PHYSICAL REVIEW B VOLUME 14, NUMBER 10 15 NOVEMBER 1976

Energy resolution and angular-broadening effects in Compton-profile anisotropy measurements*

W. R. McIntire†

Department of Physics, University of Houston, Houston, Texas 77004

(Received 19 May 1976)

The effects of detector resolution and angular broadening on γ-ray Compton-profile anisotropy measurements are studied. Angular broadening limits the experiments to scattering angles near 180°. For such angles, the resolution of the profiles improves with increase in incident photon energy E_0, up to $E_0 \sim 600$ keV. However, the slight improvement in resolution possible for $E_0 > 200$ keV does not produce an appreciable change in the accuracy of the measurements. This is demonstrated by broadening theoretical anisotropy curves with resolution functions appropriate to 60-, 160-, and 500-keV photons scattered at 180°. Although for high-incident-energy photons ($E_0 \gtrsim 2$ MeV) significant improvement in detector resolution is possible for low scattering angles, it is shown that the conditions of high E_0 and low scattering angle produce angular-broadening effects many times as significant as the detector resolution for these cases.

INTRODUCTION

The use of Ge(Li) detectors and γ-ray sources for Compton-profile measurements has extended the range of measurements to high-atomic-number samples[1-5] and has increased interest in the field. Fundamental to the success of the γ-ray experiments is the fact that the detector resolution halfwidth increases less rapidly with incident photon energy than does the Compton peak width. This leads to improvement in detector resolution relative to the peak width as higher-energy photons are used. The detector resolution width ΔE_D for scattered photons at final energy E_f is given by

$$\Delta E_D = (\sigma^2_{\text{noise}} + \alpha E_f)^{1/2} , \tag{1}$$

where ΔE_D is the full width at half-maximum height (FWHM), σ_{noise} is the preamplifier noise contribution, and αE_f is the intrinsic detector contribution.[3] For the low-incident photon energies of the x-ray experiments, the width in energy of a Compton profile is approximately proportional to the incident photon energy. The profile width divided by ΔE_D increases approximately as $E_0/(\sigma^2_{\text{noise}} + E_f)^{1/2}$, and E_f increases less rapidly than E_0. For higher-incident photon energies we must use the relativistic formula for the component of the incident electron momentum along the momentum-transfer direction

$$p_z(E_f) = mc\left(\frac{E_0 - E_f}{mc^2} - \frac{E_0}{mc^2}\frac{E_f}{mc^2}(1 - \cos 2\theta_c)\right)\Bigg/\left[\frac{E_0}{mc^2}\frac{E_f}{mc^2}(2 - 2\cos 2\theta_c) + \left(\frac{E_0 - E_f}{mc^2}\right)^2\right]^{1/2} . \tag{2}$$

Using this formula with $2\theta_c = 180°$, the peak width divided by ΔE_D increases more slowly, levels off and then actually increases for $E_0 \gtrsim 600$ keV. In this paper we discuss this saturation of the relative resolution and demonstrate the effects on Compton-profile anisotropy measurements of finite detector resolutions appropriate to 60-, 160-, and 500-keV photons.

Fukamachi and Hosoya[6] have pointed out that for higher-incident photon energies ($E_0 \gtrsim 1$ MeV), the relative resolution is greatly improved at lower scattering angles. However, at the low-scattering angles suggested, the angular-broadening effects present in an experimental measurement become much more significant than the detector resolution. Therefore angular broadening should also be considered as a function of incident photon energy and scattering angle.

DETECTOR RESOLUTION

It is instructive to plot the detector resolution FWHM both in eV (ΔE_D), and in atomic units of momentum (ΔP_D). On the scale of initial electron momentum p_z the detector resolution width is given by

$$\Delta P_D = \Delta E_D \frac{dp_z}{dE_f} . \tag{3}$$

While ΔE_D increases with an increase in photon energy, the factor dp_z/dE_f for conversion to the momentum scale is proportional to the inverse of the Compton peak width and decreases with E_0. Figure 1 shows the energy-momentum conversion factor dp_z/dE_f, ΔE_D, and ΔP_D plotted as a function of incident photon energy for $2\theta_c = 180°$. (It is shown below that experimental geometries should have $2\theta_c$ near 180°.) A number for comparison to

