

Theory of electron-pair emission from random alloys

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(Received 29 July 2002; published 20 December 2002)

A theory is developed for the treatment of correlated electron-pair emission from alloys with substitutional disorder following the impact of fast electrons. The influence of disorder on the emitted, hot-electron states is treated using the virtual-crystal approximation. Numerical results for several metallic binary alloys are presented and analyzed revealing the interplay between disorder effects and scattering dynamics. On the basis of this work conclusions are drawn on the potential of utilizing the electron-pair spectroscopy for the study of electronic collisions in random alloys.

DOI: 10.1103/PhysRevB.66.235114

PACS number(s): 79.20.Kz, 71.20.Gj

The process of the simultaneous ejection of two electrons from quantum targets induced by an impinging electron beam has been established as a powerful tool for the study of electronic correlation as well as for the mapping of electronic structure of materials. This technique which is known as the $(e,2e)$ spectroscopy (one electron in, two electrons out) has been developed and extensively applied in atomic and molecular physics.^{1,2} In contrast, it is only recently that the $(e,2e)$ approach has been utilized successfully for the theoretical and experimental studies on solids and surfaces.³⁻⁹ The $(e,2e)$ measurements from surfaces can be categorized in two classes: (1) *the transmission*¹⁰ and (2) *the reflection mode* experiments.^{3,4} In the transmission mode¹⁰ an incoming energetic electron passes through a free-standing thin film knocking out a valence-band electron. The two emitted electrons are detected on the side of the film that does not contain the incident beam, i.e., both final-state electrons propagate in the forward direction with respect to the incoming beam. For fast electrons (compared to the Fermi velocity) the scattering is well described as a direct, single encounter between the projectile and the bound electron in which case, the spectral properties of the hole can be directly related to the measured $(e,2e)$ cross section.¹⁰

The reflection mode set up, where all vacuum electrons are present at one side of the sample, avoids complications related to the preparations of thin films and allows a direct investigation of electron scattering at surfaces and adsorbates. However, since the ejected electrons are collected in the direction opposite to the incoming projectile the description of the $(e,2e)$ process requires, at least, a second-order mechanism that involves, in addition to the electron-electron interaction, a backscattering from the crystal potential.⁸ Furthermore, the energies of the electrons are rather low (0.5–500 eV). In general, this rules out a disentanglement of the scattering dynamics from the electronic properties of the target. Under certain conditions, however, the footprints of the target's electronic structure can be identified in the $(e,2e)$ cross section.^{7,9,11}

A variety of materials have been studied by the $(e,2e)$ technique, such as clean metals,^{5,6,10} metal oxides,¹² insulators,^{3,13} semiconductors,¹⁴ and more recently ferromagnets.¹¹ The aim of the present work is to provide the theoretical framework for $(e,2e)$ from disordered alloys. To our knowledge, no $(e,2e)$ experiments or theories exist for these systems. The importance of physical phenomena in-

duced by disorder is well documented (cf. Refs. 15,16 and references therein). Therefore, we concentrate here on the aspects pertinent to the $(e,2e)$ from alloys. Particular emphasis is put on the $(e,2e)$ in reflection mode from the surface of binary substitutional alloys. Because of the disorder there is a lack of translational symmetry parallel to the surface. The lattice sites are randomly occupied by atoms of two types, and consequently the Bloch wave vector \mathbf{k}_{\parallel} is not a good quantum number as it is in the ordered system. At the same time the notion of the band structure can be kept for alloys, e.g., within the Korringa-Kohn-Rostoker coherent-potential approximation¹⁷ (KKR CPA) by calculating the Bloch spectral function and identifying its peaks in the energy wave-vector space. In the high-energy transmission mode one may expect to reveal the alloys' spectral properties using $(e,2e)$, however, the disorder influences the collision dynamics, and a careful analysis of the interplay between the transition matrix elements and the target electronic properties is needed, i.e., we have to investigate how the disorder affects the quantum transition between the two-electron states involved in the $(e,2e)$ reaction. In the consideration below, we make an accent on this problem, leaving aside the problem of the alloy's band structure, which does not depend on the experimental method by which it is studied.

The paper is organized as follows. In Sec. I, we present the model for collision dynamics which explicitly accounts for a single backscattering of the fast electron. In Sec. II, the configurational average of the cross section over atomic configurations in alloys is discussed. Then, in Sec. III, we apply the derived formalism to the case of binary metallic alloys using the jellium model and the virtual-crystal approximation (VCA) to describe the electronic structure. Furthermore, we present and discuss numerical results for the energy sharing and for the angular distributions in the case of aluminum-*sp*-metal alloys. The conclusions are made in Sec. IV. Unless otherwise stated, atomic units (a.u.) are used throughout.

I. COLLISION DYNAMICS

We consider the $(e,2e)$ process where, following the impact of a fast vacuum electron of a wave vector \mathbf{k}_0 and energy E_0 , two electrons are emitted from the surface of a semiinfinite solid with wave vectors $\mathbf{k}_s, \mathbf{k}_e$ and energies E_s, E_e (see Fig. 1), hereafter the subscript $s(e)$ stands for the scattered (ejected) electron.

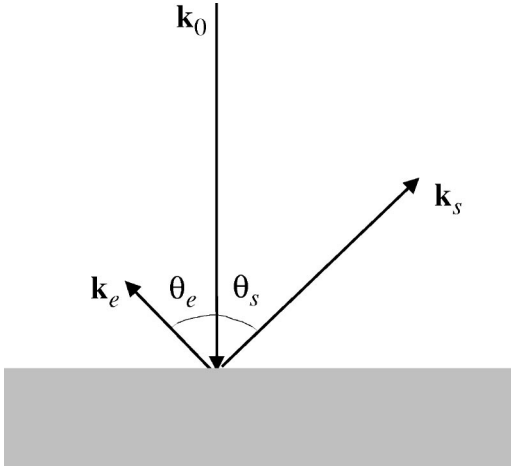


FIG. 1. A schematic representation of the $(e,2e)$ process in the normal incidence, reflection mode geometry.

In general, the spin-averaged differential cross section of this reaction is given by⁸

$$\begin{aligned} \frac{d\sigma_{(e,2e)}^{av}}{dE_s d\Omega_s dE_e d\Omega_e} &= \frac{k_s k_e}{(2\pi)^5 k_0} \sum_{\substack{i_{occ} \\ s_i s_0 \\ s_s s_e}} \\ &\times |\langle \mathbf{k}_s s_s, \mathbf{k}_e s_e | T_{(e,2e)} | \mathbf{k}_0 s_0, i s_i \rangle|^2 \\ &\times \delta(E_s + E_e - E_0 - \varepsilon_i). \end{aligned} \quad (1)$$

Here, we specified the directions of the wave vectors of the emitted electrons by the solid angles $\Omega_{s/e}$. The state vectors $|\mathbf{k}_s s_s, \mathbf{k}_e s_e\rangle$ and $|\mathbf{k}_0 s_0, i s_i\rangle$ describe, respectively, the two final-state electrons (with asymptotic wave vectors $\mathbf{k}_s, \mathbf{k}_e$ and spin projections s_s, s_e) and the initial state consisting of the projectile spinor state (with wave vector \mathbf{k}_0 and spin s_0) and the valence-band state $|i s_i\rangle$ with a spin projection s_i . The sum is taken over all occupied one-particle states of the surface with energy $\varepsilon_i = E_s + E_e - E_0$. We consider $(e,2e)$ experiments that do not resolve the spin states of the electrons. The operator $T_{(e,2e)}$ is an effective transition operator that induces the $(e,2e)$ process and is assumed to be spin independent. In the frozen-core approximation it has the formal structure

$$T_{(e,2e)} = V_s + W_{se} + (V_s + V_e + W_{se}) G_{se}^+(E_{tot}) (V_s + W_{se}), \quad (2)$$

where V_s , V_e , and W_{se} are effective (optical) electron-solid and electron-electron potentials, respectively, and $G_{se}^+(E_{tot})$ is the two-electron propagator in the potential $V_s + V_e + W_{se}$ at the total energy $E_{tot} = E_s + E_e$.

