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Modeling of the energy spectra of individual steps of the $L_{23} \rightarrow M_{2,3}M_{2,3} \rightarrow M_{2,3}VV \rightarrow VVVV$ cascade chain in MnO

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Abstract

Model calculations of the energy spectra of individual steps of the Mn $L_{23} \rightarrow M_{2,3}M_{2,3} \rightarrow M_{2,3}VV \rightarrow VVVV$ Auger cascade of MnO are described and the results compared with the results of recent Auger–Auger coincidence measurements. The spectra are modeled in terms of multiple integrations over products of the valence band density of states (VB-DOS) and an energy conserving delta function which includes hole–hole interactions in its argument. The formalism has applications to spectra of Auger transitions occurring in the later stages of Auger decay in which there are valence holes in the intermediate state preceding the transition and results in a lineshape which is proportional to an energy shifted function comprised of N_i correlation and $N_f - 1$ convolution operations over VB-DOS's where N_i and N_f are the number of valence holes in the initial and final states, respectively.

Keywords: Auger cascade; Auger lineshape; MnO

The spectra of electrons emitted as a result of Auger cascade processes [1] provide a window into the energetics of interacting multi-hole states. The Auger cascade process is initiated by a direct Auger transition that leaves one or more holes in an inner shell, this intermediate state then decays via one or more additional Auger transitions with final states that could have up to $N+1$ holes, where N is the total number of Auger transitions in the cascade.

Recent studies of the spectra associated with the later steps of the cascade chains initiated by the Mn LMV and LMM transitions in MnO, schematically shown in Fig. 1, have demonstrated that it is possible to separate out and measure individual contributions of specific Auger cascade chains in solids by using Auger–Auger coincidence spectroscopy (AACS) [2]. The AACS measurements indicated that the energy spectra associated with the Mn MVV transitions (i.e. $M_{2,3}M_{2,3} \rightarrow M_{2,3}VV$ and $M_{2,3}VV \rightarrow VVVV$) which follows the $L_{23} \rightarrow M_{2,3}M_{2,3}$ transition is ~3.5 eV broader [2,3] than the spectrum of the Mn MVV transition following the direct photoionization of an M hole. Furthermore, the AACS results indicate that the cascade-induced MVV spectra extend to energies ~10 eV above the direct MVV transitions. Details of the experimental measurements are provided elsewhere [2,3]. In this paper we provide details of a model which accounts for this additional width and energy in terms of the rearrangement of "spectator" hole(s) within the valence band. The model results in a lineshape for a transition with N_i valence holes in the initial state and N_f valence holes in the final state that is proportional to an energy shifted function comprised of N_i correlation and $N_f - 1$ convolution operations over identical valence band density of states (VB-DOS's). This formalism is a generalization of the model first used by Lander [4] for band-like CVV transitions and reduces in that case to the same energy shifted self-convolution (self-fold) of the VB-DOS as the original, more restricted theory [4].

The mechanism by which "spectator" hole rearrangement can lead to an increase in the full width of the spectra of the $M_{2,3}VV \rightarrow VVVV$ transition as compared to that of the direct $M \rightarrow VV$ transition can be understood qualitatively by referring to the schematic energy level diagram shown in Fig. 2. The hole states that lead to the lowest kinetic energy Auger electron correspond to an initial state in which the two holes are at the top of the valence band and a final state in which all four holes are at the bottom of the valence band. The states leading to the highest kinetic energy Auger emission correspond to an initial state in

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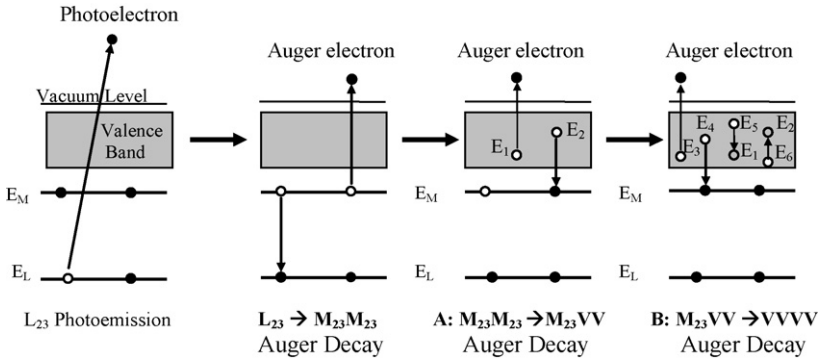