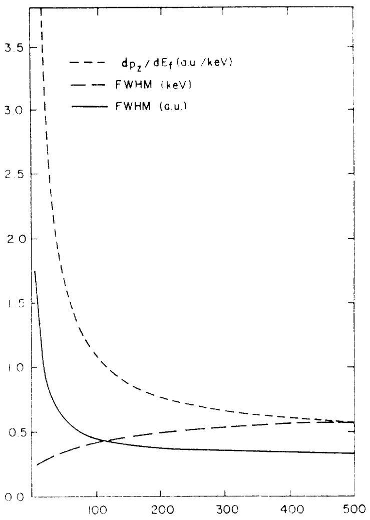

FIG. 1. Detector resolution at the Compton peak as a function of incident photon energy. Short-dashed line: dp_z/dE_f (a.u./keV); long-dashed line: ΔE_D (FWHM in keV); solid line: ΔP_D (FWHM in a.u. of momentum).

ΔP_D is the width of a free-electron parabola for Al, about 1.8 a.u.

The values of dp_z/dE_f are calculated from values of $p_z(E_f)$ vs E_f at the peak center using the relativistic formula for $p_z(E_f)$.[7] Detector resolution values were calculated for a good 10-mm active diameter Ge(Li) detector with measured FWHM of 228 eV at 5.9 keV and 508 eV at 122 keV. Reported resolutions for experiments using 60-keV,[1,8–10] 159-keV,[2] and 412-keV γ rays[11] all lie on or slightly above our calculated curve. The detector FWHM in a.u. of momentum decreases dramatically as the incident photon energy increases from the x-ray region to about 100 keV, but the curve of dp_z/dE_f vs E_0 is not hyperbolic as often assumed, and the relative resolution ΔP_D improves little for $E_0 \gtrsim 200$ keV. Going to higher-energy γ-rays at $2\theta = 180°$ does not improve the resolution very much. In fact, the calculated values of ΔP_D vs E_0 for 180° scattering reach a minimum of 0.352 a.u. for $E_0 \approx 600$ keV. This value of ΔP_D is only 10% smaller than the calculated value 0.383 a.u. for $E_0 = 200$ keV. Beyond 600 keV ΔP_D increases with E_0. This trend is seen in Fig. 4 of Ref. 6. For the detector specified above, ΔP_D approaches 0.522 a.u. as E_0 becomes infinite. It is clear that with current technology the γ-ray measurements will not exceed the best reported resolution of the x-ray scattering measurements, about 0.2 a.u. FWHM using a LiF 600 reflection for energy analysis.[12] The γ-ray experiments do, of course, have other advantages over x-ray measurements.[5]

ANGULAR BROADENING

The most straightforward way to demonstrate the effects of collecting photons scattered over a finite range of angles 2θ is to define the Compton peak shift

$$\Delta E_{2\theta}(\delta) = E_{2\theta} - E_{2\theta+\delta} , \tag{4}$$

where $E_{2\theta}$ is the energy of the center of the Compton peak for the scattering angle 2θ, $E_{2\theta+\delta}$ is the peak center of energy for scattering $2\theta+\delta$, and δ represents the angular spread. The energy of the Compton peak center is given by

$$E_{2\theta} = 12.40\ \text{keV}/(\lambda_0 + 0.0485\sin^2\theta) \tag{5}$$

for λ_0 given in angstroms. The equation is presented with numerical values for the constants hc and $2h/mc$ to stress the importance of λ_0 in the angular dependence of $E_{2\theta}$. For ^{241}Am γ rays, $E_0 = 60$ keV ($\lambda_0 = 0.208$ Å), λ_0 dominates the denominator. For ^{88}Y γ rays, $E_0 = 1836$ keV ($\lambda_0 = 0.00675$ Å), and the angular dependence of $\Delta E_{2\theta}$ is more pronounced. By considering

$$\Delta E_{2\theta}(\delta)/\Delta E_D = (E_{2\theta} - E_{2\theta+\delta})/(\sigma^2_{\text{noise}} + \alpha E_{2\theta})^{1/2} , \tag{6}$$

we standardize the values for the various sources and show the relative significance of angular broadening and detector resolution broadening as a function of E_0 and scattering angle. The calculated results for $\delta = 1°$ in 2θ are presented in Fig. 2 in

