Relaxation and screening in Auger emission: an explanation for the changes from bandlike to quasi-atomiclike CVV Auger spectra across the transition metal series

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(November 21, 2018)

Abstract

Supercell method is used to study the relaxation and screening effects during the Auger transition in metals. Our consideration is based on the assumption that when a core-hole exists long enough before the Auger transition occurs, the occupied valence states relax to screen the core-hole which results in a redistribution of the valence electrons, in particular within the atom that contains the core-hole. In order to make the interaction between the core-holes sited at different atoms negligible, the real metal is simulated by supercells repeated periodically. In each supercell one atom is considered to have a core-hole and many others without core-hole. The electronic states concerned by the Auger transition are calculated by the self-consistent full-potential linearized augmented plane wave (FLAPW) method. The occurrence of both bandlike and quasi-atomiclike Auger spectra across transition metal series is related clearly to the different responses of these metals to the existence of a core-hole depending on whether their d-bands are partially or completely filled. As examples, L$_3$VV and M$_1$VV Auger spectral profiles of Cu have been calculated in a reasonably well agreement with experiment.

PACS number(s): 79.20.Fv, 71.15.Ap, 71.20.Be

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I. INTRODUCTION

The idea of correlating Auger spectral line shapes from elemental metals with their electronic structure goes back to Lander [1]. It was shown that the Auger spectral line shape of a core-valence-valence (CVV) transition is determined by the self-convolution of the local density of (valence) states (LDOS) if the state dependence of the transition matrix elements may to a good approximation be ignored across the valence band. From the late 1970’s, efforts have been given to consider the actual variation of the matrix elements and their dependence on the angular momenta of the valence electrons [2–7]. The results showed that, based on the basic assumption of Lander with adequate consideration of the state variation of the matrix elements, reasonably good agreement between theories and experiments can be obtained for the CVV Auger spectral line form of alkali and alkaline-earth metals and silicon. Even the spin polarization of the Auger electron can be described adequately by the theory [8]. The basic feature of the CVV Auger spectra of these materials is a relatively broad peak reflecting the fact that there is a definite width for the valence band.

In contrast to the relatively prosaic CVV Auger spectral line shape of alkali and alkaline-earth metals, it is obvious from the experimental findings that the Auger spectra of some materials display quasi-atomic features on a background reflecting the presence of itinerant states [9]. The occurrence of quasi-atomiclike CVV Auger spectra is typical of some d-band materials [10]. Relying on this kind of experimental findings, Cini [11] and Sawatzky [12] developed a theory of Auger emission based on a Hubbard model. The original form of their theory is only applicable to filled band system and has been extended by many author to treat the unfilled band and multi-band cases [13–17]. In his theory Sawatzky [12] is led to the conclusion that when the effective Coulomb interaction $U$ in the Hubbard Hamiltonian is very large compared to the width of the valence band $W$, that is if $U \gg 2W$, the Auger spectra will display a relatively sharp quasi-atomiclike structure. The parameter $U$ was determined empirically from the experiments [18–21]. The obtained values increase from light (V) to heavy (Zn) 3d-transition metals. The relatively large $U$ for Cu and Zn is consistent with the fact that these metals show quasi-atomiclike sharply split structures in their valence Auger spectra, while Cr, Fe, and Ni display relatively broad bandlike
features. The most interesting thing is that the change of the CVV Auger spectral line shape from bandlike to quasi-atomiclike characteristics across the transition metal series from left to right in the periodic table occurs dramatically at Cu and Ag, respectively, for 3d and 4d transition metals, rather than gradually from left to right across the whole series. Nevertheless, the theory of Cini [11] and Sawatzky [12] cannot give a quantitative prediction that the quasi-atomiclike CVV Auger spectra just start from Cu for the 3d transition metals and from Ag for the 4d transition metal, from which the d-band starts to be filled completely.