In what follows, we treat Eq. (2) only to a first order in the electron-electron interaction W_{se} . This procedure is justified by the choice of kinematics $E_0 \gg \Delta E$ ($\Delta E \equiv E_0 - E_s$) as well as by the screening of the electron-electron interaction by the surrounding medium (which is negligible in small atomic systems). This approximation leads to the distorted-waves Born approximation (DBA),

$$T_{(e,2e)} = [1 + (V_s + V_e) G_{(s,e)}^+(E_{tot})] W_{se} [1 + G_{(s,e)}^+(E_{tot}) V_s], \quad (3)$$

where $G_{(s,e)}^+$ is the two-electron propagator in the potential $V_s + V_e$. Furthermore, in the spirit of the kinematical approximation of the LEED (low-energy electron diffraction) theory,¹⁸ we account for all possible scattering events only to a first order. This means, in addition to the electron-electron single scattering, we include in the theory those processes in which the projectile electron undergoes a single scattering from the crystal potential V_s before or after the interaction with the bound electron. Scattering of the slow electron from the crystal potential is included in the initial-state binding. Exchange effects between the two emitted electrons are also included. Under these assumptions Eq. (3) takes on the form

$$T_{(e,2e)} = (1 + V_e G_e^+) (V_s g_s^{(0)+} W_{se} + W_{se} g_0^{(0)+} V_s), \quad (4)$$

where G_e^+ is the propagator of the ejected electron in the potential V_e , $g_s^{(0)}$, and $g_0^{(0)}$ are the free propagators at energies E_s and E_0 , respectively. Here, we did not consider explicitly the simple case of the pair emission due to a single electron-electron interaction W_{se} . This process is of relevance to the transmission mode $(e,2e)$.^{19,20} In reflection mode its contribution is negligible compared to that of Eq. (4). For a more realistic description of the backscattering, we shall use in Eq. (4) renormalized propagators g_s and g_0 instead of the $g_s^{(0)}$ and $g_0^{(0)}$, respectively. So that

$$T_{(e,2e)} = (1 + V_e G_e^+) (V_s g_s^+ W_{se} + W_{se} g_0^+ V_s). \quad (5)$$

The renormalization accounts for the refraction of the electron field at the surface and for its damping inside the surface.

In Eq. (1), we couple the spins of the electrons involved in the $(e,2e)$ event to a total (conserved) electron-pair spin S . Since the transition operator (5) does not contain spin-flip terms the sum over the spin projections in Eq. (1) reduces to an averaging of the cross section over the singlet ($S=0$) and the triplet ($S=1$) channels,²¹ i.e.,

$$\begin{aligned} \frac{d\sigma_{(e,2e)}^{av}}{dE_s d\Omega_s dE_e d\Omega_e} &= \frac{1}{4} \frac{d\sigma_{(e,2e)}}{dE_s d\Omega_s dE_e d\Omega_e} \Big|_{S=0} \\ &+ \frac{3}{4} \frac{d\sigma_{(e,2e)}}{dE_s d\Omega_s dE_e d\Omega_e} \Big|_{S=1}, \end{aligned} \quad (6)$$

where

$$\begin{aligned} \frac{d\sigma_{(e,2e)}}{dE_s d\Omega_s dE_e d\Omega_e} \Big|_{S=0} &= \frac{k_s k_e}{(2\pi)^5 k_0} \sum_{i_{occ}} \{ |\langle \mathbf{k}_s, \mathbf{k}_e | T_{(e,2e)} | \mathbf{k}_0, i \rangle|^2 \\ &\pm |\langle \mathbf{k}_e, \mathbf{k}_s | T_{(e,2e)} | \mathbf{k}_0, i \rangle|^2 \} \\ &\times \delta(E_s + E_e - E_0 - \varepsilon_i). \end{aligned} \quad (7)$$

Thus, and from Eq. (5), the basic quantity from which the $(e,2e)$ cross section derives has the form

$$\frac{d\sigma_{(e,2e)}}{dE_s d\Omega_s dE_e d\Omega_e} = \frac{k_s k_e}{(2\pi)^5 k_0} \sum_{i_{occ}} |\langle \chi_{\mathbf{k}_e} | M(\mathbf{k}_s, \mathbf{k}_0) | \chi_i \rangle|^2 \times \delta(E_s + E_e - E_0 - \varepsilon_i), \quad (8)$$

where $|\chi_{\mathbf{k}_e}\rangle = (1 + G_e^- V_e) |\mathbf{k}_e\rangle$ is the time-reversed scattering state of the ejected electron under the action of the potential V_e , $|\chi_i\rangle$ is the state of the bound electron, and

$$M(\mathbf{k}_s, \mathbf{k}_0) = \langle \mathbf{k}_s | V_s g_s^+ W_{se} + W_{se} g_0^+ V_s | \mathbf{k}_0 \rangle \quad (9)$$

can be regarded as an effective one-electron transition operator.

Rewriting Eq. (6) as

$$\frac{d\sigma_{(e,2e)}}{dE_s d\Omega_s dE_e d\Omega_e} = \frac{k_s I_e}{(2\pi)^3 k_0} \quad (10)$$

with

$$I_e = \frac{k_e}{(2\pi)^2} \sum_{i_{occ}} |\langle \chi_{\mathbf{k}_e} | M(\mathbf{k}_s, \mathbf{k}_0) | \chi_i \rangle|^2 \delta(E_s + E_e - E_0 - \varepsilon_i), \quad (11)$$

it becomes evident that this formula (11) is equivalent to the expression given by the golden rule for the energy and angular resolved photocurrent, except for the transition operator. Instead of the dipole electron-photon interaction in a photoemission process, in $(e,2e)$ one has to deal with the effective operator given by Eq. (9).

In the case of solids with a translational symmetry parallel to the surface, the state $|\chi_{\mathbf{k}_e}\rangle$ is nothing else but a time-reversed LEED state.²² Thus, Eq. (11) can be evaluated as done in the one-step model of photoemission and the well-developed algorithms can be employed for calculating the photocurrent substituting the dipole electron-photon operator by Eq. (9).

