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2 HAMBURG 52 · NOTKESTIEG 1

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The Li K absorption edge was measured with yield spectroscopy at liquid nitrogen temperature. The broad feature hitherto considered to be the edge is shown to be a combination of a sharp absorption edge corresponding to a 0.18 eV wide Li K core level and a rising density of states at the Fermi level.

The shape of the Li K absorption edge has been extensively discussed since it was first observed in 1937.[1] The theoretical interest was caused by the strong deviation of both the Li K emission and absorption edge from the expected sharp Fermi step. Several approaches to the Li K edge problem have been made[2-7] among which the final state interaction theory put forward by Mahan, Nozieres and de Dominicis (MND) is presumably the most attractive one.[3,4]

This many body theory predicted a rounding of the Li K edge and thus seemed to explain both the similarity of emission and absorption edges and their considerable width. The theory has recently been critizized by Dow and co-workers in a series of papers.[7-10] Tests of the theory (dependence of the edge shape on momentum transfer[11] and temperature[12]) have been performed and did not follow the predictions, thus casting doubt on the explanation of the edge shapes by the MND final state interaction theory.

An alternative to the MND theory is a simple one electron band theory. The transition density for Li K absorption was calculated in great detail by McAllister.[5] This density is virtually a product of the matrix element and the p-symmetric part of the conduction states, which is sampled by the absorption process from the s-like inner shell. Because of the hitherto observed broad structureless absorption threshold[1,11,12,13] this one electron model appeared to be inappropriate. It was maintained by Dow et al.[7] that in the framework of the one electron theory the observed threshold shape could only be fitted under the assumption of an extreme 1s-core level width of about 0.5 eV. An electron phonon interaction mechanism which would produce such a width was proposed,[7] exact calculations, however, have not yet been reported. It is shown in this letter that the Li K absorption edge when observed at liquid nitrogen temperature (LNT) has a shape, which allows for a straightforward single electron explanation.

Measurements of the partial photoyield of massive specimens of Li were performed under UHV conditions. The photoyield was shown to be proportional to the absorption coefficient in the vacuum ultraviolet except for the shape of a smoothly varying background.[14] Synchrotron radiation and a special monochromator with a fixed excit beam[15] served as a light source. More details are given in Ref. 12. The only change in the experimental set up described there was a modification of the sample holder permitting measurements at LNT.

Figure 1 shows the Li K absorption edge at LNT, a model potential density of states (DOS) calculation by Shaw and Smith[16] and McAllister's calculation[5] of the transition density to p-symmetric final states. The Fermi levels of both calculations have been adjusted. In the relevant energy intervall the transition density should be proportional to the p-symmetric DOS since a possible small variation of the matrix element can be neglected. The predominantly p-symmetric character of the eigenfunction near the Brillouin zone boundary[18] is reflected by the excellent agreement between model potential DOS and experiment concerning the positions of the extrema.

Figure 2 shows one of the original spectra which led to the interpretation of the Li K absorption threshold given here. The results have very recently been confirmed by total yield measurements.[19] Obviously there is a steep rise at the onset followed by a significant decrease of ascent. The bend observed at 55 eV photon energy cannot be explained by the MND theory[3,4] or by core level broadening[7] but it finds a suggestive explanation in the shape of the transition density[5] and the model potential DOS.[16] It is therefore argued that the Li K absorption edge extends from the onset of absorption to the bend and is followed by DOS structure.

Assuming tentatively a quadratic superposition of the resolution function of the monochromator ($\sim$ 0.11 eV FWHM at 55 eV) and contributions to the edge width inherent in Li a Li K core level width of about 0.18 eV is obtained. A width of this order of magnitude can be explained by Auger lifetime broadening; a lower bound of this effect was calculated to be 0.13 eV.[20]

The experimental results demonstrate that the Li K absorption edge at LNT can be interpreted entirely in terms of one electron band theory. The width of the edge is in qualitative agreement with calculations of lifetime broadening due to the Auger KVV decay of the 1s core hole. Core level broadening caused by lattice relaxation (∿0.06 eV at LNT) might be involved.[6] The assumption of a large core level width due to indirect electron phonen interaction[7] is obviously unnecessary. The observed temperature broadening[12] has to be reinterpreted in the light of this new result and will be discussed elsewhere.[19] Edge rounding due to the MND final state interaction theory[3,4] is not observed and a possible contribution to the edge width caused by this many body effect must have a value far less than 0.1 eV. Such a small influence of the many body effect on the edge width is consistent with OPW-calculations by Longe [21] based on this theory. It is furthermore in agreement with recently published experimental results on the Cs N_5 edge, which also did not exhibit edge rounding.[22]

