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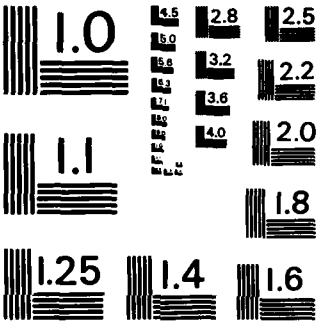

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The C KVV Auger lineshape of graphite is quantitatively interpreted. Localization, static and dynamic screening effects, and intrinsic plasmon loss effects are discussed in the context of the theoretical model and found to contribute significantly to the lineshape.

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THE AUGER LINESHAPE OF GRAPHITE

By

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SUMMARY ABSTRACT -- The Auger Lineshape of Graphite

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The Auger lineshape of graphite has been the subject of considerable recent study (see ref. 1 and references therein). Although much of this attention has been due to graphite's novel intercalation properties, the graphite Auger spectrum is itself of interest as a model for studying initial-state, core-hole screening and final-state, hole-hole correlation effects in aromatic systems.

The first attempt at obtaining an accurate C(KVV) lineshape for graphite was reported by Smith and Levinson [2]. An attempt at quantitatively interpreting their lineshape was recently reported by Murday, et al. [3]. The major conclusion of this work was that the Auger spectrum was well characterized by a simple self-fold of the graphite density of states (DOS) which would imply a small and uniform value of the final state hole-hole repulsion energy for all graphite transitions and a negligible contribution from static and dynamic screening effects.

We have obtained the Auger spectrum for POCO graphite from data taken in two separate laboratories and on three

different types of electron-energy analyzers. These separate data were independently corrected for the effects of secondary-electron background and extrinsic losses. A typical spectrum is shown as curve a in Fig. 1. Considerable care was taken to ensure that the absolute energy scale was accurate and that the lineshape is as free as possible from experimental and data-reduction artifacts. This spectrum shows significant differences from that reported by Smith and Levinson [2] which we attribute to an improper loss deconvolution of their experimental data [1]. This improper data handling resulted in incorrect assumptions in the subsequent theoretical analysis of Murday, et al. [3].

In Fig. 1, our C(KVV) lineshape (curve a) is compared to a model (curve b) which consists of the self-convolution of the graphite one-electron density of states including atomic values for the symmetry-determined Auger matrix elements and assuming no initial-state screening and noninteracting final-state holes. The one-electron partial DOS (σ_s, σ_p, π_p) were determined empirically [3] from x-ray emission spectra, x-ray photoemission spectra, and an assumed electron configuration of $sp^2\pi$. The model lineshape differs considerably from that of the experiment with intensity missing in the model function at both the high- and low-energy ends of the spectrum and there are significant differences in relative intensity throughout the main body of the line.

To characterize these discrepancies, we have considered both the static and dynamic aspects of initial- and final-state screening which are included in the model lineshape of Fig. 1c. The static polarization effect of initial-state screening has a negligible influence on the lineshape. However, valence electron shake up into the core excitonic level places charge in an energy region where very little exists in ground-state graphite giving rise to significant new intensity in the Auger lineshape just below the Fermi level. Modeling the dynamic Auger effect by the inclusion of a delta-function DOS at the Fermi energy and assuming that the valence/core excitonic electron participates in the Auger process along with a valence electron (Fig. 1g), results in a dramatic improvement between the measured (Fig. 1a) and model (Fig. 1c) lineshapes in the high-energy region.

The distorting effect on the predicted lineshape resulting from the hole-hole interaction in the Auger final state has been modeled using the Cini expression [4,5]. We have assumed that the empty portions of the σ and π bands are separated sufficiently from each other and from the filled portions to permit the use of the Cini filled-band formalism by including screened hole-hole repulsion parameters for the $\sigma^*\sigma$ (Fig. 1d), $\sigma^*\pi$ (Fig. 1e), and $\pi^*\pi$ (Fig. 1f) contributions. Under these assumptions we find effective hole-hole interaction energies of 2.2 eV for two holes in the σ band, 1.5 eV for one hole each in the σ and π bands, and 0.6 eV for both holes in the π band. The application of the Cini expression results in considerable improvement of the model lineshape of Fig. 1c in the region below the principal maximum.