II. CONFIGURATIONAL AVERAGE OF THE CROSS SECTION

In this section, we present the $(e,2e)$ theory for random alloys. For simplicity, we consider a substitutionally disordered binary alloy $A_x B_{1-x}$ of two components A and B with concentration $c_A = x$ and $c_B = 1 - x$, respectively. The condition $c_A + c_B = 1$ of full randomness neglects any sort of statistical correlation in the occupation of the lattice sites. Furthermore, here we do not treat effects related to positional disorder. In general, the potential at site \mathbf{R}_i of the lattice depends on the occupation of all other sites. A simplification frequently used in the theory of alloys is the neglect of local environment effects by employing the single-site approximation. This approximation states that the one-electron potential at site \mathbf{R}_i depends only on the occupation at \mathbf{R}_i by the atom of the type A or B .

Expressing the crystal potential V_s as a sum of muffin-tin potential functions V_j^s located at sites \mathbf{R}_i yields $V_s = \sum_j V_j^s$. Now, we introduce occupation indices ξ^j where the random numbers $\xi^j = 1$ if the site j is occupied by the atom of type A

and $\xi^j = 0$ if j is occupied by the atom of type B . The on-site potential can be presented as

$$V_s^j = \xi^j V_s^{jA} + (1 - \xi^j) V_s^{jB}. \quad (12)$$

The configurational average $\langle \xi^j \rangle$ of ξ^j (hereafter, we use the angle brackets $\langle \dots \rangle$ for configurationally averaged quantities) is given by the probability that the atom A occupies the site j , i.e., $\langle \xi^j \rangle = x$ where x is the concentration of A .

The simplest single-site method for the treatment of disordered alloys is the VCA which consists of writing for Eq. (12)

$$V_s^j = x V_s^{jA} + (1 - x) V_s^{jB}. \quad (13)$$

The second step beyond VCA is the average t-matrix approximation (ATA) which accounts for multiple scattering from $V_s^{jA/B}$, i.e., one operates with t-matrices $t_s^{jA/B}$ rather than with single potentials. Obviously, the single-scattering potential approximation (VCA) becomes accurate at higher energies where multiple scattering events become less important. The next stage in sophistication beyond ATA is the coherent-potential approximation (CPA) in which the ATA is performed self-consistently. This is required in particular for the evaluation of the ground-state properties of alloys and has been implemented in standard band-structure computer codes,²³ like the (linear muffin-tin orbitals) LMTO CPA,²⁴ and KKR CPA.²⁵ Since the effects of disorder on the electronic structure are akin to the material under study and has been well investigated in the past,^{15,16} we concentrate here on the aspects that are directly related to the $(e,2e)$ process, namely, the influence of disorder on the scattering dynamics of the electron pairs. As the energy of the detected electrons is well above the vacuum level, the VCA approach provides a good starting point, in particular in the low-concentration limit and for the case where the strengths of the potentials V_s^{jB} and V_s^{jA} are of the same order. It should be noted however, that, in general, methods using the single-site approximation (e.g., VCA, ATA, CPA) are not capable of describing statistical fluctuations in the chemical composition and do not account for short-range order effects, such as disorder-induced localization of states and formation of magnetic moments.

For the calculations of the $(e,2e)$ cross section from alloys, we write at first the matrix element (9) as a sum over the lattice sites

$$M(\mathbf{k}_s, \mathbf{k}_0) = \sum_j M_j(\mathbf{k}_s, \mathbf{k}_0), \quad (14)$$

where

$$M_j(\mathbf{k}_s, \mathbf{k}_0) = \langle \mathbf{k}_s | V_s^j g_s^+ W_{se} + W_{se} g_0^+ V_s^j | \mathbf{k}_0 \rangle. \quad (15)$$

As a consequence of Eq. (12), we deduce

$$M_j(\mathbf{k}_s, \mathbf{k}_0) = \xi^j M_{jA}(\mathbf{k}_s, \mathbf{k}_0) + (1 - \xi^j) M_{jB}(\mathbf{k}_s, \mathbf{k}_0). \quad (16)$$

Substitution of Eq. (14) into Eq. (10) yields

$$\frac{d\sigma_{(e,2e)}}{dE_s d\Omega_s dE_e d\Omega_e} = \frac{k_s k_e}{(2\pi)^5 k_0} \sum_{jj'} \langle \chi_{\mathbf{k}_e} | M_j(\mathbf{k}_s, \mathbf{k}_0) \times A^-(\varepsilon) M_{j'}^+(\mathbf{k}_s, \mathbf{k}_0) | \chi_{\mathbf{k}_e} \rangle. \quad (17)$$

Here, we introduced the one-electron spectral function

$$A^-(\varepsilon) = \sum_{i_{occ}} |\chi_i\rangle \langle \chi_i| \delta(\varepsilon - \varepsilon_i), \quad \varepsilon = E_s + E_e - E_0. \quad (18)$$

Performing configurational average of Eq. (17), we decouple the on-site quantities related to the different electrons:

$$\begin{aligned} & \langle \chi_{\mathbf{k}_e} | M_j(\mathbf{k}_s, \mathbf{k}_0) A^-(\varepsilon) M_{j'}^+(\mathbf{k}_s, \mathbf{k}_0) | \chi_{\mathbf{k}_e} \rangle \\ &= \langle \langle \chi_{\mathbf{k}_e} | \langle M_j(\mathbf{k}_s, \mathbf{k}_0) \rangle A^-(\varepsilon) \langle M_{j'}^+(\mathbf{k}_s, \mathbf{k}_0) \rangle | \chi_{\mathbf{k}_e} \rangle \rangle \\ &+ \delta_{jj'} \{ x \langle \langle \chi_{\mathbf{k}_e} | M_{jA}(\mathbf{k}_s, \mathbf{k}_0) A^-(\varepsilon) M_{jA}^+(\mathbf{k}_s, \mathbf{k}_0) | \chi_{\mathbf{k}_e} \rangle \rangle \} \\ &+ (1-x) \langle \langle \chi_{\mathbf{k}_e} | M_{jB}(\mathbf{k}_s, \mathbf{k}_0) A^-(\varepsilon) M_{jB}^+(\mathbf{k}_s, \mathbf{k}_0) | \chi_{\mathbf{k}_e} \rangle \rangle \} \\ &- \langle \langle \chi_{\mathbf{k}_e} | \langle M_j(\mathbf{k}_s, \mathbf{k}_0) \rangle A^-(\varepsilon) \langle M_{j'}^+(\mathbf{k}_s, \mathbf{k}_0) \rangle | \chi_{\mathbf{k}_e} \rangle \rangle \}. \end{aligned} \quad (19)$$

