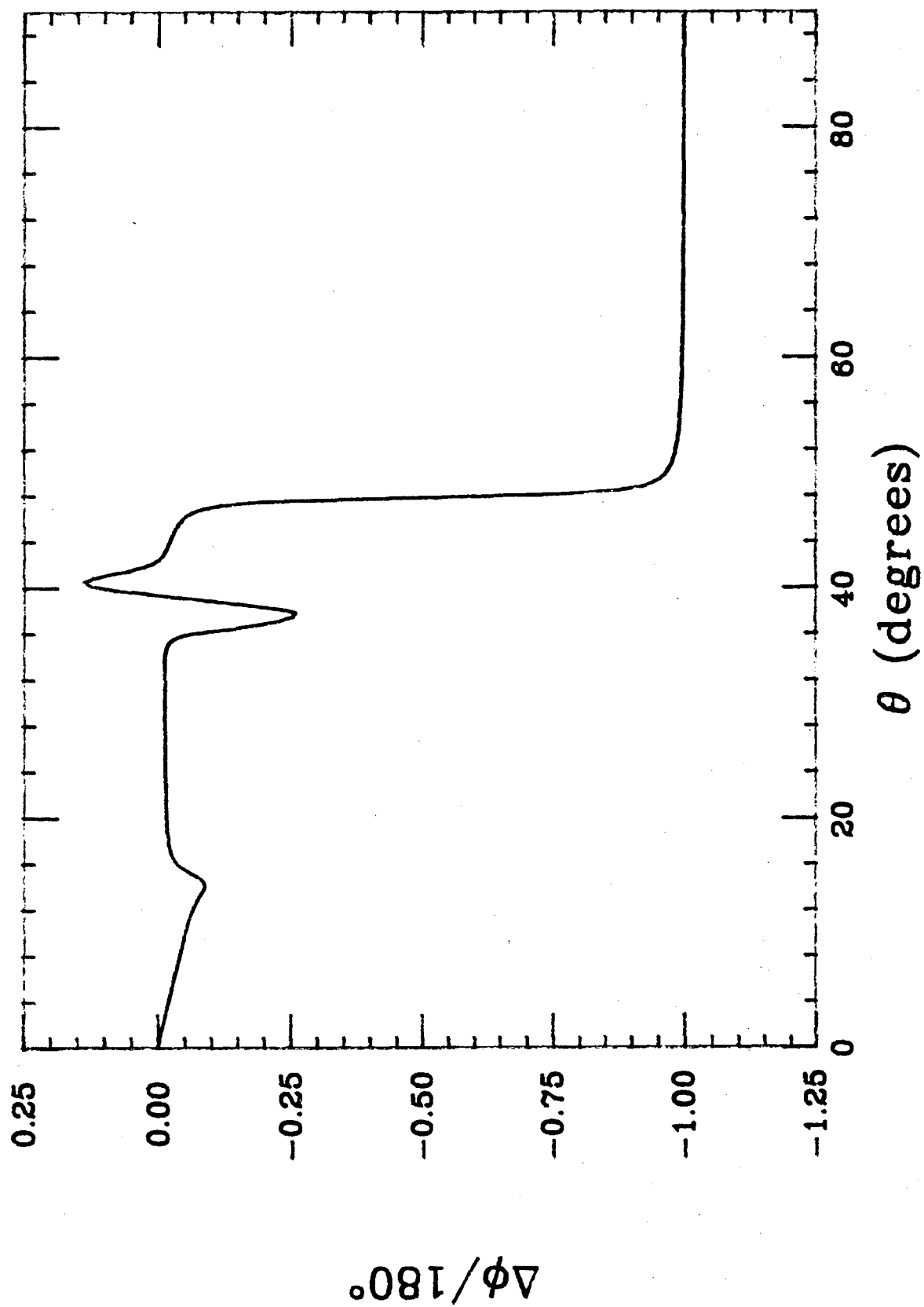


FIGURE 3c