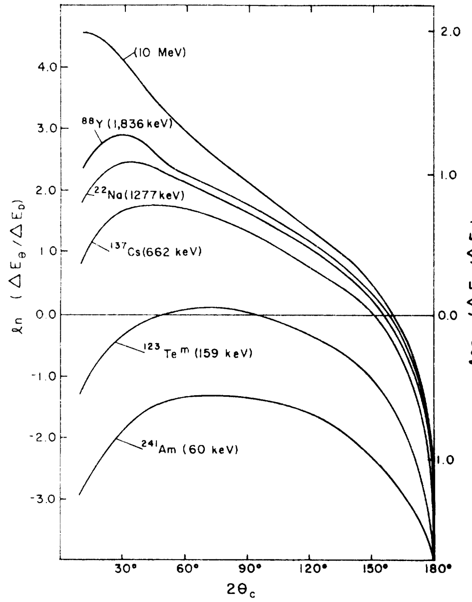

FIG. 2. Ratio of angular broadening to detector broadening, $\Delta E_\theta/\Delta E_D$, as a function of scattering angle. A logarithmic scale is used to include a range of incident energies and to show the effects near 180 ° as well as at low-scattering angles.

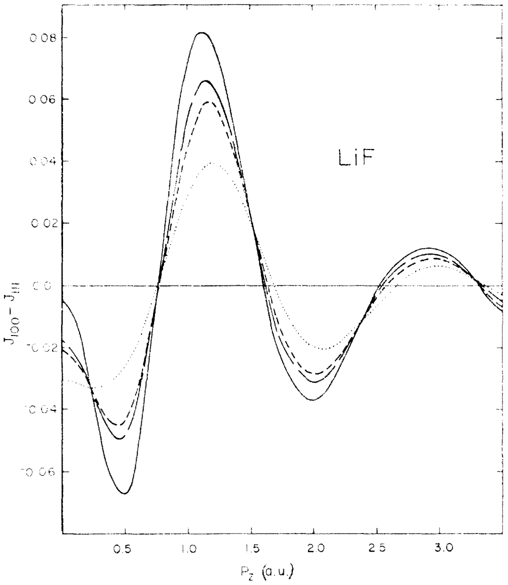

FIG. 3. Theoretical and resolution-broadened J_{100}-J_{111} anisotropy for LiF. Solid line: theoretical anisotropy; long-dashed line: broadened by $E_0 = 500$-keV resolution function; short-dashed line: broadened by the $E_0 = 160$-keV resolution function; dotted line: broadened by the $E_0 = 60$-keV resolution function.

which a logarithmic scale has been used to adequately represent the different cases. In particular we would point out that for ^{88}Y γ rays scattered at $2\theta \approx 50°$, for which the relative detector resolution is improved by approximately 30% over that of ^{123}Te^m at 180°,[6] the angular broadening over the narrow 1° range is more than an order of magnitude greater than the detector resolution broadening. In using 10-MeV photons with $2\theta = 40°$ to gain a relative detector resolution twice as good as that for ^{123}Te^m at 180°, one would incur angular broadening for a 1° range of 2θ which would be 38 times as broad as the detector broadening. For $E_0 > 500$ keV, ΔP_D may be improved for low-scattering angles, but the angular broadening prohibits experiments at these low angles unless very narrow collimation is used with a significant and probably prohibitive decrease in counting rates.

For the lower-energy γ-ray sources, the angular broadening for a 1° angular range is much smaller than the detector resolution width for $2\theta \gtrsim 170°$. Larger angular ranges can be employed with these sources to increase count rates. With higher-energy γ rays, angular broadening would contribute a significant amount to the total instrumental broadening of the Compton peak, and narrower collimation would be required for the same total resolution.