This means that we neglect all two-electron on-site correlated terms in the configurational average. We have assumed also in Eq. (19) that

$$M_j(\mathbf{k}_s, \mathbf{k}_0) = \langle \mathbf{k}_s | V_s^j | g_s^+ \rangle \langle W_{se} \rangle + \langle W_{se} \rangle \langle g_0^+ | V_s^j | \mathbf{k}_0 \rangle, \quad (20)$$

i.e., we have neglected fluctuation terms containing $g_r^+ - \langle g_r^+ \rangle$ ($r=s,0$) and $W_{se} - \langle W_{se} \rangle$. So, we obtain for the configurationally averaged cross section

$$\begin{aligned} \left\langle \frac{d\sigma_{(e,2e)}}{dE_s d\Omega_s dE_e d\Omega_e} \right\rangle &= \left\langle \frac{d\sigma_{(e,2e)}^{coh}}{dE_s d\Omega_s dE_e d\Omega_e} \right\rangle \\ &+ \left\langle \frac{d\sigma_{(e,2e)}^{incoh}}{dE_s d\Omega_s dE_e d\Omega_e} \right\rangle, \end{aligned} \quad (21)$$

where the terms

$$\begin{aligned} \left\langle \frac{d\sigma_{(e,2e)}^{coh}}{dE_s d\Omega_s dE_e d\Omega_e} \right\rangle &= \frac{k_s k_e}{(2\pi)^5 k_0} \sum_{jj'} \langle \langle \chi_{\mathbf{k}_e} | \langle M_j(\mathbf{k}_s, \mathbf{k}_0) \rangle \times A^-(\varepsilon) \langle M_{j'}^+(\mathbf{k}_s, \mathbf{k}_0) \rangle | \chi_{\mathbf{k}_e} \rangle \rangle, \end{aligned} \quad (22)$$

and

$$\begin{aligned} & \left\langle \frac{d\sigma_{(e,2e)}^{incoh}}{dE_s d\Omega_s dE_e d\Omega_e} \right\rangle \\ &= \frac{k_s k_e}{(2\pi)^5 k_0} \sum_j \{ x \langle \langle \chi_{\mathbf{k}_e} | M_{jA}(\mathbf{k}_s, \mathbf{k}_0) \times A^-(\varepsilon) M_{jA}^+(\mathbf{k}_s, \mathbf{k}_0) | \chi_{\mathbf{k}_e} \rangle \rangle \} \\ &+ (1-x) \langle \langle \chi_{\mathbf{k}_e} | M_{jB}(\mathbf{k}_s, \mathbf{k}_0) A^-(\varepsilon) M_{jB}^+(\mathbf{k}_s, \mathbf{k}_0) | \chi_{\mathbf{k}_e} \rangle \rangle \} \\ &- \langle \langle \chi_{\mathbf{k}_e} | \langle M_j(\mathbf{k}_s, \mathbf{k}_0) \rangle A^-(\varepsilon) \langle M_j^+(\mathbf{k}_s, \mathbf{k}_0) \rangle | \chi_{\mathbf{k}_e} \rangle \rangle \}. \end{aligned} \quad (23)$$

are the coherent and incoherent contributions to the cross section that arise from the coherent and the incoherent backscattering of the fast projectile electron, respectively. In Eqs. (22) and (23) we have in accordance with Eq. (16)

$$\langle M_j(\mathbf{k}_s, \mathbf{k}_0) \rangle = x M_{jA}(\mathbf{k}_s, \mathbf{k}_0) + (1-x) M_{jB}(\mathbf{k}_s, \mathbf{k}_0). \quad (24)$$

Note that we do not specify here the model for the configurational average related to the bound and ejected electron in the right hand sides of Eqs. (22) and (23). For example, it can be given by the VCA or KKR CPA. Moreover, different approximations can be employed for the bound- and ejected electron states.

III. RESULTS AND DISCUSSION

In this section, we apply the above formulas to the $(e,2e)$ from (001) face of aluminum-*sp*-metal alloys. We use the VCA implemented in jellium model to evaluate the configurational average in Eqs. (22) and (23). For aluminum-*sp*-metal alloys the use of VCA is justified by the weak electron scattering. The details of the calculations of the cross section given by Eq. (21) are presented in the Appendix. To make our analysis unambiguous, we avoid uncertainties related to the use of an *ad hoc* finite life times and energetic positions of the quasiparticles by considering emission from the Fermi level. The muffin-tin crystal potentials used for the present calculations are determined from self-consistent density-functional calculations within the local-density approximation.

Figure 2 shows the energy sharing distribution between the two emitted electrons for a certain total energy of the electron pair. Considering the case of clean aluminum ($x=1$) one observes a structure in the region $0.5 > |(E_s - E_e)/E_{tot}|$ and two structures in the regions $1 \geq |(E_s - E_e)/E_{tot}| > 0.5$ which correspond, respectively, to the electron-pair diffraction with the reciprocal-lattice vectors $\mathbf{g}_{||} = (00)$ and $\mathbf{g}_{||} = \pm(11)$.^{5,26} Transforming the relative energy scale in Fig. 2 into wave vector one, the width of the structure centered at equal energy sharing is given by $2k_F$. The diffraction picture is preserved in the case of alloys if we neglect the incoherent part of the cross section (23), because then both electrons see the virtual ordered lattice given by VCA. The effect of alloying on the coherent part of the cross section (22) is only a very slight change in the Fermi momentum for $\text{Al}_{0.85}\text{Mg}_{0.15}$ and $\text{Al}_{0.9}\text{Li}_{0.1}$, which is not seen for $\text{Al}_{0.985}\text{Pb}_{0.015}$ due to a very small concentration of Pb. As anticipated, the inclusion of Eq. (23) into Eq. (21) does not affect the results for $\text{Al}_{0.85}\text{Mg}_{0.15}$ since the difference between on-site muffin-tin potentials [see Eq. (12)] of the constituents is small. But in the case of $\text{Al}_{0.9}\text{Li}_{0.1}$ and especially $\text{Al}_{0.985}\text{Pb}_{0.015}$ the big difference between the on-site muffin-tin potentials induces a strong incoherent backscattering of the projectile electron. This changes qualitatively the energy sharing distribution curves. In particular, the diffraction structure corresponding to $\mathbf{g}_{||} = (00)$ is much less pronounced in contrast to the case when we neglect the disorder effect on the backscattering of the projectile electron. This reflects the

