Self-consistent theory of scattering at disordered interfaces in layered nanostructures

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A self-consistent theory of electron scattering at the real disordered interfaces in the layered nanostructures is developed. This theory generalizes, particularly, the well known quantum mechanics results for the electron transmission through and reflection from the perfect potential steps/wells/barriers on the case of the intermixed (alloylike) interfaces. The closed analytical expressions for the probabilities of the specular and diffuse electron transmission and reflection at a single disordered interface are obtained in the self-consistent single-site coherent potential approximation (CPA) and the effective mass approximation for the electronic spectra of different layers. The exact (in the adopted approximations) quantum mechanical transmission amplitude for the electron traveling through two disordered interfaces of a trilayer is also obtained. These results allow studying the interfacial scattering at any angle of an electron incidence at an interface, any materials making up a multilayer (any potential profile and effective masses) and any concentrations of atoms mixed at an interface (particularly, at a nonzero average defect scattering strength). It is shown that the diffuse scattering (caused by the imaginary part of the coherent potential) vanishes at the grazing (with a very small perpendicular to an interface component of velocity) electron incidence at an interface leading to practically specular reflection from an interface (channeling affect). The specular scattering also dominates at close to normal to an interface electron incidence and small interfacial scattering potential fluctuations (from its average value). The diffuse scattering diminishes the specular transmission but may increase or decrease the specular reflection at a disordered interface and permits scattering to the areas (of the parallel to an interface electron momentum component) inaccessible for specular scattering at the perfect interfaces. The obtained specular transmission probability over a potential well of a metallic trilayer exhibits additional (to the conventional resonance states) oscillations caused by the real (average) part of the coherent interfacial potential. The interface roughness associated with the long-range layers' thicknesses fluctuations is accounted for through the semiclassical approximation for the obtained specular transmission probability through a metallic trilayer. For the case of an insulating spacer the obtained tunneling magnetoresistance (TMR) ratio may be expressed (for thick spacer) in the Slonczewski-type form but with the electron polarization and interface factors defined by the electron transmission probabilities (for different spin channels) through a spacer with disordered interfaces. The obtained results are believed to be important for the giant magnetoresistance (GMR) and TMR effects in the real nanostructures with disordered interfaces.

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I. INTRODUCTION

Transport phenomena in the artificial structures consisting of alternating magnetic and nonmagnetic layers, each of a few atomic layers thick, have been attracting a great deal of interest especially since the discovery of the giant magnetoresistance[1] (GMR) and tunneling magnetoresistance (TMR) effects.[2,3] These phenomena come from spin-dependent scattering (SDS) of the electrons (caused by the magnetic layers' density of state asymmetry at the Fermi energy) within the bulk of magnetic layers and at the interfaces between layers.

When the layer thicknesses are less than the spin-diffusion length (a spin-flip scattering is absent), spin-dependent scattering by defects and a spin-dependent electronic structure of a multilayer or sandwich give rise to the GMR [in the current perpendicular to plane (CPP) geometry] and TMR effects. The influence of a band structure on the GMR and TMR may be separated from the effect of spin-dependent scattering by the bulk defects in the ballistic regime, when the thicknesses of the layers are less than the electron mean free path [this condition is also essential for exhibiting the GMR in the current-in-plane (CIP) geometry]. The quantum scattering from quantum wells/barriers plays an important role in an explanation of the GMR/TMR in the case of ballistic regime. In the diffusive transport regime, when the sample dimensions are much larger than the electron mean free path, it is difficult to separate contributions of SDS by defects and spin-dependent electronic structure to the GMR and TMR.

There have been a number of works treating the GMR and TMR in the layered nanostructures with perfect interfaces. In the CPP geometry they are mainly based on an exact evaluation of the Kubo formula or related to that the Landauer formalism allowing the calculation of the conductances in terms of the electron transmission probabilities. For perfect interfaces, when there is two dimensional periodicity in the plane of the layers, the momentum of an electron parallel to the layers $\mathbf{k}_{\|}$ is conserved and, therefore, the Bloch electron may be only specularly transmitted through or reflected from the interfaces.