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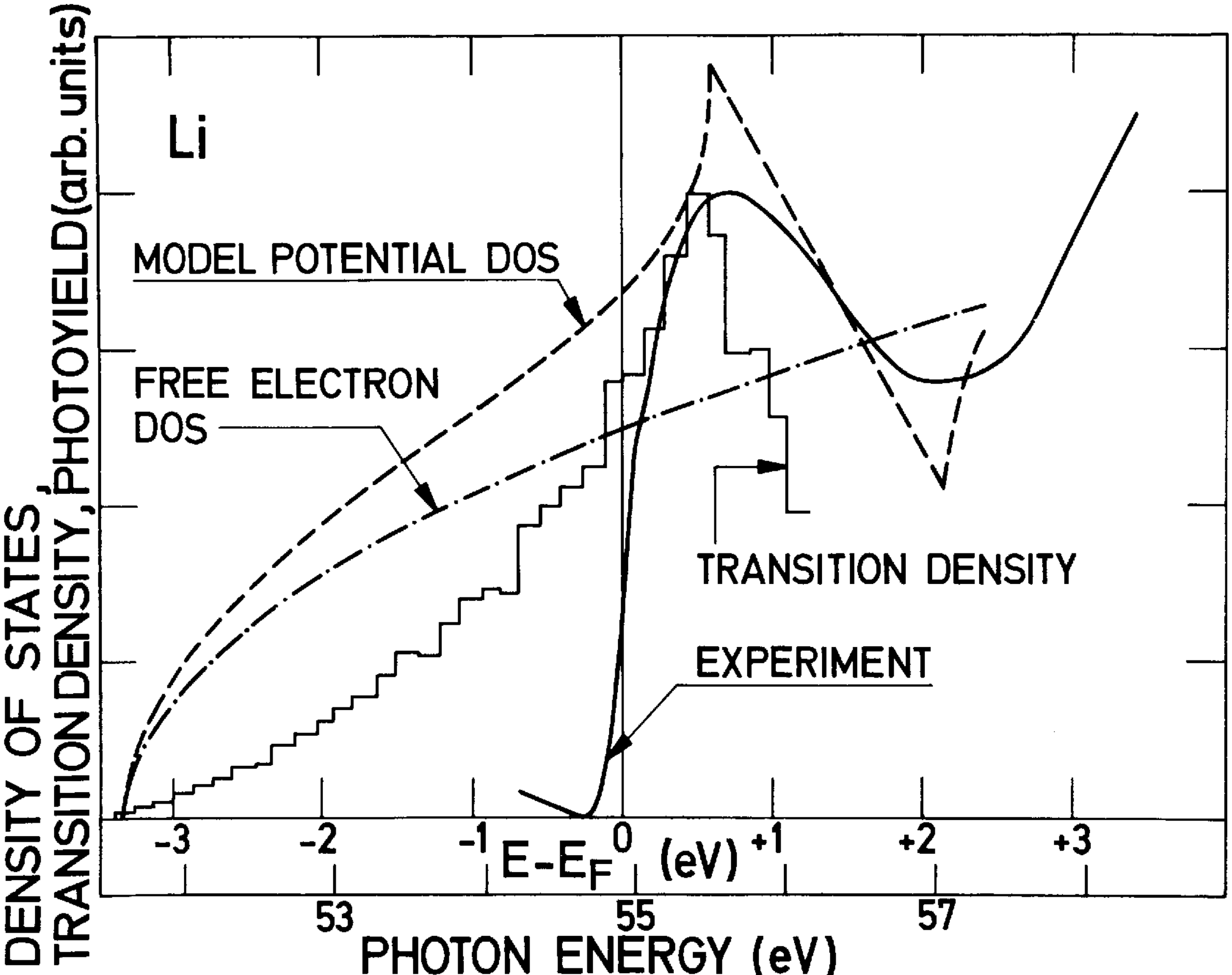
Figure Captions

Fig. 1 Li K absorption edge measured with yield spectroscopy at LNT. Included is a) The free electron DOS and the model potential DOS calculated by Shaw and Smith.[16] The 3.32 eV Fermi energy was reported by Lee[17] and differs from the free electron value by a factor of 0.856.[16] b) The transition density to p-symmetric final states as calculated by McAllister.[5]

Fig. 2 Li K absorption edge at LNT, original x-y recorder trace obtained with counting technique and ratemeters, the time constant was 0.3 sec.