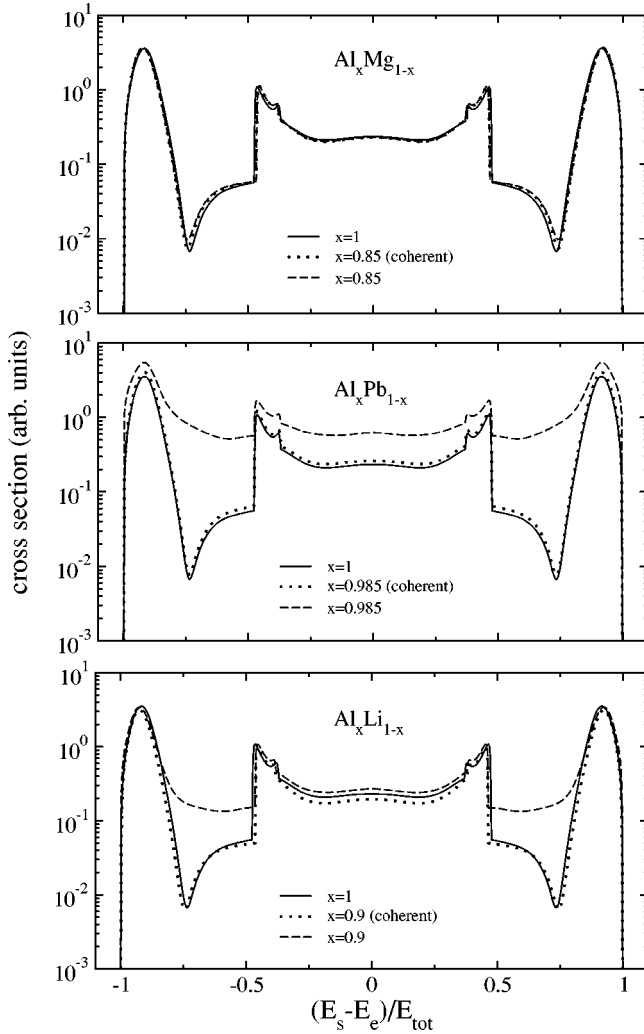


FIG. 2. The energy sharing distribution between an electron pair with a fixed total energy E_{tot} . The incidence projectile electron energy is $E_0 = 200$ eV and the (001) fcc face of the alloy is considered. The electron emission occurs from the Fermi level, i.e., $E_{tot} = E_0 - \Phi$ (Φ is the work function). The polar emission angles are $\theta_s = \theta_e = 45^\circ$ (see Fig. 1), whereas the azimuthal electrons' emission angles are $\varphi_s = 0^\circ$ and $\varphi_e = 180^\circ$ with respect to x axis directed along [100].

violation of the conservation law for the surface parallel wave vector of electron pair.

With respect to the Fig. 2, we note that, in general, for a correct description of the characteristic structure around equal energy sharing, we have to take into account the correlations between two electrons which are beyond the dynamical model suggested in Sec. I (e.g., as done in Ref. 27). For unequal energy sharing $|(E_s - E_e)/E_{tot}| \sim 1$ our dynamical model is appropriate. The results depicted in Fig. 2 are less influenced by the interelectronic correlation even when the two electrons escape with the same speed because the mutual emission angle of the electron pair is rather large.²⁷

In Fig. 3 the angular distribution of the ejected electron is shown for the same alloys and concentrations as in Fig. 2. The energy sharing condition $E_e = 0.1E_{tot}$ is chosen to ensure the applicability of the dynamical model. In addition, it

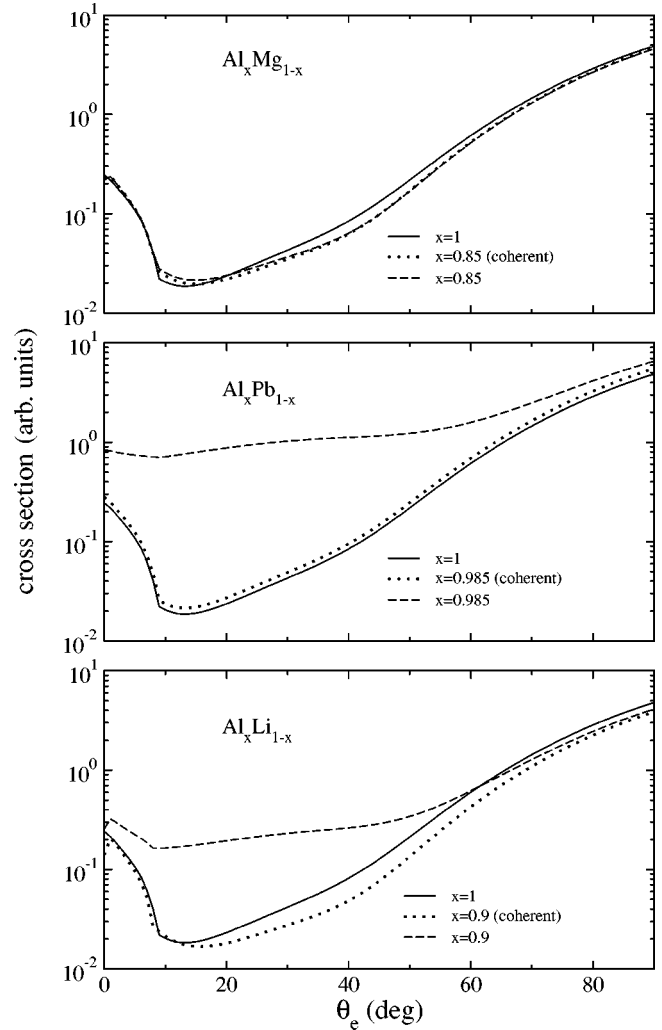


FIG. 3. The angular distribution of a slow electron with an energy $E_e = 0.1E_{tot}$ ejected from the Fermi level. The incident electron energy is $E_0 = 200$ eV. The other emission angles are $\theta_s = 45^\circ$, $\varphi_s = 0^\circ$, and $\varphi_e = 180^\circ$.

turns out that in this condition the magnitude of the cross section is particularly high. As noted in Fig. 2, there is almost no difference between the cross section results for pure Al and for $Al_{0.85}Mg_{0.15}$. For $Al_{0.9}Li_{0.1}$ and $Al_{0.985}Pb_{0.015}$ the effect of the incoherent backscattering of the projectile electron due to the disorder is much more pronounced than in Fig. 2. Indeed, in this case, the diffraction pattern is destroyed implying a loss of conservation of the surface parallel wave vector of the bound electron.

Since in Fig. 3, the ejected electron is slow its angular distribution is broad and slightly structured. This is to be contrasted with Fig. 4 where the angular distribution of the fast scattered electron is shown. One can see here the well pronounced peaks. Again the effect of the incoherent backscattering is very strong in the case of $Al_{0.9}Li_{0.1}$ and $Al_{0.985}Pb_{0.015}$, and it is absent in the case of $Al_{0.85}Mg_{0.15}$.

Finally, we note that the numerical results presented in Figs. (2–4) show almost no difference between the pure metal case and the case of alloying, when only coherent backscattering is taken into account. This is due to the simi-

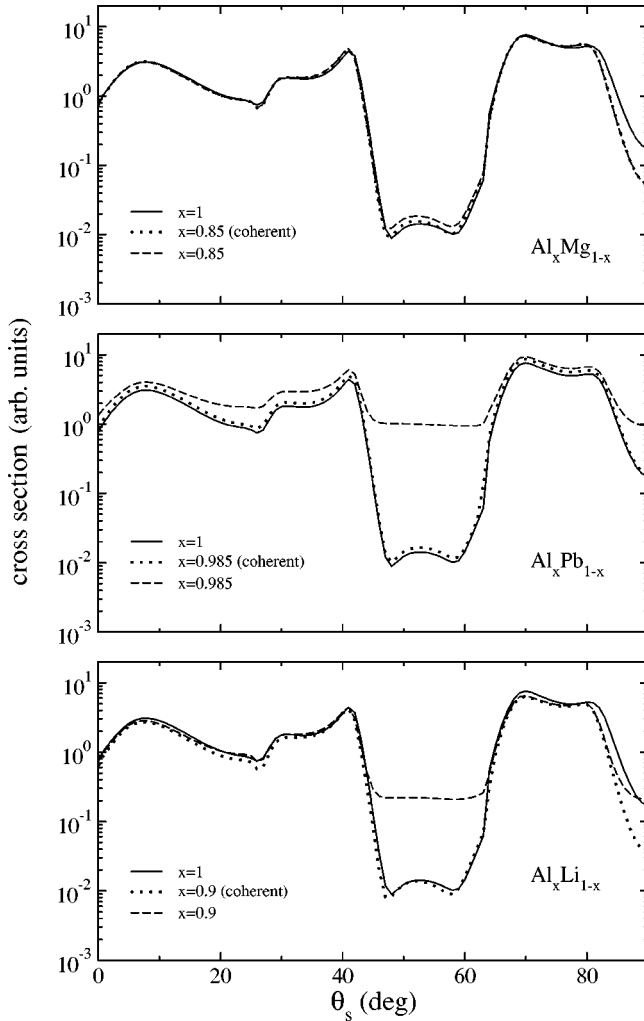


FIG. 4. The angular distribution of the fast scattered electron with energy $E_s = 0.9E_{tot}$. The other angles are $\theta_e = 45^\circ$, $\varphi_e = 180^\circ$, and $\varphi_s = 0^\circ$.

larity of electronic structure of the sp metals which have been chosen here to insure the validity of the present model.