For such a case Schep *et al.*[4] calculated the GMR for a

perfect infinite superlattice using an *ab initio* band structure and found that in the ballistic regime for electrons (no scattering by defects at all) the GMR in the CPP geometry can be as large as in the diffusive regime when scattering by defects plays a decisive role in determining the resistance. Thus, an important role of a difference in electronic structure between parallel and antiparallel configurations of magnetic multilayers and of scattering from quantum wells in explaining the GMR has been demonstrated. Mathon *et al.*[5] calculated the ballistic CPP GMR of a Co/Cu/Co trilayer using realistic tight-binding bands fitted to *ab initio* band structures of Cu and Co. They found that the CPP GMR without impurity scattering can be as high as 90% and is due solely to specular quantum scattering of electrons from perfectly flat Co/Cu interfaces. Quantum interference effects lead to oscillations of the CPP GMR with the spacer and ferromagnet thickness.[5,6]

The importance of specular scattering has been also demonstrated by recent experiments that have used oxide layers to enhance specular scattering and increase the GMR in spin valves and magnetic multilayers.[7]

The giant magnetoresistance up to 40% is also exhibited by two ferromagnetic metals separated by an insulating nonmagnetic layer.[8,9] This tunneling magnetoresistance effect is conditioned by electrons' tunneling across the insulating spacer.[10] Recent calculations[11] and[12] have predicted extremely large TMR for certain systems based on the assumption of transverse momentum conserving (i.e., specular) transmission through interfaces.

An essential question then arises whether and how all above-mentioned predictions are affected by interfacial disorder. Advances in both molecular dynamics simulations and experimental techniques allowing now the crucial information on the structure of multilayer interface regions.[13,14] These studies show that the interfaces in some technologically important multilayers can be viewed as locally crystalline with interdiffusion of different atom species within a few layers of the interface. Based on these results, we will adopt for the interfacial structure a model of a disordered alloy made of atoms of the adjacent layers. When an interfacial disorder is present, the in-plane component of the electron wave vector may be no longer conserved and the effects of disorder on the specular and arising diffuse scattering of an electron at an interface are to be studied.

Standard semiclassical approaches characterize diffuse scattering at interfaces with a specularity constant which is the fraction of electrons that are specularly scattered. Most of these approaches (beginning from the method used by Fuchs over 60 years ago[15,16]) assumed that the probability for diffuse scattering was independent of the angle of incident (or equivalently of $\mathbf{k}_{\|}$) of the electron on the interface and of whether the electron was transmitted through or reflected from the interface.[17,18]

In the recent paper[19] the specular and diffuse transmission and reflection probabilities have been obtained for the interfacial scattering within a free electron model with a steplike interface (potential profile) in which random point scatterers are confined to the interfacial plane. It has been found that a specularity constant is not a constant, but depends on the angle of the electron incident at the interface (on $\mathbf{k}_{\|}$) and is different for reflected and transmitted electrons. To the lowest (second) order of perturbation theory in the scattering (impurity) potential the dependence of specular and diffuse scattering on $\mathbf{k}_{\|}$ has been obtained. For more realistic model in which Bloch electrons encounter a Co/Cu interface approximated by substitutional disorder and treated within the coherent potential approximation (CPA), the transmission and reflection probabilities in dependence on $\mathbf{k}_{\|}$ have also been numerically calculated using the Layer Korringa-Konh-Rostoker (LKKR) technique.[20]

