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Photoemission Studies of NaBr†

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The recently calculated densities of states for the NaBr valence and conduction bands are compared with the observed energy distributions of photoemitted electrons. The effective width of the observed structure is found to be in agreement with the calculations.

It has been shown recently by Kunz and Lipari[1] that the density of electronic states of the valence and conduction bands can be calculated for NaBr. The results of the calculations were compared with those of optical and x-ray-emission studies[2,3] and were found to be in reasonable agreement with experiment. However, it was apparent that further comparison could be made if more experimental information on the density of states of NaBr were available. In this note, we present photoelectron spectra for a more detailed comparison with the calculations. With optical excitation of sufficiently high energies, we have observed energy distributions of photoemitted electrons which show structures that are characteristic of the valence and conduction bands of NaBr.

The photoemission measurements were made on evaporated NaBr films with dispersed uv radiation of energy above 12 eV. In order to avoid contamination of the sample, the films were prepared in a vacuum of 10^{-7}–10^{-8} Torr and measurements were performed *in situ* immediately after evaporation. The dispersed radiation was provided by a vacuum-uv monochromator using a helium-continuum source. The ac method[4] was used to obtain the energy distributions of photoemitted electrons. The quantum yield of NaBr has been measured at photon energies between 12 and 23 eV,[5] but the energy distribution of the photoelectrons from NaBr had not been investigated in this spectral region.

The observed energy distributions of the photoemitted electrons for photon energies above 14 eV are shown in Fig. 1. The cutoff on the left represents the vacuum level, which is 8.0±0.1 eV above

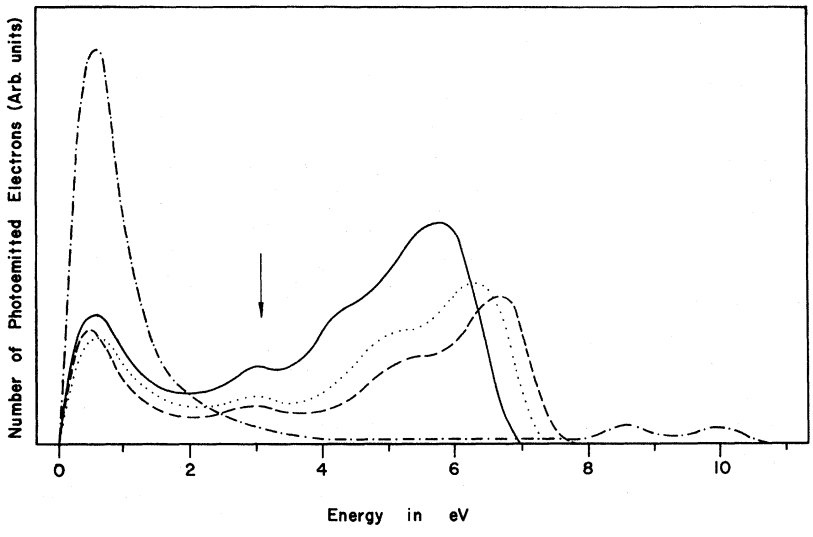

FIG. 1. Energy distributions of photoemitted electrons from NaBr for different photon energies: solid curve, 14.8 eV; dotted curve, 15.3 eV; dashed curve, 15.9 eV; dot-dashed curve, 19.1 eV. The vacuum level is located at zero energy. A conduction-band structure is shown at approximately 3 eV above the vacuum level.

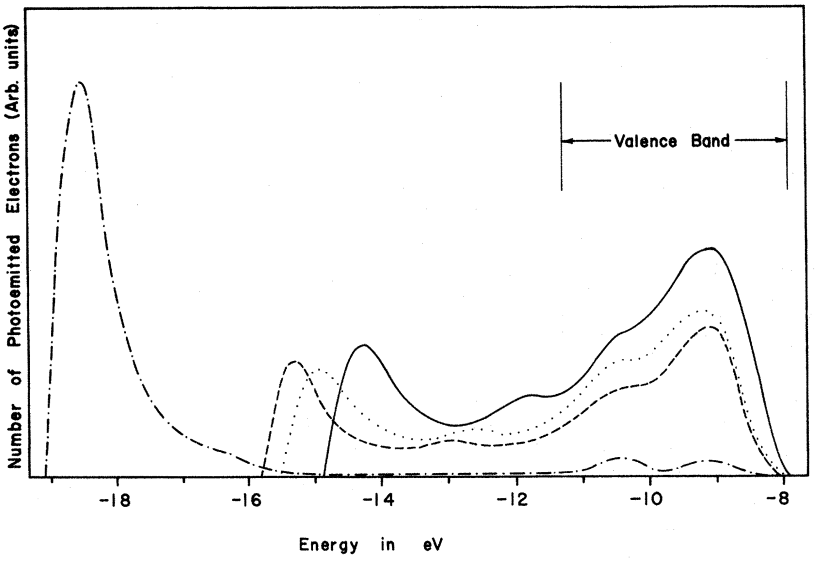

FIG. 2. The structure in the density of states for the valance band of NaBr is illustrated by the energy distributions of the photoelectrons. The distribution curves are plotted with the cutoff on the right located at the highest occupied states below the vacuum level. The curves are for the same photon energies shown in Fig. 1.

the valence band. It can be seen that there is a small peak in the distribution which does not shift with increasing photon energy. We interpret this peak as a high density of states in the conduction band of NaBr.[6] The effective width and energy of this structure 3.0 ± 0.2 eV above the vacuum level agree with the calculations of Kunz and Lipari.[1] The distribution curves also show high-energy peaks which move in energy by an amount equal to the increase in photon energy. These peaks can be attributed to electrons optically excited from the high density of states of the $4p$ valence band of NaBr. Since the high-energy peaks shift according to the equal-increment rule, the predominant transitions from the valence band of NaBr are probably nondirect.[6,7] The three peaks associated with the valence- and conduction-band structure are just resolved for a photon energy of 14.8 eV. This demonstrates the importance of probing the electronic states with photons of suitable energies.

In order to illustrate the structure of the valence band, the distribution curves of Fig. 1 are plotted with the energy scale of each distribution shifted according to the difference of photon energy. As shown in Fig. 2, the cutoff on the right represents the highest occupied states below the vacuum level. Relatively high optical densities of states are observed at 1.2 ± 0.2 and 2.5 ± 0.2 eV below the top of the valence band. The effective base width of the valence band is found to be 3.5 ± 0.5 eV, which is in good agreement with the calculated results. However, the separation of the observed peaks appears to be smaller than the calculated value of about 2 eV.[1]

It should be mentioned that the low-energy peak near the vacuum level is due to scattered electrons. The enhancement of this peak at photon energies above 16 eV is associated with the suppression of the high-energy peaks. This change in relative height is due to inelastic collisions.[8,9]

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