We will show by an \textit{ab initio} calculation why the quasi-atomiclike CVV Auger spectra start from Cu and Ag respectively for the 3d and 4d series. The relaxation and screening effects are the main factors in our consideration. The relaxation and screening effects has been investigated by many authors since the late 1970’s. In the early study of Barth and Grossmann [22], considerable changes in the LDOS caused by the relaxation and screening effects was predicted by means of an empirical model. However, after taking the dynamical screening into account, the static screening around the core-ionized site has less influences on the spectra profiles of the x-ray emission and CVV Auger transition of the simple metals [22,23,6], resulting in the so-called final-state rule. The effects of screening on the Auger spectral line shape of metallic Mg was studied by Davies \textit{et al.} [4] also using an empirical method. Cluster method and transition state were applied by Kucherenko [24] to the investigation of the influence of relaxation effects on the shape of the Auger spectra of metals. A modified excited atoms model was used to predict relaxation and Auger parameter shifts between free atoms and elemental solids for Na and Mg [27]. The screening effect was also considered by Yuan \textit{et al.} [8] to find it’s influence on the spin polarization of Auger electrons from K and Cr metals. Most recently, Weightman [28] discussed the screening and correlation effects in CVV and CCV Auger processes of Si. The localized nature of the final states and the delocalized nature of the screening in semiconductors have influences on both CVV and CCV Auger spectra profiles. In the present work, relaxation and screening effects will be studied by using a supercell method and a definite relation will be found between the occurrence of the bandlike or quasi-atomiclike CVV Auger spectra and the qualitatively different response of the valence band electrons to screen the core-
hole. As examples, L_{3}VV and M_{1}VV Auger spectral profiles of Cu will be calculated to see to what extent the present theory can reproduce experimental observations.

II. THEORETICAL METHOD

Both the initial and final Auger states are excited (mutually degenerate) N-electron states that can be described within a generalized density functional theory \cite{27}. The key idea of density functional theory resides in mapping the interacting N-electron system onto that of a noninteracting N-electron system having the same spin-resolved one-particle densities as the original one but moving in a modified external potential. The noninteracting wave function has the form of a Slater determinant. The approach used in the following is based on the assumption that the transition matrix elements describing the Auger process can, to a good approximation, be calculated by using the pertinent initial- and final-state determinants instead of the true N-electron wave function. As a consequence, the following calculations concern only one-electron states by which these Slater determinants differ. As for the electronic states of the metals we are considering, we employ the full-potential linearized augmented plane wave (FLAPW) code WIEN95 \cite{28} to calculate the itinerant valence and semi-core solutions to the Kohn-Sham equations. The FLAPW method requires a subdivision of the crystal into sufficiently large, but non-overlapping concentric spheres (atomic spheres) around the atomic nuclei and an interstitial region between these spheres. Inside the atomic sphere the one-electron state of band index \( n \) is given by

\[
\psi_n(\epsilon_n, \vec{k}, \vec{r}) = \sum_L \sum_{\nu=0}^1 c_L^{(n)}(\epsilon_n, \vec{k}) R_{l\nu}(\epsilon_l, r) Y_L(\hat{r}) \chi_{\sigma_n} \tag{1}
\]

where spherical harmonics are denoted by \( Y_L(\hat{r}) \), \( L = (l, m) \). The quantity \( \chi_{\sigma_n} \) represents a unit spinor for the spin orientation \( \sigma_n = \pm 1 \). The function \( R_{l0}(\epsilon_l, r) \) is regular at the origin and solves the radial part of the Kohn-Sham-type equation for \( E = \epsilon_l \), \( R_{l1}(\epsilon_l, r) \) denotes its normalized energy derivative.

