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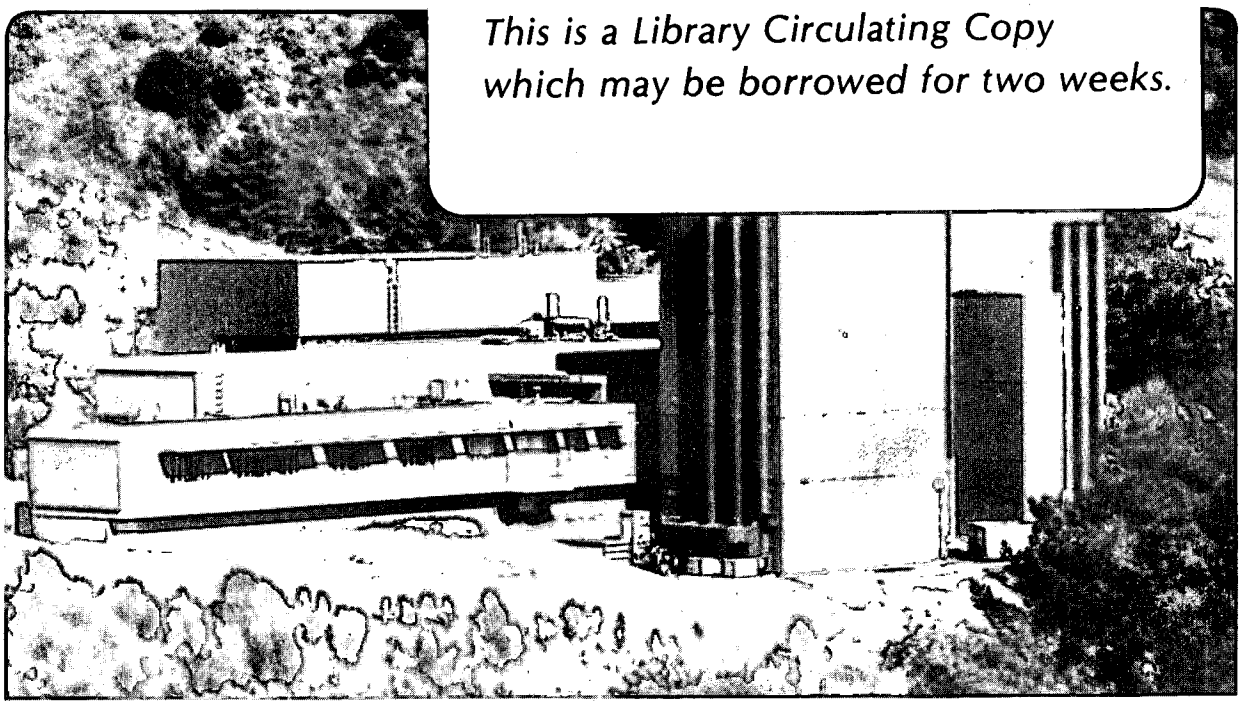

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PLASMON LINESHAPE ANALYSIS IN EELS OF SEMICONDUCTORS

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Many materials display plasmon peaks in their low-loss EELS spectra. The plasmon peak shape, energy, and linewidth are characteristic of each material and are sensitive to the outer-shell electron density and details of the electronic band and energy-level structures. As these properties are a function not only of the composition but also the structure and chemistry of a sample, plasmon spectroscopy can potentially become a materials characterization tool which goes beyond the elemental analyses provided by EDXS and ionization-edge EELS. However, analysis of plasmon spectra requires considerably more sophistication than either of the aforementioned techniques due to the possibility of overlapping spectrum features, the prevalence of plural scattering, and the difficulty in detecting and characterizing the often subtle differences between the plasmon spectra of similar materials. As yet, no systematic approach to plasmon analysis analogous to that available commercially for EDXS or EELS core-edge analysis has been developed. We present here an approach which, for the simple case of semiconductors, makes some progress in this direction.