In this paper, we generalize the perturbational approach of Ref. 19 in a way allowing for analytical treatment of electron scattering at a disordered interface in the cases when the conventional perturbation theory may not work. Particularly, it is the case when electrons strike an interface at the angles which are essentially different from the normal (perpendicular to the interface) ones, i.e., when the electron perpendicular velocities (in the neighboring layers) are small, and when the perpendicular velocities in the neighboring layers are close to each other (see Ref. 19). It is obviously important to account for such (grazing) electrons not only in the current-in-plane geometry (CIP GMR) but also for CPP GMR when integrating over all contributing electron channels ($\mathbf{k}_{\|}$) in the Landauer formalism. We will adopt the effective-mass approximation (EMA) for electronic spectrum used in Ref. 21 and introduce the coherent potential for disordered (alloy-like) interfaces allowing for treating the electron interfacial scattering self-consistently. It will enable us to develop a theory valid at all (relative to the interface plane) electron velocities and to obtain the closed expressions for electron specular and diffusive transmission and reflection probabilities for a single disordered interface averaged over all the arrangements of different atoms interdiffused at the interface.

The Green function representation of the transmission and reflection amplitudes shows[19] that the probability for the specular scattering at the disordered interface is defined by the average scattering T matrix, while the probability for diffuse scattering is given by the deviation of T matrix (from its average value). We introduce the self-consistency condition (implying that a single-site average T matrix vanishes) making it possible to separate the specular scattering from the diffuse one and express the specularity factor through the one-particle effective-medium Green function (its self-energy coincides with the coherent potential) alone and also providing the equation for the coherent potential (self-energy) of the reference medium. This fact distinguishes our approach from that of Refs. 21 and 19. It will be shown that the flux removed from the specular scattering by the diffuse scattering is defined by the imaginary part of the coherent potential and decreases with the electron perpendicular (to the interface) velocity. Thus, if the real part of the coherent potential (the average interfacial potential in the first approximation) is much bigger than the imaginary part (the fluctuations of the average scattering potential are small), the specular scattering may dominate. Note, that in the previous papers, Refs. 21, 22, and 19, the interfacial disorder has been characterized by the zero average potential and, therefore, the real and imaginary parts of the one-particle Green function's self-energy are of the same order of magnitude and defined (in the first approximation) by the interfacial poten-

tial average square fluctuations. The dependencies of the specular transmission and reflection probabilities (defined by the two-particle effective-medium Green function) on the angle of electron incidence at the interface ($\mathbf{k}_\parallel$) are plotted.

In the framework of the adopted model we have also managed to obtain the exact transmission amplitude for a freelike electron (considered in the EMA) passing through two disordered interfaces of a trilayer. This amplitude accounts for both the specular and diffuse scatterings and for all quantum interference effects. Introduction of the coherent potential, defined self-consistently, allows one to derive from the obtained exact transmission amplitude the exact formula for the specular part of the electron transmission probability. In the case of a metallic spacer this transition probability contains in the denominator an additional [to conventional $\propto\sin^2(k_2^\perp d)$] oscillating term, proportional to $\sin(2k_2^\perp d)$ ($k_2^\perp$ is the perpendicular to an interface electron momentum in a spacer and d is the spacer thickness). This additional term is caused by the real part of the interfacial coherent potential (average impurity potential). Both real and imaginary parts of the interfacial coherent potential lead to the modification of the transmission probability for a trilayer with perfect interfaces obtained in Ref. 23. For two identical metallic layers (separated by a metallic spacer) the obtained specular transmission probability reduces to the expression which generalizes the well known from the textbooks formula describing the electron transmission over a potential well (see, e.g., Ref. 24). The obtained formula contains in the denominator the square combination of the conventional $\sin(k_2^\perp d)$ term (responsible for resonance transmission) and the $\cos(k_2^\perp d)$ term, relative contribution of which is defined by the real part of the interfacial coherent potential. The semiclassical version of the specular transmission probability (with no oscillating terms caused by quantum interference effect) for a trilayer with rough interfaces is also considered. The obtained specular transmission probabilities are plotted as the functions of $\mathbf{k}_\parallel$.