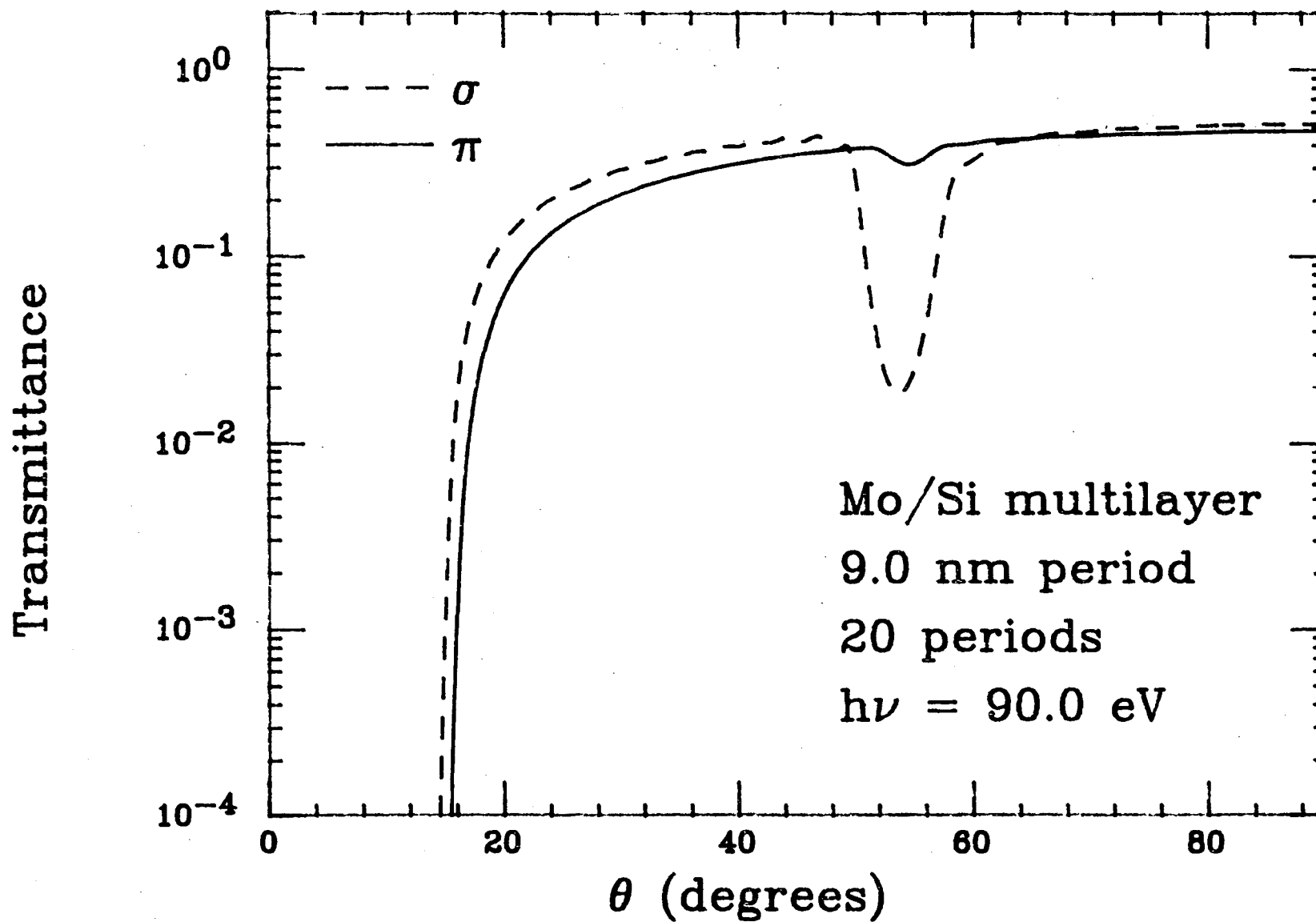


FIGURE 4a

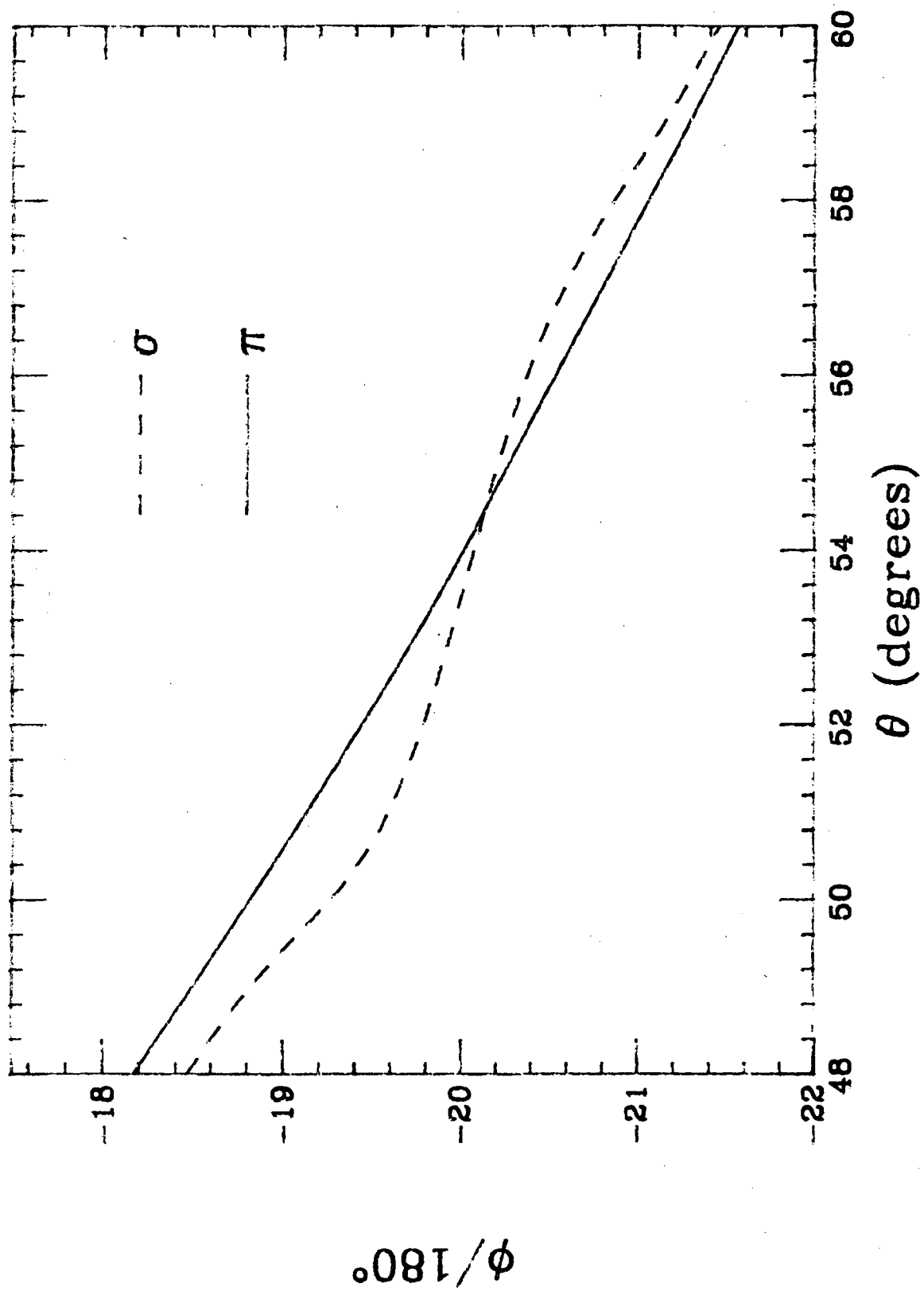