RESOLUTION EFFECTS IN COMPTON-PROFILE ANISOTROPY MEASUREMENTS

How significant are the differences in resolution for different γ-ray sources? Figure 3 shows our theoretical $J_{100} - J_{111}$ anisotropy for LiF,[13] and the results of broadening the theoretical curve with the instrumental broadening functions (assumed Gaussian) corresponding to experiments using 60-, 160-, and 500-keV γ rays scattered at 180°. This theoretical curve, when broadened with the actual resolution function of Berggren, Martino, Eisenberger and Reed,[14] fits their experimental results well,[13] so it represents a typical crystalline anisotropy , one which is also comparable in magnitude and in sharpness to those observed in Cu and Ni simple-crystal measurements.[15]

Although the sharp peak in the anisotropy at $p_z = 0.0$ would be nearly obscured by instrumental broadening for a 60-keV experiment, the general nature at the anisotropy curve including curve crossings and peak positions would be evident in measurements using 60-keV γ rays from an ^{241}Am source. Much better resolution can be obtained by using a ^{123}Te^m source with 159-keV γ rays. Such an experiment can better resolve sharp peaks in the anisotropy such as that at the origin. The curve crossings, peak positions, and peak intensities are also more adequately resolved. Going to higher-incident photon energies ($200 < E_0 \lesssim 600$ keV) does produce a slight improvement in the relative resolution, but even with $E_0 = 500$ keV, there is little change in the relative resolution and in the resolution-broadened theoretical curve, when compared to those obtained for 160-keV photons from ^{123}Te^m.

OPTIMUM γ-RAY SOURCE ENERGIES

Although the resolution of γ-ray Compton-profile measurements improves with an increase in incident photon energy up to $E_0 \sim 600$ keV, the slight improvement in resolution possible for using $E_9 > 200$ keV does not produce an appreciable change in the accuracy of Compton-profile anisotropy measurements. Greater counting rates may be obtainable with high E_0 due to the lower photoelectric absorption, particularly in high-atomic-number samples, but the resolution difference is not significant. For still higher energies, the experimental resolution at $2\theta = 180°$ actually decreases with an increase in E_0, the limit as $E_0 \rightarrow \infty$ of ΔP_D being slightly greater than 0.5 a.u. Although improved detector resolution ΔP_D is possible for high-energy γ rays ($\gtrsim 2$ MeV) scattered at low angles,[6] the angular broadening for such cases will dominate the experimental broadening unless extreme collimation is used at a great loss in counting rates.

Thus optimum experimental conditions will involve incident photons in the energy range of 150 to 600 keV scattered at angles near 180°. Lower E_0 degrades the relative detector resolution and for higher energies the angular broadening becomes significant even near 180° unless very narrow collimation is used. Within the incident photon energy range above, the relative detector resolution is not of principal importance. Selection of an optimum γ-ray source should be based on intensity factors such as photoelectric absorption, detector efficiency, and acceptable angular range.

---

*Research supported by the U.S. Energy Research and Development Administration.

†Present address: Chemical Engineering Div. Argonne National Laboratory, Argonne, Ill. 60439.

[1] J. Felsteiner, R. Fox and S. Kahane, Phys. Lett. A 33, 442 (1970).

[2] B. W. Batterman, W. R. McIntire, H. Cole, and F. W. Chambers, American Crystallographic Association Meeting, Ames, Iowa, 1971 (unpublished).

[3] W. R. McIntire, Pittsburgh Diffraction Conference, 1971 (unpublished).

[4] T. Fukamachi and S. Hosoya, Phys. Lett. A 38, 341 (1972).

[5] P. Eisenberger and W. A. Reed, Phys. Rev. A 5, 2085 (1972).

[6] T. Fukamachi and S. Hosoya, Phys. Status Solidi A 15, 629 (1973).

[7] M. Cooper and B. Williams, Philos. Mag. 25, 1499 (1972).

[8] W. R. McIntire and B. W. Batterman, Phys. Status Solidi B 63, 621 (1974).

[9] T. Paakkari, S. Maninen, O. Inkinen, and E. Liukkonen, Phys. Rev. B 6, 351 (1972).

[10] T. Fukamachi and S. Hosoya, Phys. Lett. A 41, 416 (1972).

[11] P. Pattison, M. Cooper and J. R. Schneider (unpublished).

[12] W. C. Phillips and R. J. Weiss, Phys. Rev. 171, 790 (1968).

[13] B. I. Ramirez, W. R. McIntire, and R. L. Matcha, J. Chem. Phys. 65, 906 (1976).

[14] K.-F. Berggren, F. Martino, P. Eisenberger, and W. A. Reed, Phys. Rev. B 13, 2296 (1976).

[15] P. Eisenberger and W. A. Reed, Phys. Rev. B 9, 3242 (1974).