Obtained in this paper exact (in the adopted model) electron transmission amplitude for an electron passing through a spacer (and two disordered interfaces) from one layer to another is also applicable to the case of an insulating spacer. The specular part of the transmission probability, derived from this exact amplitude, is a generalization of that for the perfect interfaces (see Refs. 25 and 26) in a sense that the electron velocities in all three layers are renormalized by the real and imaginary parts of the interfacial coherent potential. For a small barrier factor (thick spacer) the specular TMR may be written in the Slonczewski form[10] but with the modified by the coherent impurity potential polarization and interface factors. It is also shown, that in the case of a small barrier factor the total TMR (with account for both the specular and diffuse scattering) may be presented in the Slonczewski-type form with the generalized electron polarization defined by the difference between the spin majority and spin minority average (over imperfections configurations) electron transmission probabilities.

The plan of the paper is as follows. In Sec. II a general theory of an interfacial specular and diffuse scattering at a single disordered interface in the EMA and single-site CPA is given. This theory is extended in Sec. III to the case of a trilayer. The specular transmission probability for a metallic spacer is considered in Secs. III A and III B (semiclassical case), while that for an insulator spacer is treated in Sec. III C. The obtained results are summed up in Sec. IV.

II. TRANSMISSION THROUGH AND REFLECTION FROM A SINGLE DISORDERED INTERFACE

Let us first consider an electron scattering at a single disordered interface between two metals, that is important for the GMR effect. To obtain more analytical results, we will consider the materials in the EMA. The EMA is suitable for s electrons in the ferromagnetic (FM) materials, which primarily mediate a current, and for the majority d electrons. This approximation is especially appropriate for now actively considered dilute magnetic semiconductors (DMS) as the promising spintronics materials. Thus, our consideration may also be applied to the semiconductor/semiconductor and metal/semiconductor interfaces. The interfacial disorder is modelled by the short-range scattering centers located in the interface plane (y,z) and giving rise to the scattering potential $V(x,y,z)$. For the case of material and spin dependent electron's effective mass $m^*(x)$ and arbitrary conduction-band profile $U(x)$ (axis x is directed perpendicular to the interface) the Schrodinger equation for a single-electron state in the EMA reads

$$\left[-\frac{\hbar^2}{2}\nabla\frac{1}{m^*(x)}\nabla+U(x)+V(x,y,z)\right]\psi(x,y,z)=E\psi(x,y,z). \tag{1}$$

By expanding the wave function in the complete set of the transverse wave functions $\phi_{\mathbf{k}_\parallel}(\rho)$,

$$\psi(x,\rho)=\sum_{\mathbf{k}_\parallel}c_{\mathbf{k}_\parallel}(x)\phi_{\mathbf{k}_\parallel}(\rho),\ \phi_{\mathbf{k}_\parallel}(\rho)=\frac{e^{i\mathbf{k}_\parallel\rho}}{\sqrt{A}}, \tag{2}$$

where $\rho=(y,z)$, $\mathbf{k}_\parallel=(k_y,k_z)$, and A is the area of the interface, Eq. (1) may be reduced to the following one-dimensional equation for the longitudinal wave function $c_{\mathbf{k}_\parallel}(x)$ (see, e.g., Ref. 21)

$$\left(\frac{\partial}{\partial x}\right)\frac{1}{m^*(x)}\left(\frac{\partial}{\partial x}\right)c_{\mathbf{k}_\parallel}(x)+\frac{k^{\perp^2}(x)}{m^*(x)}c_{\mathbf{k}_\parallel}(x)=\sum_{\mathbf{k}'_\parallel}V_{\mathbf{k}_\parallel\mathbf{k}'_\parallel}(x)c_{\mathbf{k}'_\parallel}(x). \tag{3}$$