Li
MODEL POTENTIAL DOS
FREE ELECTRON DOS
TRANSITION DENSITY
EXPERIMENT
DENSITY OF STATES, TRANSITION DENSITY, PHOTOYIELD (arb. units)
-3
-2
-1
0
+1
+2
+3
E-E_F (eV)
53
55
57
PHOTON ENERGY (eV)

Fig. 1

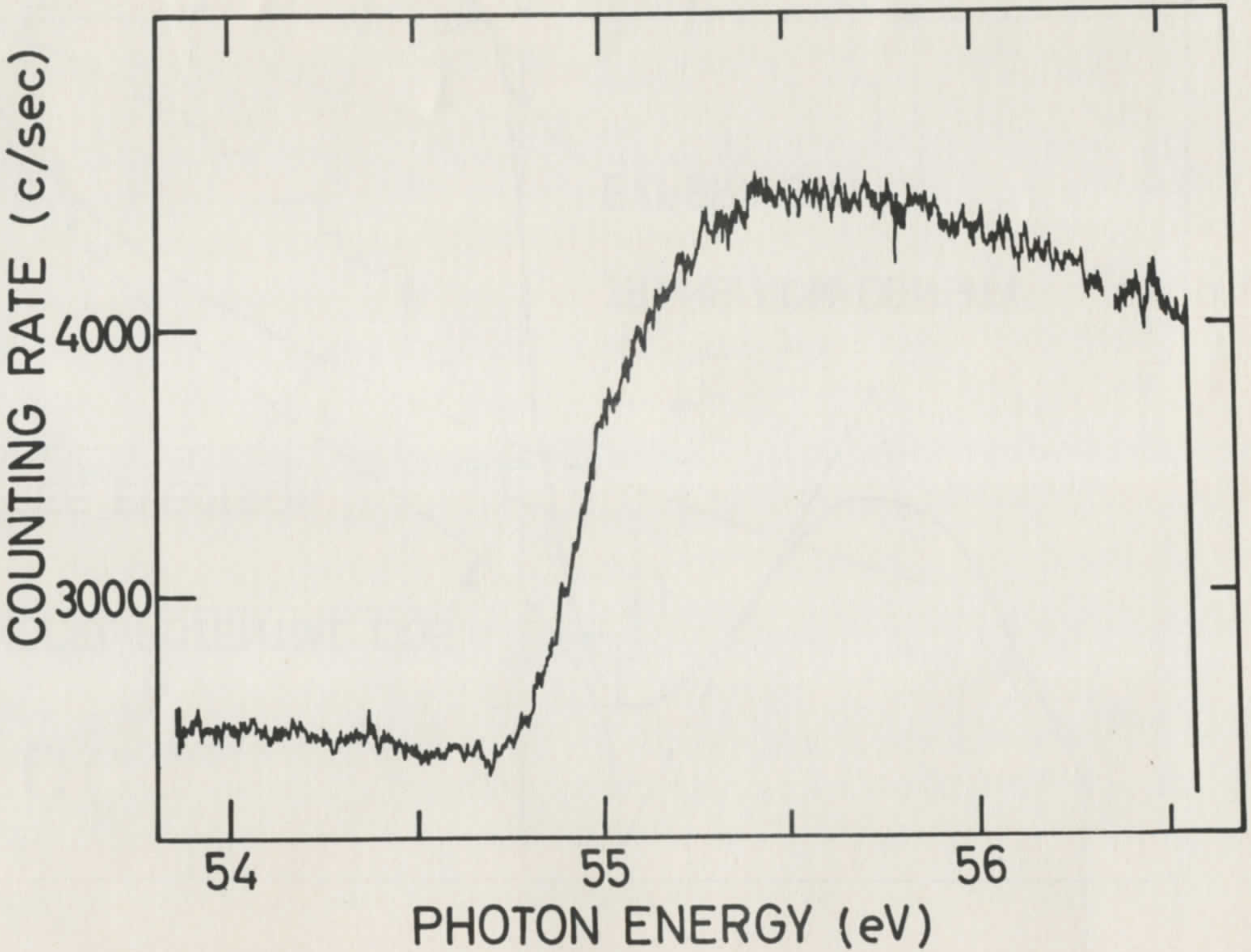


Fig. 2