The main features of the proposed method are 1)elimination of plural scattering via Fourier-log deconvolution and 2)use of a theoretical plasmon lineshape model.[1] The theoretical model is well suited for least-squares (χ^2) fitting to measured single-loss profiles and has the following functional form with 3 adjustable parameters:

$$I_p(E) = \frac{CE\ln(2E_0/E)}{(E_p^2-E^2)^2 + \Gamma_p^2 E^2}$$

where E is the energy loss, E_0 is the incident beam energy, and C, E_p, and Γ_p are the adjustable parameters related to the plasmon peak intensity, energy, and linewidth (FWHM), respectively. χ^2-fits of this model to the plasmon spectra of four different semiconductors are shown in Fig.1. The correspondence between model and data is clearly quite good. Excess counts in the data on the low side of the plasmon peak are due to surface plasmon excitations neglected in the above model. On the high side, d-shell transitions contribute distinct features in the spectra of GaAs, InP, and InAs. Fitted values of the critical parameters E_p and Γ_p appear in Table 1. In order to avoid the influence of the finite spectrum resolution on the measured plasmon linewidth, the model is convoluted with a measured zero-loss peak before comparison with the measured spectrum to obtain χ^2. Although the theoretical basis of this analytical procedure assumes angle-integrated (image-mode) spectra, it has been found to give good results for collection semi-angles as small as 6-7mrad for specimens less than 1 inelastic mean free path in thickness.

Use of a theoretical lineshape model enhances plasmon analysis in two ways. First, since the fitting procedure is based upon the statistically well-defined χ^2 minimization procedure, the values of the lineshape parameters E_p and Γ_p output by the fit represent the most accurate and precise values allowed by statistics.[2] In fact, assuming suitable precision in the calibration of the spectrum energy scale, the plasmon energy and linewidth can, in principle, be measured to a precision better than either the energy resolution or energy increment per channel of the spectrum (Table 1). The precision of the numerical results allows subtle differences in plasmon energy or damping (via linewidth) due to chemical or structural distinctions between two material samples to be reliably detected. In addition to yielding the most precise possible characterization of the plasmon lineshape, comparison of measured plasmon EELS spectra with the above model can aid in the identification of additional contributions to the low-loss EELS spectrum besides the main plasmon contribution. For example, figure 2a shows the single-scattering profile measured from an AlAs sample which had been partially oxidized by exposure to atmospheric conditions. The best χ^2 fit of the above lineshape model to the main peak of the spectrum (13-18eV) is given by the dotted curve. An additional energy-loss mechanism appears to contribute counts to the high side of the main plasmon peak. Assuming plasmon excitations in the oxide layer contribute these counts (AlAs has no d-shell transitions at such low energies), a 2-plasmon model, formed by summing two terms of the above form and comprising six adjustable parameters, was matched to the data. A near-perfect fit results (Fig. 2b). Although E_p=23-26eV and Γ_p=10-20eV for

Al_2O_3, the lineshape parameters found for the secondary peak (Fig. 2c), E_p=19.3eV and Γ_p=8eV, are consistent with previous findings of incomplete Al oxidation in AlAs exposed to O_2.[3] Hence, a true deconvolution of overlapping plasmon signals, analogous to Gaussian deconvolution applied to x-ray peaks, can be achieved with this analytical approach.[4]

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4. Support of the Division of Materials Sciences, Office of Basic Energy Sciences, U.S. Department of Energy under contract DE-AC03-76-SF00098 is gratefully acknowledged.