Here, the perpendicular wave vector $k^\perp(x)$ and the matrix element of the scattering potential $V_{\mathbf{k}_\parallel\mathbf{k}'_\parallel}(x)$ are defined as

$$k^{\perp^2}(x)=\frac{2m^*(x)}{\hbar^2}[E-U(x)]-\mathbf{k}_\parallel^2,$$

$$V_{\mathbf{k}_\parallel\mathbf{k}'_\parallel}(x)=\frac{2}{\hbar^2}\int d\rho\phi^*_{\mathbf{k}_\parallel}(\rho)V(x,\rho)\phi_{\mathbf{k}'_\parallel}(\rho). \tag{4}$$

At this stage we will take a different approach from the paper[21] approach. It is useful to introduce the translationally

invariant generally nonhermitian single-site (coherent) potential σ^0 defining the corresponding translationally invariant interfacial reference medium (hereinafter index 0 refers to the interface located at $x=0$). Thus, let us present the scattering interfacial potential in the following way:

$$V(x,\rho)=\sum_{\alpha}(\tilde{\gamma}_{\alpha}^{0}+\sigma^{0})\delta(x)\delta(\rho-\rho_{\alpha}). \tag{5}$$

Here, a summation is over all randomly distributed δ-impurity scatterers located at the interface ($x=0$) with the transverse positions ρ_α and the strength $\gamma_\alpha^0=\tilde{\gamma}_\alpha^0+\sigma^0$, where $\tilde{\gamma}_\alpha^0=\gamma_\alpha^0-\sigma^0$. If all disorder is at the interface [as it is assumed by Eq. (5)], then the values γ_α^0 can be estimated via the on-site potentials in the first, U_1, and second, U_2, materials. The rectangular potential profile is determined by $U(x)=U_1(x<0)$ and $U(x)=U_2(x>0)$ and can be related to γ_α^0 as $\gamma_\alpha^0\sim(|U_1-U_2|/2)(a/2)^3$, where a is the lattice constant. Accordingly, the material and spin dependent electron mass $m^*(x)$ in the ith material is labeled m_i (m_1 for $x<0$ and m_2 for $x>0$).

The matrix element of the scattering potential (5) is

$$V_{kk'}(x)=V_{kk'}\delta(x),\quad V_{kk'}=\frac{2}{\hbar^2}[\Sigma^0\delta_{kk'}+V_{kk'}^0],$$

$$\Sigma^0=n_i^0\sigma^0,\quad V_{kk'}^0=\sum_{\alpha}(V_{\alpha}^0)_{kk'},$$

$$(V_{\alpha}^0)_{kk'}=\frac{1}{A}\tilde{\gamma}_{\alpha}^0 e^{-i(k-k')\rho_{\alpha}}, \tag{6}$$

where $n_i^0=N_i^0/A$ is the interface impurity density (N_i^0 is the number of interfacial defects) and for the sake of simplicity we henceforth denote $\mathbf{k}_\parallel$ as k.

Use of Eq. (6) and integration of Eq. (3) across the $\delta(x)$ function from 0^- to 0^+ yields

$$\frac{1}{m_2}\left[\frac{dc_k(x)}{dx}\right]_{0^+}-\frac{1}{m_1}\left[\frac{dc_k(x)}{dx}\right]_{0^-}=\frac{2}{\hbar^2}\sum_{k'}(\Sigma^0\delta_{kk'}+V_{kk'}^0)c_{k'}(0). \tag{7}$$

Equation (7) defines the discontinuity of the wave function $c_k(x)$ derivative caused by electron scattering at the interface ($x=0$) disorder.