The Auger transition rate \( P_{fi}^{a,d} \) can be cast into the Golden Rule form \cite{29}

\[
P_{fi}^{a,d}(a, d) \propto \sum_{\vec{k}, \vec{n}, \sigma_a, m_{sa}} | M_f^{\sigma_t, \sigma_a, m_{sa}}(\vec{k}, \vec{n}, \sigma_a, m_{sa}) \rangle \langle M_i^{\sigma_t, \sigma_a, m_{sa}}(\vec{k}, \vec{n}, \sigma_a, m_{sa}) |^2 \delta(\epsilon_d - \epsilon_{n'}(\vec{k'})) - \epsilon_n(\vec{k}) + \epsilon_a + \Delta \epsilon(\vec{k}' \vec{n'}; \vec{k}, \vec{n}) \tag{2}
\]
where \( \sigma_d = \pm 1 \) refers to the two spin orientations of the outgoing electron. The spin quantum number of the core-hole spinor state \( \psi_a(\vec{r}) \) is denoted by \( m_{sa} \) \((= \pm \frac{1}{2})\) referring to the total angular momentum \( j_a = l_a + m_{sa} \) of the spin-orbit split core-hole doublet states. \( \Delta \epsilon(\vec{k}'n'; \vec{k}, n) \) represents the non-averaged interaction between the two holes after the Auger transition occurs \([12]\). It can be calculated by using the wave functions of the two concerned states:

\[
\Delta \epsilon(\vec{k}'n'; \vec{k}, n) = \langle \psi_b^*(\vec{r}_1)\psi_c^*(\vec{r}_2) \bigg| \frac{1}{|\vec{r}_1 - \vec{r}_2|} \bigg| \psi_b(\vec{r}_1)\psi_c(\vec{r}_2) \rangle + \delta_{\sigma_b,\sigma_c} E X \tag{3}
\]

where \( \psi_b(\vec{r}) \) is given by Eq.(1). \( E X \) represents the exchange part. By using the expansion given in Eq.(1), the above element can be expressed in details as:

\[
\Delta \epsilon(\vec{k}'n'; \vec{k}, n) = \sum_{L_b} \sum_{L_c} \sum_{L'_b} \sum_{L'_c} \sum_l \frac{4\pi}{2l + 1} G(L'_b, L_b, L) G(L_c, L'_c, L)
\]

\[
\times \sum_{\nu_b=0} \sum_{\nu_c=0} \sum_{\nu'_b=0} \sum_{\nu'_c=0} c_{L_b,\nu_b}^b c_{L_c,\nu_c}^c c_{L'_b,\nu'_b}^b c_{L'_c,\nu'_c}^c F_{\nu_b,\nu'_b,\nu'_c,\nu_c}(l_b, l_c, l'_b, l'_c) + \delta_{\sigma_b,\sigma_c} E X \tag{4}
\]

in which \( G(L'_b, L_b, L) \) represent the Gaunt integrals and \( F_{\nu_b,\nu'_b,\nu'_c,\nu_c} \) is shorthand for

\[
F_{\nu_b,\nu'_b,\nu'_c,\nu_c}(l_b, l_c, l'_b, l'_c) = \int_0^{r_0} R_{l_b,\nu_b}(r_1) R_{l'_b,\nu'_b}(r_1) \left[ \frac{1}{r_1^{l+1}} \int_0^{r_1} r_2^{l+2} R_{l_c,\nu_c}(r_2) R_{l'_c,\nu'_c}(r_2) dr_2 \right]
\]

\[
+ r_1^{l} \int_{r_1}^{r_0} \frac{1}{r_2^{l+2}} R_{l_c,\nu_c}(r_2) R_{l'_c,\nu'_c}(r_2) dr_2 \] \( dr_1 \). \tag{5}