Fig. 1. Energy level diagram illustrating the $L_{2,3} \rightarrow M_{2,3}M_{2,3} \rightarrow M_{2,3}VV \rightarrow VVVV$ cascade chain.

which both valence holes are at the bottom of the band and a final state in which all four holes are at the top of the valence band. If the width of the valence band is taken to be W, it may be seen from consideration of the highest and lowest energy Auger transitions illustrated in Fig. 2 that the full width (FW) of the Auger transition with two valence holes in the initial state and four valence holes in the final state is $6W$. This should be compared to a FW of $2W$ for a direct Auger transition involving only two final state valence holes and no initial state valence holes or a transition in which the energy of the spectator holes is held fixed during the cascade-induced transitions.

It is interesting to note that the cascade transition can result in the emission of electrons with higher kinetic energies than electrons emitted in the direct Auger decay. This "extra" energy is made available when holes in the valence band in an intermediate state in the cascade are filled with valence electrons from higher up in the valence band during the next step in the cascade.

The lineshapes of the cascade spectra are modeled using multiple integrations over a product of N_{tot} identical VB-DOS's (where $N_{tot} = N_i + N_f$) and an energy conserving delta function. Integration of this product results in a function, $N(KE)$, which is proportional to the number of all possible initial and final state valence hole combinations that result in an Auger electron with a kinetic energy, KE. The assumptions underlying this model are that the valence holes created in previous cascade steps remain available to participate in subsequent cascade steps and that the Auger transition probabilities are independent of the energies of the valence holes within the band.

The argument of the energy conserving delta function is determined by equating initial and final state energies in a given Auger transition. For the transition labeled A in Fig. 1 ($M_{2,3}M_{2,3} \rightarrow M_{2,3}VV$), this yields:

$$2E_M + U_{pp} = E_M + E_1 + E_2 + 2U_{pd} + U_{dd} + KE_{Auger} + \phi \quad (1)$$

where $2E_M$ is the total energy of the two initial M_{23} holes, and E_M, E_1 and E_2 are the energies of the final state core and valence holes, respectively, and U_{dd}, U_{pp}, U_{pd} and ϕ are the valence–valence, core–core, valence–core hole–hole interaction energies and the work function, respectively.

Within this model, spectrum A is given by

$$N_A(KE) \propto \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \rho(E_1)\rho(E_2)\delta(KE + E_2 + E_1 - E_M + U_1)\,dE_1\,dE_2 = \rho * \rho(KE - E_M + U_1) \quad (2)$$

where $U_1 \equiv 2U_{pd} + U_{dd} - U_{pp} + \phi$.

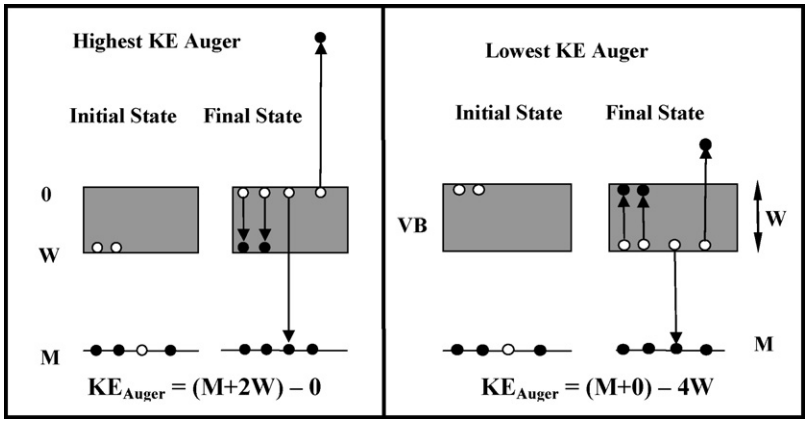

Fig. 2. Energy level diagram illustrating the valence hole configurations associated with the highest and lowest kinetic energy electrons associated with the $M_{2,3}VV \rightarrow VVVV$ Auger cascade step. The valence band is assumed to have a width W. For simplicity we have referenced the zero of energy to the top of the valence band.