IV. CONCLUSION

We have considered and analyzed theoretically the $(e,2e)$ process in the reflection mode from the surface of binary substitutional alloys. The present study is focused on the disorder effects on the scattering dynamics of the correlated electron pair. The numerical calculations of the cross sections for several alloys of aluminum with sp metals have been performed using VCA implemented within the jellium model to treat the bound- and the ejected electron states. Based on numerical calculations, we deduced that if the difference between the muffin-tin potentials of the constituents of the alloy is small, one can neglect the incoherent back-scattering of the fast projectile electron and evaluate the transition operator (9) with the average muffin-tin atomic potential. In this case it is possible to use the algorithm of the one-step model photoemission²⁸ based on KKR CPA substituting the dipole operator by the effective operator (9) aver-

aged in the spirit of VCA. This can be done for the numerical treatment of $(e,2e)$ from surfaces of such alloys as, for example, $\text{Cu}_x\text{Ni}_{1-x}$ and $\text{Ag}_x\text{Pd}_{1-x}$. On the other hand, if the difference between the muffin-tin atomic potentials of the constituents is not small, a more elaborate numerical treatment is required. In this case, the direct information on the alloy's electronic band structure is overshadowed by the effect of disorder on the scattering dynamics of the correlated electron pair. In particular, the direct information on the wave vector of the occupied bound-electron states may be lost. Nonetheless, it is possible to implement the algorithm²⁸ into numerical evaluation of the cross section (21) in order to extract the information on alloy's electronic band structure. The above main conclusions of our analysis imply that the incoherent effects in $(e,2e)$ restrict the class of disordered systems whose electronic structure can be studied directly by the present technique. The cases studied in this work do not confirm the long-standing expectations that, compared to photoemission, the $(e,2e)$ method is particularly good for the study of the disordered systems due to its ability to measure the real momentum of the bound electron (recall that in photoemission the crystal momentum is measured). In this respect, the high-energy transmission mode geometry seems to be more promising.²⁹ The other important point, which should be mentioned in connection with our analysis, is that, we did not consider the case of disordered surface structure deposited on clean crystalline substrate. The coherent electron-pair scattering off the substrate combined with the finite electron escape depth can provide direct access to the spectral properties of the disordered surface. However, each particular case of such disordered system requires particular elaborate numerical analysis in order to answer the question, whether the $(e,2e)$ method could be utilized for the detailed study of its electronic structure or not.

ACKNOWLEDGMENTS

We are grateful to Josef Kudrnovský, Jürgen Henk, and Patrick Bruno for the fruitful discussions and consultations and especially to Arthur Ernst, who provided us the data on the one-electron muffin-tin potentials from *ab initio* KKR band-structure calculations.

APPENDIX: MODEL OF METALLIC ALLOY

For the evaluation of Eq. (21), we have to determine the configurationally averaged states for the bound and for the slow ejected electrons. In addition an expression of the potentials V_s^j and $\langle W_{se} \rangle$ is needed. In this appendix, we present a procedure for the evaluation of these quantities.

Let us consider a semiinfinite metallic alloy filling the space in the negative z direction. Within the jellium model, the effective one-electron potential V_e is a step like one, i.e.,

$$V_e = -V_0 \theta(-z).$$

For a clean metallic material, we have

$$V_0^C = E_F^C + \Phi^C (C=A,B),$$

where E_F^C and Φ^C are the Fermi energy and the work function, respectively. The application of the virtual-crystal approximation in the case of an alloy yields

$$V_0 = xV_0^A + (1-x)V_0^B.$$

The wave functions and energy spectrum of an electron subject to this potential are

$$\chi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}_{\parallel}\mathbf{r}_{\parallel}} \{ \theta(z) B_{k_z} e^{-\gamma z} + \theta(-z) (e^{ik_z z} + A_{k_z} e^{-ik_z z}) \},$$

$$E_{\mathbf{k}} = \frac{1}{2} (k_{\parallel}^2 + k_z^2) - V_0, \quad (\text{A1})$$

where

$$A_{k_z} = \frac{k_z - i\gamma}{k_z + i\gamma}, \quad B_{k_z} = \frac{2k_z}{k_z + i\gamma}, \quad \gamma = \sqrt{2V_0 - k_z^2},$$

and $\sqrt{2V_0} \geq k_z \geq 0$. The Fermi energy is, thus, given by $E_F = (3\pi^2 n)^{2/3}/2$ with the concentration of valence electrons $n = N/v$. Here, $N = xN_A + (1-x)N_B$ and v are, respectively, the number of valence electrons and the volume per atom in the alloy. Constructing the wave function of slow ejected electron with energy $E_e = k_e^2/2$, we account for the damping of the electron wave inside the solid by adding small imaginary component iV_{0i} ($V_0 \gg V_{0i} > 0$) to the alloy's potential. Thus, the wave function is given by

$$\chi_{\mathbf{k}_e}(\mathbf{r}) = e^{i\mathbf{k}_e \cdot \mathbf{r}} \{ \theta(z) e^{ik_{e,z}z} + \theta(-z) e^{\alpha z} (A_1 e^{ik'_{e,z}z} + A_2 e^{-ik'_{e,z}z}) \}, \quad (\text{A2})$$

where

$$A_1 = \frac{k'_{e,z} + k_{e,z} + i\alpha}{2k'_{e,z}}, \quad A_2 = \frac{k'_{e,z} - k_{e,z} - i\alpha}{2k'_{e,z}}, \quad \alpha = \frac{V_{0i}}{k'_{e,z}} \approx \frac{1}{\lambda_e},$$

$$k'_{e,z} = \sqrt{\frac{k_{e,z}^2 + 2V_0 + [(k_{e,z}^2 + 2V_0)^2 - 4V_{0i}^2]^{1/2}}{2}} \approx \sqrt{k_{e,z}^2 + 2V_0},$$

with λ_e being the length of the inelastic mean-free path.