With CVV Auger transitions one is dealing with a core-hole state that is, to a good approximation, confined to the pertaining atom. The intra-atomic transition, in which the final two holes located in the same atom with the initial core-hole, contributes the dominant part to the Auger spectra. Hence the integration over the \( r \)-dependent functions may be restricted to the atomic sphere of that atom without causing considerable errors. The matrix elements on the right-hand side of Eq.(2) can be split into two portions

\[
M_{fi}^{(\sigma_d,\sigma_a,m_{sa})}(\vec{k}', n'; \vec{k}, n) = D_{abcd}^{(m_{sa})} \delta_{\sigma_a,\sigma_i} \delta_{\sigma_c,\sigma_d} - E_{abcd}^{(m_{sa})} \delta_{\sigma_a,\sigma_i} \delta_{\sigma_c,\sigma_d} \tag{6}
\]

where \( D_{abcd}^{(m_{sa})} \) and \( E_{abcd}^{(m_{sa})} \) denote, respectively, the so-called direct and exchange portion of the transition matrix element. The details for the calculations of the transition matrix element can be found in our previous paper \([8]\).
III. RESULT AND DISCUSSION

It is well known that the CVV Auger spectra of transition metals with partially filled d-bands like Cr, Fe, Ni and Pd etc. show relatively broad bandlike features, while the spectra of transition metals with completely filled d-bands like Cu, Zn and Ag are conspicuous by sharp quasi-atomiclike structures. The approach used by Cini [11] and Sawatzky [12] to explain the quasi-atomiclike Auger spectra is based on a Hubbard-type Hamiltonian that contains the parameter $U$ describing the effective Coulomb interaction and another parameter $W$ referring to the band width. If $U \gg 2W$, it was shown by these authors that the two-hole density of states splits into a broad and a narrow structure. The occurrence of the latter is correlated with the observed quasi-atomiclike Auger peaks. By exploiting certain experimental findings it can be made evident that Cu and Zn are associated with a larger ratio $U/2W$ compared to the other 3d-transition metals.

The theory of Cini [11] and Sawatzky [12] can qualitatively explain the change from bandlike to quasi-atomiclike Auger emission as one goes from the light to the heavy 3d-transition metals. Nevertheless, due to the model Hamiltonian and the empirical parameters involved in their theory, they cannot predict in a sense of an ab initio way that the change of the CVV Auger spectrum from bandlike to quasi-atomiclike features occurs just from Ni to Cu [30] rather than somehow earlier or later in the 3d transition series by noting the fact that the ratio $U/2W$ increases monotonously from Fe to Zn [18]. We have therefore reexamined this problem from a first-principles point of view. Our considerations are based on the two-step model of the Auger electron emission. An initial core-hole is first generated by the absorption of an incoming photon or by impact with some other particle. If that core-hole exists long enough before the Auger transition occurs, the occupied valence states relax to screen the core-hole which results in a redistribution of the valence electrons, in particular within the atom that contains the core-hole.

In our theoretical treatment, a core-hole state can be obtained by simply putting one less electron in the considered core orbital. In order to make the interactions between the core-hole negligible, supercell method is employed, in which an enough large unit cell containing one atom with a core-hole and many other atoms without core-hole is repeated periodically, and we take electronic structure calculations with many chemically same atoms per unit
cell. In our calculations, except for the unit cell being chosen much larger than the usual one there is not any change made on the real crystal structure, and except for one less electron being putted in a core orbital of a specific atom, there are not any other extra environmental conditions taken on the supercell. Therefore, after an enough large unit cell is used, we carry out an \textit{ab initio} calculation. The accuracy of the calculation is examined by having the supercell results being the same as the simple crystal calculation when the core-hole state does not exist. We take the atom having the core-hole at the center of the unit cell, and take the unit cell large enough to have the LDOS of the atoms at the corner of the cell being nearly the same of the simple crystal. By this way, we have, in a unit cell, up to sixteen atoms for the Bcc and Hcp metals and thirty two atoms for Fcc crystals. The unit cell is a simply cubic one for Bcc and Fcc crystals, and a hexagonal one for the Hcp cases.