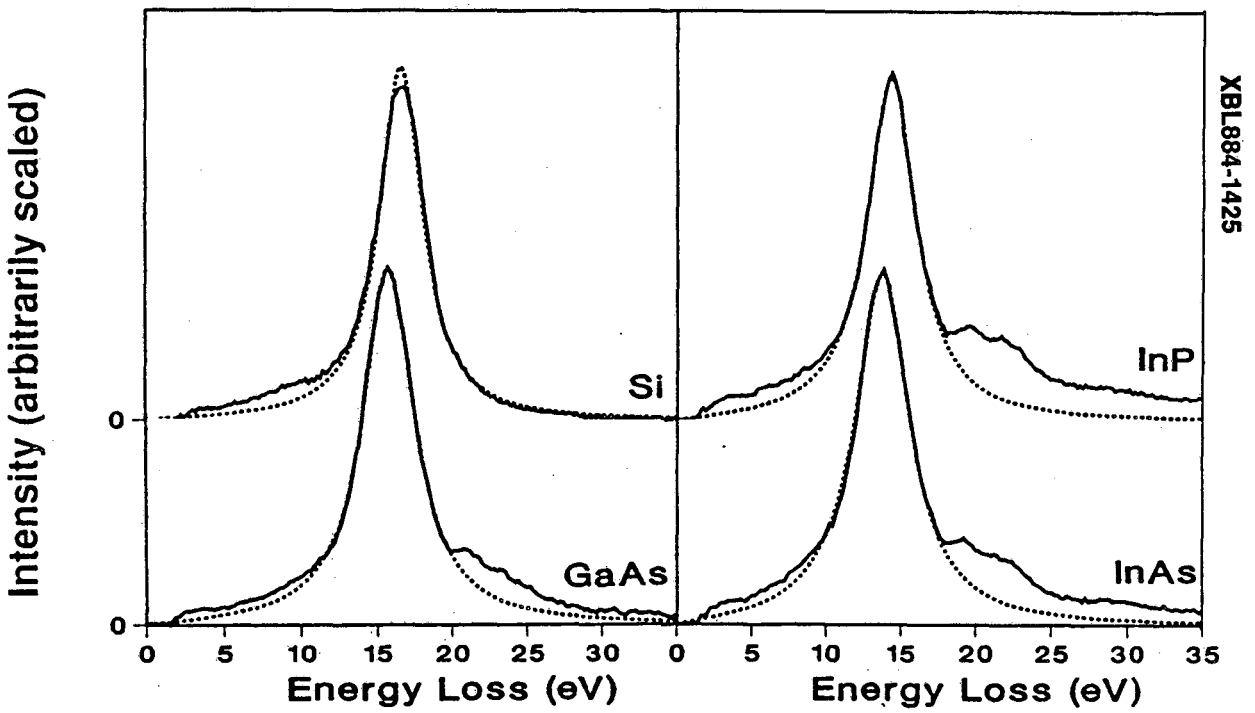

FIG. 1.--Comparison of measured single-loss profiles (solid) and plasmon lineshape models obtained from χ^2 fits (dotted) for Si, InP, GaAs, and InAs.

	E_p (±.04eV)	Γ_p (±.1eV)
Si	16.82	3.25
GaAs	16.09	4.0
InP	14.65	4.1
InAs	14.08	4.1
AlAs	15.81	3.7

TABLE 1.--Lineshape parameter values for various semiconductors obtained from χ^2 fit of lineshape model. Energy scale calibration based on Si $L_{2,3}$=99.8eV.

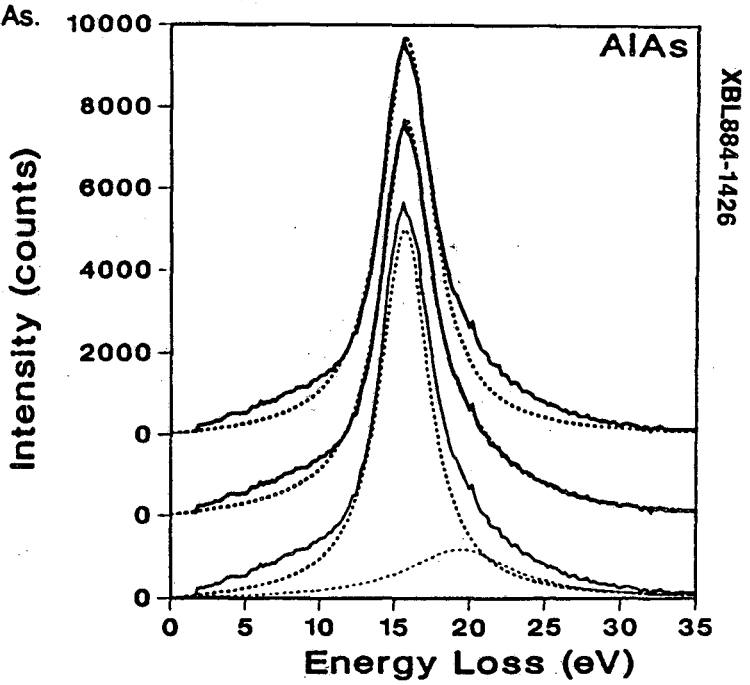

FIG. 2.--AlAs exposed to air. Single-loss profile (solid) compared with a)1-plasmon model, b)2-plasmon model, and c)individual components of b) (dotted).

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