

1. Characteristic energy losses in Al. (a) Electron reflection experiment; photoelectron experiment (upper curve $\times 3$).

L' electron with kinetic energy $E(K-LL')$. The energy conservation law thus gives:

$$E(K) - E(L) = E^*(L') + E(K - LL') \quad (1)$$

where $E(K)$ and $E(L)$ are respectively the binding energies of the K and L electrons, and $E^*(L')$ is the binding energy (in the so-

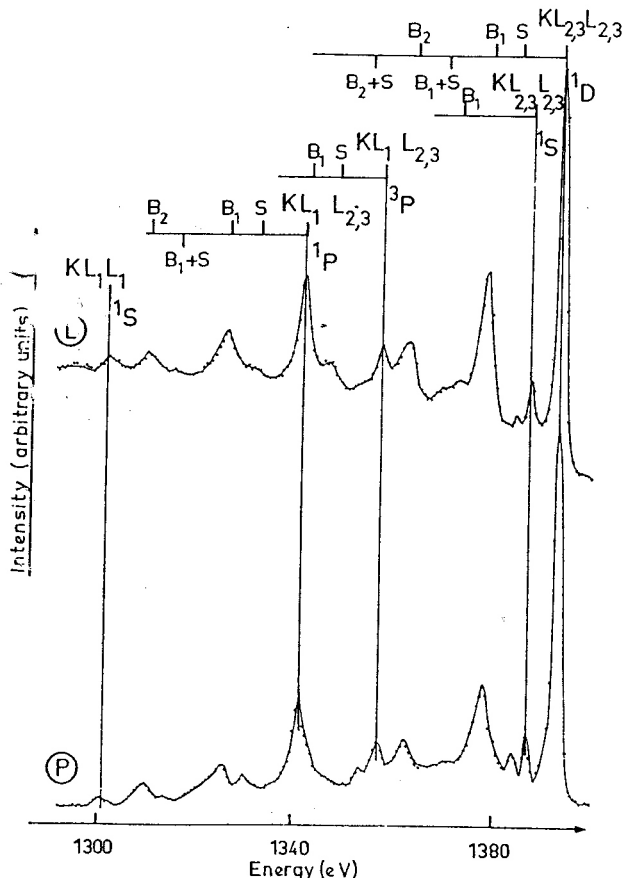


Fig. 2. Al *K*-LL Auger spectra: photon induced (L) and electron induced (P).

Table I. *Al K-LL Auger electron kinetic energies (referenced to the Fermi level; values in eV)*

Auger line	E (L lab)	E (P lab)	E (theory)
$K-L_{2,3}L_{2,3} (^3P)$	Not obs.	Not obs.	(1 398.1) ^a
$K-L_{2,3}L_{2,3} (^1D)$	1 393.2	1 393.1	1 393.5
$K-L_{2,3}L_{2,3} (^1S)$	1 387.2	1 387.1	1 386.6
$K-L_1L_{2,3} (^3P)$	1 357.2	1 357.2	1 358.5
$K-L_1L_{2,3} (^1P)$	1 341.4	1 341.6	1 342.3
$K-L_1L_1 (^1S)$	1 302.0	1 302.6	1 304.0

^a Forbidden in *LS* coupling.

lid) of an L' electron in an atom with an L hole. So the kinetic energy of the Auger electron can be written as:

$$E(K-LL') = E(K) - E(L) - E^*(L') \quad (2)$$

The last contribution of this equation is given by:

$$E^*(L') = E(L') + C(LL'; T) - R \quad (3)$$

because $E^*(L')$ is different from the binding energy $E(L')$ by R , which takes into account the so-called electronic relaxation following the creation of the L hole, and by $C(LL'; T)$, the coupling energy between the L and L' holes in the final state T [7]. Finally, the K - LL' Auger electron kinetic energy is:

$$E(K-LL'; T) = E(K) - E(L) - E(L') - C(LL'; T) + R \quad (4)$$

The $C(LL'; T)$ term of eqs. (3) and (4) can be calculated in LS coupling [4] using the Slater-Condon integrals F^k and G^k given by a nonrelativistic Hartree-Fock calculation [3], the effect of relativity being weak in this atomic number region. The two-hole coupling energies for the different final states T are given in Table II.

The term R in eqs. (3) and (4) can be considered as the sum of an atomic relaxation energy R_a and of an extra-atomic relaxation energy R_o [7]:

$$R = R_a + R_e \quad (5)$$

R_a represents the reduction of the binding energy of an L' electron due to the relaxation which follows the creation of the L hole in a free atom. In the "equivalent core" approximation [13], R_a is twice the reorganization energy for the ionization of an L' electron [5]. This reorganization energy is the difference between the orbital energy given by a Hartree-Fock calculation and the true binding energy, which is the difference between the total energy of the atom and that of the ion. Gelius' calculations for Al [14] give $R_a \approx 12.2$ eV for a $2s$ electron and $R_a \approx 14.2$ eV for a $2p$ electron.

The L hole creation also modifies the electronic distribution in the solid. The relaxation energy R_e associated with this process can be evaluated using the excitonic model proposed by Ley

Table II. Two-hole coupling energies (eV) in Al K-LL Auger spectrum (LS coupling)

LL'	L_1L_1	$L_1L_{2,3}$	$L_{2,3}L_{2,3}$			
T	1S	1P	3P	1S	1D	$(^3P)^a$
$C(LL'; T)$	39.8	48.6	32.4	49.4	42.5	$(37.9)^a$

^a Forbidden in *LS* coupling.