We first confine ourselves to describe the relaxed electron distribution after the core-hole excitation. The characteristics of the valence electronic states can be seen from the LDOS of the concerned atoms. The bandlike or quasi-atomiclike features of the Auger spectra can be extracted from the LDOS of the structural calculations. The valence band was appropriately filled higher up to ensure charge neutrality of the system. This is just equal to exciting the core electron to the valence band instead of the vacuum states. From Figs. 1 to 9, we show the LDOS obtained for Sc, Ti, Cr, Fe, Ni, Cu, Zn, Pd and Ag to see the changes of the LDOS induced by the existence of a core-hole from light to heavy elements across the 3d transition series, in particular the changes of the LDOS from Ni to Cu and from Pd to Ag as examples of the transition between the two kind responses to screen the core-hole. The plots refer to the density of states of the pertinent atom with a core-hole by the solid lines, to that of the atoms at the corner of the unit cell without the core-hole by the dot lines, and to the LDOS of the perfect crystals by the long-short dashed lines. Obviously, from Sc to Ni and Pd the relaxation only changes the distribution of the density of states within the valence band, although much higher values of the LDOS are observed at the bottom of the d-bands for Ni and Pd, which will result in a relatively narrow Auger line shape. In contrast to the above metals, for Cu, Zn and Ag the relaxation leads to a sharply peaked structure strongly shifted away from the original d-band complex.
While the latter contains sizable p-type portions, the peaked structure is almost purely d-type. The position of the sharp structure falls into the gap between the onset of the s-p valence band and the lower lying 3p-core level band. If one could gradually enlarge the unit cell, the peak would more and more attain the form of a delta-function reflecting the fact that one is dealing with a d-type quasi-atomiclike impurity state. Therefore, the Auger transition closely resembles that of a free atom. The quasi-atomiclike splitting one observes with the respective peak can hence easily be understood as a final state effect that results from the coupling in the open 3d-shell after the Auger transition has taken place. Spin polarized calculations are carried out for Cr, Fe and Ni to consider the antiferromagnetic and ferromagnetic properties of these metals.

The difference response of the valence electrons to the relaxation effects comes from the different occupations of the screening electrons to s and p or d orbitals. For the full filled d-band metals, the screening electrons can only go to the s and p orbitals, which lies above the d-band, and the strong core potential on the d-band cannot be screened effectively. Due to the strong attractive core potential, the d-band moves towards a much lower energy and display a typical localized state characteristics. For the partially filled d-band metals, the screening electrons mainly occupy the empty d orbitals resulting in a more effective screening on the core attractive potential for the d-band, and the band structure of the d electrons remains unchanged with a definite width of the band. As examples, we consider the changes of the valence charge inside the atomic sphere caused by relaxation for Pd and Ag. The valence charge inside the atomic sphere with the core-hole increases 1.003 and 0.718 for Pd and Ag respectively. The increased charge of 1.003 of Pd distributes 0.039 in s-wave, 0.042 in p-wave, and 0.921 in d-wave, while the increased charge of 0.718 of Ag has 0.150 in s-wave, 0.159 in p-wave and 0.408 in d-wave. The results support the fact that for Pd most of the increased charge to screen the core attractive potential comes from the d partial waves, while for Ag most of the increased charge to screen the core attractive potential comes from the s and p partial waves and the main part is outside the atomic sphere. Because of the very small DOS at the Fermi energy, the screening radius of Ag is much larger than that of Pd, i.e. we have the delocalized nature of screening for the full filled d-band transition metals. The increased d partial charge inside the atomic sphere
for Ag is mainly attributed to the contraction of the d orbital caused by the strong core attractive potential.