To arrive at a semianalytical results, we parametrize the potential V_s^j by a functional form corresponding to a Coulomb potential of the ion at lattice site j statically screened by the electrons in the alloy, i.e.,

$$V_s^{jC} = \frac{Z_C \exp(-\lambda_C |\mathbf{r}_s - \mathbf{R}_j|)}{|\mathbf{r}_s - \mathbf{R}_j|}, \quad (C=A,B). \quad (\text{A3})$$

The parameters Z_C and λ_C can be considered as the ionic charge and the screening constant, respectively, and \mathbf{R}_j stands for the coordinate of ion at lattice site j . The values of the parameters Z_C and λ_C are determined from a fit of Eq. (A3) to the one-electron muffin-tin potential obtained from self-consistent density-functional calculations within the local-density approximation. For the materials studied in this work, these *ab initio* potentials are well described by the analytical two-parameter expression (A3). Defining the potential $\langle W_{se} \rangle$, we neglect the effects of dynamical screening and account only for the static screening within the Thomas-Fermi model

$$\langle W_{se} \rangle = \frac{\exp(-\lambda_{TF} |\mathbf{r}_s - \mathbf{r}_e|)}{|\mathbf{r}_s - \mathbf{r}_e|}, \quad (\text{A4})$$

where λ_{TF} is the Thomas-Fermi screening constant. Now, we consider the propagators of the fast electron in Eq. (15). In the wave-vector space, the effects of the surface refraction and damping of the electron field can be incorporated into the propagators as follows

$$\begin{aligned} & \langle \langle \mathbf{k}_r + p' | g_r^+ | \mathbf{k}_r + p \rangle \rangle \\ &= \delta(p - p') \langle g_r^+ (\mathbf{k}_r + p) \rangle \\ &= \frac{\delta(p - p')}{E'_r - \frac{(\mathbf{k}_{r,\parallel} + p_{\parallel})^2}{2} - \frac{(k'_{r,z} + p_z)^2}{2} + iV_{0i,r}}, \quad (r=s,0), \end{aligned} \quad (\text{A5})$$

where $E'_r = E_r + V_0$ and $k'_{r,z} = \sqrt{k_{r,z}^2 + 2V_0}$ are, respectively, the energy and the wave vector normal to the surface of the refracted electron. The potential $iV_{0i,r}$ accounts for the damping.

Considering Eq. (A1), we can present the configurationally averaged spectral function (18) as follows

$$\langle A^-(\varepsilon) \rangle = f(\varepsilon) \sum_{\mathbf{k}} |\chi_{\mathbf{k}}| \langle \chi_{\mathbf{k}} | \delta(\varepsilon - E_{\mathbf{k}}), \quad (\text{A6})$$

where $f(\varepsilon)$ is the Fermi distribution function. Substituting Eq. (A6) into Eqs. (22) and (23), we receive

$$\begin{aligned} & \left\langle \frac{d\sigma_{(e,2e)}^{coh}}{dE_s d\Omega_s dE_e d\Omega_e} \right\rangle = \frac{k_s k_e}{(2\pi)^5 k_0} f(\varepsilon) \sum_{\mathbf{k}} \delta(\varepsilon - E_{\mathbf{k}}) \\ & \quad \times \left| \sum_j \langle \chi_{\mathbf{k}_e} | \langle M_j(\mathbf{k}_s, \mathbf{k}_0) \rangle | \chi_{\mathbf{k}} \rangle \right|^2, \end{aligned} \quad (\text{A7})$$

and

$$\begin{aligned} & \left\langle \frac{d\sigma_{(e,2e)}^{incoh}}{dE_s d\Omega_s dE_e d\Omega_e} \right\rangle = \frac{k_s k_e}{(2\pi)^5 k_0} f(\varepsilon) \sum_{\mathbf{k}} \delta(\varepsilon - E_{\mathbf{k}}) \\ & \quad \times \sum_j \{ x | \langle \chi_{\mathbf{k}_e} | M_{jA}(\mathbf{k}_s, \mathbf{k}_0) | \chi_{\mathbf{k}} \rangle |^2 \\ & \quad + (1-x) | \langle \chi_{\mathbf{k}_e} | M_{jB}(\mathbf{k}_s, \mathbf{k}_0) | \chi_{\mathbf{k}} \rangle |^2 \\ & \quad - | \langle \chi_{\mathbf{k}_e} | \langle M_j(\mathbf{k}_s, \mathbf{k}_0) \rangle | \chi_{\mathbf{k}} \rangle |^2 \}. \end{aligned} \quad (\text{A8})$$

1. Evaluation of $d\sigma_{(e,2e)}^{coh}$

Let us consider the on-site matrix element in Eq. (A7)

$$\begin{aligned} \langle \chi_{\mathbf{k}_e} | \langle M_j(\mathbf{k}_s, \mathbf{k}_0) \rangle | \chi_{\mathbf{k}} \rangle &= \int d\mathbf{Q} e^{i\mathbf{Q}\mathbf{R}_j} \langle V_s(\mathbf{Q}) \rangle \langle W_{se}(\mathbf{q} - \mathbf{Q}) \rangle \\ & \quad \times S_{\mathbf{k}_e, \mathbf{k}}(\mathbf{q} - \mathbf{Q}) [\langle g_s^+(\mathbf{k}_s + \mathbf{Q}) \rangle \\ & \quad + \langle g_0^+(\mathbf{k}_0 - \mathbf{Q}) \rangle] \end{aligned} \quad (\text{A9})$$

where, in accordance with Eqs. (A1)–(A5),

$$\begin{aligned} \langle V_s(\mathbf{Q}) \rangle &= xV_s^A(\mathbf{Q}) + (1-x)V_s^B(\mathbf{Q}) \\ &= \frac{4\pi x Z_A}{Q^2 + \lambda_A^2} + \frac{4\pi(1-x)Z_B}{Q^2 + \lambda_B^2}, \end{aligned} \quad (\text{A10})$$

$$\langle W_{se}(\mathbf{q}-\mathbf{Q}) \rangle = \frac{4\pi}{(\mathbf{q}-\mathbf{Q})^2 + \lambda_{TF}^2}, \quad \mathbf{q} = \mathbf{k}_0 - \mathbf{k}_s, \quad (\text{A11})$$

$$\langle g_s^+(\mathbf{k}_s + \mathbf{Q}) \rangle = \frac{1}{E'_s - \frac{(\mathbf{k}_{s,\parallel} + \mathbf{Q}_{\parallel})^2}{2} - \frac{(k'_{s,z} + Q_z)^2}{2} + iV_{0i,s}}, \quad (\text{A12})$$

$$\langle g_0^+(\mathbf{k}_0 - \mathbf{Q}) \rangle = \frac{1}{E'_0 - \frac{(\mathbf{k}_{0,\parallel} - \mathbf{Q}_{\parallel})^2}{2} - \frac{(k'_{0,z} - Q_z)^2}{2} + iV_{0i,0}}, \quad (\text{A13})$$

and

$$\begin{aligned} S_{\mathbf{k}_e, \mathbf{k}}(\mathbf{q}-\mathbf{Q}) &= \langle \chi_{\mathbf{k}_e} | e^{i(\mathbf{q}-\mathbf{Q})\mathbf{r}_e} | \chi_{\mathbf{k}} \rangle \\ &= \delta^{(2)}(\mathbf{k}_{\parallel} + \mathbf{q}_{\parallel} - \mathbf{Q}_{\parallel} - \mathbf{k}_{e,\parallel}) S_{k_{e,z}, k_z}(q_z - Q_z), \end{aligned} \quad (\text{A14})$$

with

$$\begin{aligned} S_{k_{e,z}, k_z}(q_z - Q_z) &= \frac{B_{k_z}}{\gamma + i(k_{e,z} - q_z + Q_z)} \\ &+ \frac{2\alpha + i(k_z + k_{e,z} + q_z - Q_z)}{[\alpha + i(k_z + q_z - Q_z)]^2 + k_{e,z}'^2} \\ &+ \frac{A_{k_z}[2\alpha + i(k_{e,z} + q_z - Q_z - k_z)]}{[\alpha + i(q_z - Q_z - k_z)]^2 + k_{e,z}'^2}. \end{aligned} \quad (\text{A15})$$