The final area of disagreement in the model lineshape consists of a shoulder-like feature on the low-energy side of the Auger line centered ~240 eV which is not accounted for by localization effects. We suggest, on the basis of more recent work by Cini and D'Andrea [6], that this structure is due to a plasmon effect intrinsic to the two-hole final state in the Auger process. The adequate characterization of this feature will undoubtedly require a theoretical model which includes multiple, partially-filled bands with the inclusion of dynamical final-state effects. A full account of the present work has been submitted elsewhere [1].

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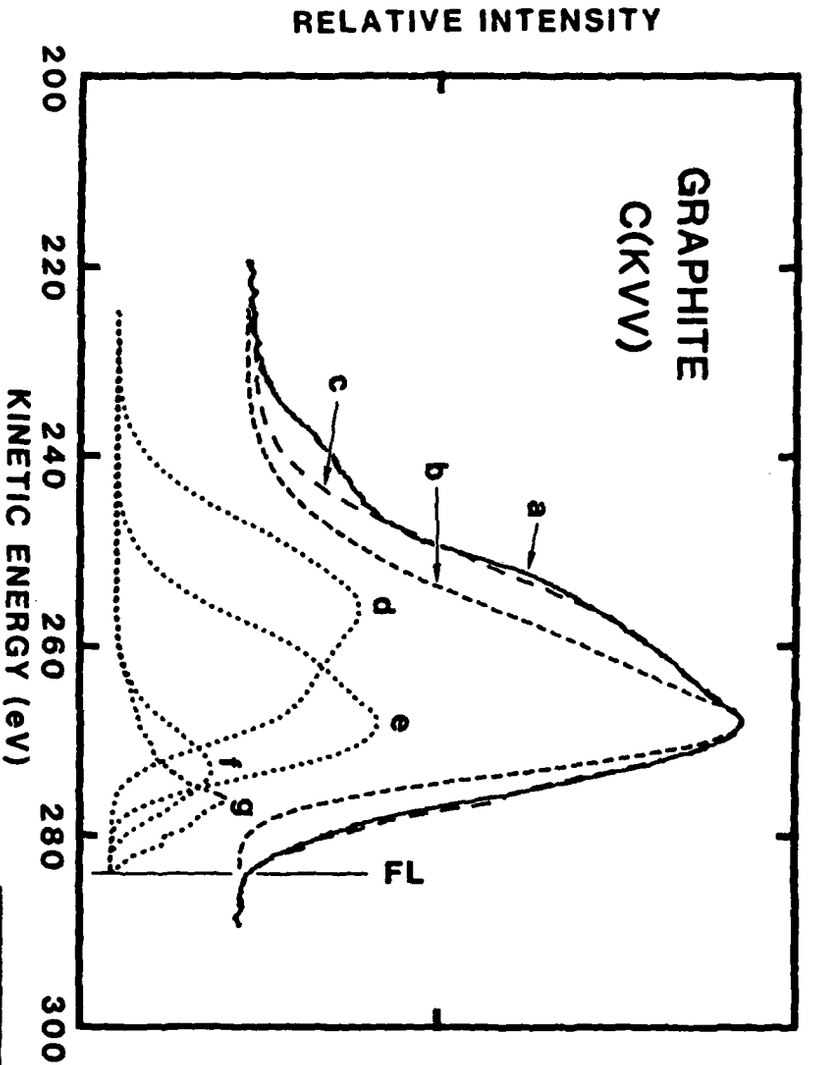
Figure Caption

Figure 1. A comparison of the experimental C(KVV) Auger lineshape (curve a) of POCO graphite, the model lineshape (curve b) using the one-electron approximation with no hole-hole interaction, and the model lineshape (curve c) which includes initial-state screening, the Fermi level valence/core excitonic state, and the hole-hole interaction distortion calculated through the use of the Cini expression [4,5]. The contributions to the model lineshape of curve c from the σ*σ, σ*π, and π*π self-folds, all distorted with the Cini expression, are shown as curves d, e, and f, respectively, and the contribution of the valence/core excitonic state is shown as curve g. Curve c is the sum of d, e, f, and g. The Fermi level (FL), after the addition of the C(1s) binding energy (284.6 eV), is also shown.



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