As examples, we also calculated the $L_3$MM and $M_1$VV Auger spectra of Cu as described by the Golden Rule of Eq.(2). In the calculation, if we neglect the Coulomb interaction between the two final holes, we will have an $\delta$-function type spectra as a result of the self-convolution of the LDOS shown in Fig. 6 by the solid line. In Figs. 10 and 11, we give the calculated Auger spectra by including the $\Delta \epsilon$ in Eq.(2). The result shows some structures that is similar to those obtained by the experiments [31–33]. The structures and their separations observed and labeled as B, D and E by Madden et al. [32] for the $L_3$VV transition are reproduced quite well by our calculations. Difference in the details of the relative height of the peaks B and E can be found between our theory and the experiment of Madden et al. [32], but the relative intensities of B and E agree much better with the latest measured result of Sarma et al. [31] with subdued satellites in the left side of the main peak D. Please be noted that the $L_3$VV and $M_1$VV spectra are obtained with different electronic wavefunctions, which are calculated by using the supercell model with a core-hole, respectively, in $L_3$ and $M_1$ core orbitals. Apparent difference between the $L_3$VV and $M_1$VV spectral profiles are revealed by both the present theory and the experiment [32].

The Auger spectra obtained without the screening effects is also presented in Figs. 10 and 11 by the dashed lines. It is obvious that the much more broader line shape cannot reproduce the experimental observations. The main features of the $L_3$MM and $M_1$VV Auger spectra of Cu is the relatively sharp peaks, which is called atomiclike and corresponds to the localized characteristics of the concerned electron states. The separated peaks, for example, of the $L_3$MM Auger spectra is the multiplet split caused by the hole-hole interaction in the final state. With a core-hole, the localization of the initial states for the full filled d-band transition metals have been seen clearly from the LDOS in the Figs. 6,7 and 9. The position of the localized initial states are well below the normal valence band. After the Auger transition, there is not hole in the core, but there are two holes in the final states. If the dynamical screening is as significant as in the simple sp metals, the final two hole states should be very close to the valence electron states of the ground
metal. Nevertheless, the dynamical screening in the full filled d-band transition metals is much less effective than that in the simple metals. The reason will be given in the following discussions. Therefore, the final two hole states of the CVV Auger transition of Cu should be much more localized compared with the ground valence states. In order to simplify the calculations (with orthogonal orbitals), we use the initial states, in a good approximation, to replace the true final orbitals. The multiplet split caused by the hole-hole interaction in the final state is also taken into account in the present treatment by including the $\Delta \epsilon$ term in Eq. (2), and the present calculations are not exactly one-electron model in the normal sense. Even in the normal one-electron model, one usually does not give the same results with and without the core-hole screening. According to Lander [1], the Auger spectral line shape of a CVV Auger transition is determined by the self-convolution of the LDOS. We have shown that the LDOS’s of the full filled d-band transition metals with and without the core-hole screening are dramatically different. The more broader line shape of the dashed lines in Figs. 10 corresponds to the much wider valence band of the perfect crystal, and the relatively higher intensity of the right peak is also consistent with the shape of the LDOS. We do not give the absolute values of the kinetic energy of the Auger electron, because the local-density-approximation (LDA) cannot predict reliable energy distance between core state and valence band.

In the present study, we did not consider the competing of the Auger emission to the screening because of the fact that in most metals the valence screening is a faster process than a CVV Auger emission. We did not consider the dynamical screening either. The dynamical screening would most likely have some influences on the Auger emission spectra. In some previous studies of the dynamical screening effect [22, 23, 24], final state rule had been arrived for simple metals by using a dynamical approach [24]. The rule states that the CVV Auger spectral profiles of the simple metals are most determined by the LDOS of the ground state valence band and that the screening effect around the core-hole state before the Auger transition are compensated significantly by the dynamical screening. Nevertheless, this conclusion derived for simple metals cannot be applied to the transition metals without modifications, because some of the transition metals, for examples Cu and Zn, have quite different valence band structure. For these transition metals, the density of
state at the Fermi level has very small values compared with the simple metals and other transition metals with partially filled d-band. Therefore, the screening behavior of these transition metals is somehow like to that in semiconductors, which results in localized final states and delocalized screening \[^{26,35}\] on the core-hole before the Auger transition and on the valence double hole after the Auger transition. When we apply the final state rule to the transition metal like Cu and Zn with a full filled d-band, the final states should be a localized atomiclike impurity states rather than the ground state of the metals. This kind of final states satisfy the requirement of Cini-Sawatzky theory for the occurrence of the atomiclike CVV Auger spectra naturally, because of the very small band width of the localized states. For the simplicity of the calculations, we use the initial states with a core-hole as the final states. The dynamical screening will cause changes in the details of the Auger spectral profiles we presented in Fig.10 and 11, but the left improvement between theory and experiment will not be dramatic or qualitative.