Performing the sum over the lattice sites j of the matrix elements (A9) and then integrating over \mathbf{Q}_{\parallel} , we derive

$$\langle M_{\mathbf{k}_e, \mathbf{k}}(\mathbf{q}) \rangle = \sum_{l, \mathbf{g}_{\parallel}} \delta^{(2)}(\mathbf{k}_{\parallel} + \mathbf{q}_{\parallel} - \mathbf{g}_{\parallel} - \mathbf{k}_{e,\parallel}) \langle M_{k_{e,z}, k_z}^{l, \mathbf{g}_{\parallel}}(\mathbf{q}) \rangle, \quad (\text{A16})$$

where

$$\begin{aligned} \langle M_{k_{e,z}, k_z}^{l, \mathbf{g}_{\parallel}}(\mathbf{q}) \rangle &= e^{i\mathbf{g}_{\parallel} \mathbf{t}_{\parallel}^l} \int dQ_z e^{iQ_z z_l} \langle V_s(\mathbf{g}_{\parallel}, Q_z) \rangle \\ &\times \langle W_{se}(\mathbf{q}_{\parallel} - \mathbf{g}_{\parallel}, q_z - Q_z) \rangle S_{k_{e,z}, k_z}(q_z - Q_z) \\ &\times [\langle g_s^+(\mathbf{k}_{s,\parallel} + \mathbf{g}_{\parallel}, k_{s,z} + Q_z) \rangle \\ &+ \langle g_0^+(\mathbf{k}_{0,\parallel} - \mathbf{g}_{\parallel}, k_{0,z} - Q_z) \rangle], \end{aligned} \quad (\text{A17})$$

and the sums are taken over the lattice planes l with coordinates z_l ($z_l < 0$ and $z_0 = -d_z/2$, where d_z is the interplane spacing) and the reciprocal lattice vectors \mathbf{g}_{\parallel} parallel to the surface, \mathbf{t}_{\parallel}^l stands for the parallel displacement of the l th plane with respect to the reference point in the surface. The integration in Eq. (A17) can be carried out analytically via residues technique.⁸ Thus, the final expression for (A7) reads

$$\begin{aligned} \left\langle \frac{d\sigma_{(e,2e)}^{coh}}{dE_s d\Omega_s dE_e d\Omega_e} \right\rangle &= \frac{k_s k_e}{(2\pi)^5 k_0} f(\varepsilon) \\ &\times \sum_{\mathbf{g}_{\parallel}} \frac{\theta[2(\varepsilon + V_0) - (\mathbf{q}_{\parallel} - \mathbf{k}_{e,\parallel} - \mathbf{g}_{\parallel})^2]}{k_z^0} \\ &\times \left| \sum_l \langle M_{k_{e,z}, k_z}^{l, \mathbf{g}_{\parallel}}(\mathbf{q}) \rangle \right|^2, \end{aligned} \quad (\text{A18})$$

where $k_z^0 = \sqrt{2(\varepsilon + V_0) - (\mathbf{q}_{\parallel} - \mathbf{k}_{e,\parallel} - \mathbf{g}_{\parallel})^2}$.

2. Evaluation of $d\sigma_{(e,2e)}^{incoh}$

Let us present Eq. (A8) in the form

$$\begin{aligned} \left\langle \frac{d\sigma_{(e,2e)}^{incoh}}{dE_s d\Omega_s dE_e d\Omega_e} \right\rangle &= \frac{k_s k_e}{(2\pi)^5 k_0} f(\varepsilon) \sum_{\mathbf{k}} \delta(\varepsilon - E_{\mathbf{k}}) \\ &\times \{x L_{\mathbf{k}_e, \mathbf{k}}^A(\mathbf{k}_s, \mathbf{k}_0) \\ &+ (1-x) L_{\mathbf{k}_e, \mathbf{k}}^B(\mathbf{k}_s, \mathbf{k}_0) \\ &- \langle L_{\mathbf{k}_e, \mathbf{k}}(\mathbf{k}_s, \mathbf{k}_0) \rangle\}, \end{aligned} \quad (\text{A19})$$

where

$$L_{\mathbf{k}_e, \mathbf{k}}(\mathbf{k}_s, \mathbf{k}_0) = \sum_j |\langle \chi_{\mathbf{k}_e} | M_j(\mathbf{k}_s, \mathbf{k}_0) | \chi_{\mathbf{k}} \rangle|^2, \quad (\text{A20})$$

with $L = L^A, L^B$, and $\langle L \rangle$ corresponding to $M_j = M_{jA}, M_{jB}$, and $\langle M_j \rangle$, respectively. It is straightforward to deduce that

$$L_{\mathbf{k}_e, \mathbf{k}}(\mathbf{k}_s, \mathbf{k}_0) = \sum_l |M_{k_{e,z}, k_z}^{l, \mathbf{K}_{\parallel}}(\mathbf{q})|^2, \quad (\text{A21})$$

where $M_{k_{e,z}, k_z}^{l, \mathbf{K}_{\parallel}}(\mathbf{q})$ is given by Eq. (A17) with the corresponding potential V_s (V_s^A , V_s^B , or $\langle V_s \rangle$) and $\mathbf{K}_{\parallel} = \mathbf{q}_{\parallel} + \mathbf{k}_{\parallel} - \mathbf{k}_{e,\parallel}$. Substitution of Eq. (A21) into Eq. (A19) yields

$$\begin{aligned} \left\langle \frac{d\sigma_{(e,2e)}^{incoh}}{dE_s d\Omega_s dE_e d\Omega_e} \right\rangle &= \frac{k_s k_e k}{(2\pi)^5 k_0} f(\varepsilon) \int_0^{\pi/2} d\theta_k \sin\theta_k \\ &\times \int_0^{2\pi} d\varphi_k \sum_l \{x |M_{k_{e,z}, k_z}^{l, \mathbf{K}_{\parallel}}(\mathbf{q}) \\ &\times [|M_{k_{e,z}, k_z}^{l, \mathbf{K}_{\parallel}}(\mathbf{q})|_A^2 + (1-x) |M_{k_{e,z}, k_z}^{l, \mathbf{K}_{\parallel}}(\mathbf{q})|_B^2 - \\ &\times \langle M_{k_{e,z}, k_z}^{l, \mathbf{K}_{\parallel}}(\mathbf{q}) \rangle|^2 \}, \end{aligned} \quad (\text{A22})$$

where $k = \sqrt{2(\varepsilon + V_0)}$ and $k_z = k \sin\theta_k$.

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