FIGURE 4b

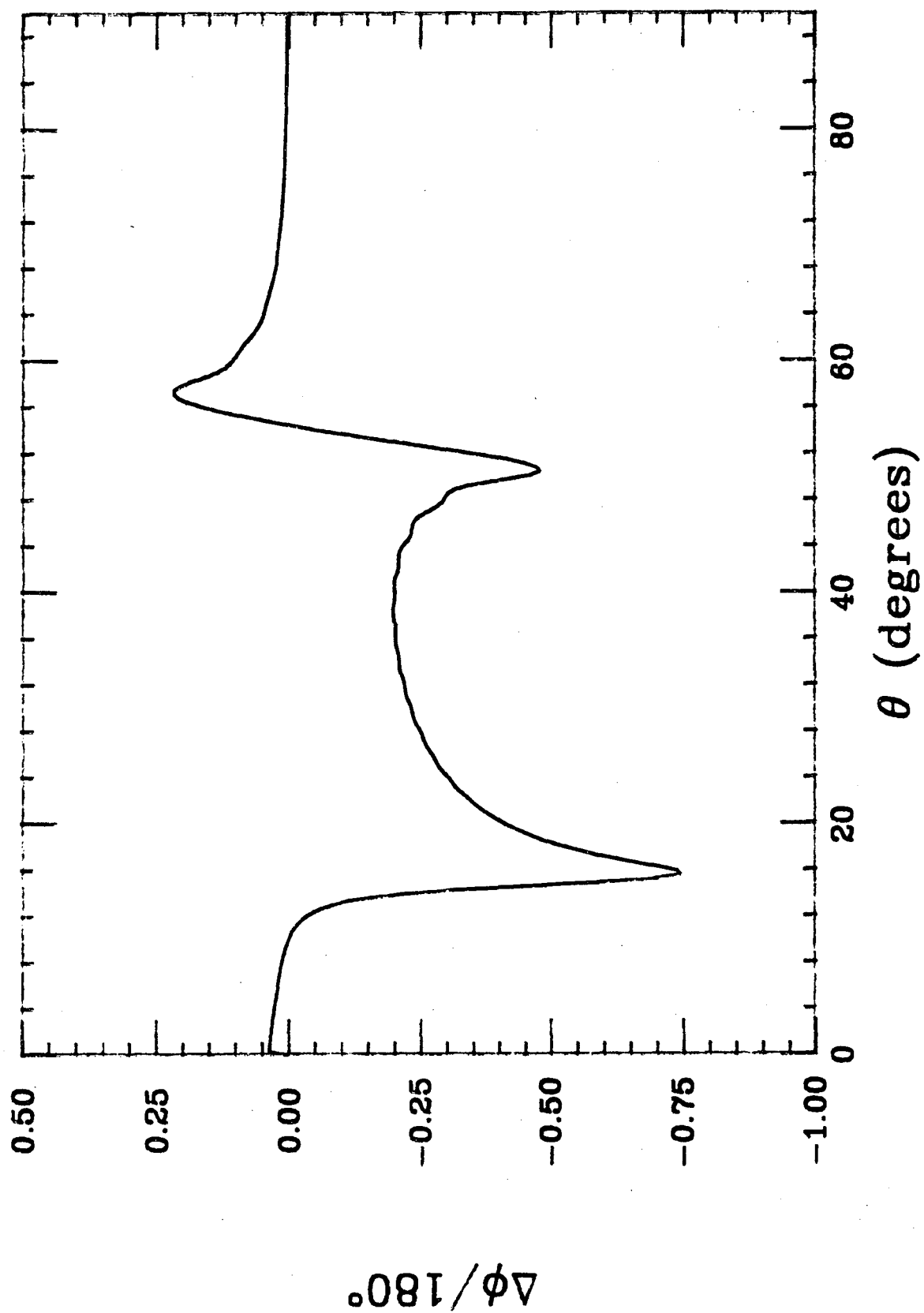


FIGURE 4c

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