In conclusion, it may be stated that the occurrence of bandlike and quasi-atomiclike features of the CVV Auger spectral line shape across the 3d and 4d transition metals can be correlated with the distinctly different behavior of d-transition metals in screening a core-hole, the mechanism crucially depending on whether their d-bands are partially or completely filled.

ACKNOWLEDGMENTS

The author is very grateful to the very helpful discussion with L. Fritsche. This work was supported by the National Science Fund for Distinguished Young Scholars under Grant No. 10025416 and also by the National Natural Science Foundation of China under Grant No. 19974075 and 59971064.
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Figure Captions:

**FIG. 1.** Local density of states (LDOS) of Sc metal. The solid line refer to the atom in the center of the unit cell with a core-hole, the dot line to the atoms at the corner of the unit cell, and the long-short dashed line to the atom in a perfect crystal. The Fermi energy is chosen to be zero and indicated by the vertical thin long dashed line.

**FIG. 2.** Same as Fig. 1 but for Ti.

**FIG. 3.** Same as Fig. 1 but for Cr. Please note that a spin-dependent calculation has been performed to consider the antiferromagnetic property of the metal below $T_N$.

**FIG. 4.** Same as Fig. 1 but for Fe. Please note that a spin-dependent calculation has been performed to consider the ferromagnetic property of the metal.

**FIG. 5.** Same as Fig. 1 but for Ni. Please note that a spin-dependent calculation has been performed to consider the ferromagnetic property of the metal.

**FIG. 6.** Same as Fig. 1 but for Cu. Please note that an additional $\delta$-function type structure is generated far below the original d-band for the atom with a $L_3$ core-hole, which indicates that localized physical impurity states are generated by the strong attractive core potential.

**FIG. 7.** Same as Fig. 1 but for Zn. Please note that similar structure has been generated as in the case of Cu.

**FIG. 8.** Same as Fig. 1 but for Pd. Please note that relatively sharp structure appears at the bottom of the d-band for the atom with a $L_3$ core-hole, but the band feature does not change anymore, reflecting the fact that Pd is not a full-filled d-band metal.

**FIG. 9.** Same as Fig. 1 but for Ag. The existence of a core-hole affects the valence electrons in a similar way as for Cu and Zn.

**FIG. 10.** The $L_3VV$ Auger spectra of Cu. The solid line refer to the results with the influence of the core-hole state, the dashed line to the results of a perfect crystal calculation.

**FIG. 11.** The same as in Fig.10 but for the $M_1VV$ Auger spectra of Cu.
Fig. 2

Energy (eV)

Local Density of States

Ti

Energy (eV)
Fig. 3

Local Density of States

$Cr$

spin–up

spin–down

Energy (eV)
Fig. 4

Local Density of States

Energy (eV)

-7.5 −5 −2.5 0 2.5

Fe

spin-up

spin-down
Fig. 5

Local Density of States

Energy (eV)

spin-up

spin-down

Ni

Energy (eV)
Fig. 7

Local Density of States

Energy (eV)

Zn
Fig. 8

Local Density of States

Energy (eV)

Pd
Fig. 11

-10  -5  0  5  10  15  20
Relative Energy (eV)

0  0.5  1  1.5
Relative Intensity

M_1VV