The longitudinal wave function $c_k(x)$ is defined as

$$c_k(x)=\frac{1}{\sqrt{v_1}}\delta_{kk'}e^{ik_1^{\perp}x}+\frac{1}{\sqrt{v_1}}r_{kk'}^{(1,2)}e^{-ik_1^{\perp}x},\quad x<0$$

$$=\frac{1}{\sqrt{v_2}}t_{kk'}^{(1,2)}e^{ik_2^{\perp}x},\quad x>0, \tag{8}$$

where $v_i=v_i(k)=\hbar k_i^{\perp}(k)/m_i$ is a perpendicular to the interface electron velocity dependent through the perpendicular wave vector $k_i^{\perp}(k)=\sqrt{(2m_i/\hbar^2)(E-U_i)-k^2}$ ($i=1,2$) of the parallel to the interface component k of the electron wave vector. The wave function $c_k(x)$ (8) with transverse momentum k results from the contribution of particles incoming to the interface in the first material with parallel momentum k' and transmitted to the state k in the second material with the amplitude $t_{kk'}^{(1,2)}$ or reflected from the interface with the second material with the amplitude $r_{kk'}^{(1,2)}$. The fluxes carried by the longitudinal parts of the wave function (8) are normalized to unity. The incident wave with k' gives rise to an infinite set of propagating (for real $k_i^{\perp}$) and evanescent (for imaginary $k_i^{\perp}$) modes. The wave function (8) is valid for both propagating and evanescent states (the latter ones are exponentially localized at the interface).

In order to obtain the transmission $t_{kk'}^{(1,2)}$ and reflection $r_{kk'}^{(1,2)}$ amplitudes one should match at the interface the wave functions $c_k(x)$ and their derivatives for $x<0$ and $x>0$. Thus, the continuity equation (at the interface $x=0$) for the wave function (8) should be combined with the equation which follows from Eqs. (7) and (8). The solution of these equations results in the following exact expression (in matrix notations) for the electron transmission amplitude $t^{(1,2)}$ through a single interface (located at $x=0$) between materials 1 and 2 with randomly distributed pointlike scatterers (compare with that from Ref. 21)

$$t^{(1,2)}=t^0=[I+i\Gamma^{(1,2)}]^{-1}\tilde{t}^{(1,2)}=\sum_{n=0}^{\infty}[-i\Gamma^{(1,2)}]^n\tilde{t}^{(1,2)}. \tag{9}$$

Here, $\tilde{t}^{(1,2)}$ is the transmission amplitude through a translationally invariant interface characterized by the single-site (coherent) potential σ^0, when the in-plane (parallel to an interface) electron's wave vector component k is conserved (specular scattering), with the matrix elements in k representation

$$\tilde{t}_{kk'}^{(1,2)}=2\frac{\sqrt{v_1v_2}}{v_1+v_2+i\frac{2}{\hbar}\Sigma^0}\delta_{kk'}, \tag{10}$$

I is a unity matrix with matrix elements $I_{kk'}=\delta_{kk'}$ and $\Gamma^{(1,2)}$ describes a scattering caused by the difference $\tilde{\gamma}_\alpha^0=\gamma_\alpha^0-\sigma^0$ which gives rise to the diffuse scattering (mixing between different transverse modes, when an in-plane momentum k is no longer conserved)

$$\Gamma_{kk'}^{(1,2)}=\frac{2}{\hbar}\frac{\sqrt{v_2}}{\left(v_1+v_2+i\frac{2}{\hbar}\Sigma^0\right)\sqrt{v_2'}}V_{kk'}^0, \tag{11}$$

where

$$v_i'=v_i(k')=(\hbar/m_i)k_i^{\perp}(k'),$$

$$k_i^{\perp}(k')=\sqrt{(2m_i/\hbar^2)(E-U_i)-k'^2}$$

(i.e., the velocity superscript corresponds to that of the variable k). As it follows from Eq. (6), V_{kk}^0 is the average fluctuation of interface impurity potential, which can be taken zero.

It is easy to represent the transmission amplitude (9) as

$$t_{kk'}^{(1,2)} = i\hbar\sqrt{v_2 v_1'}\,G_{kk'}^{(1,2)+}. \tag{12}$$

Here, the (retarded) Green function $G_{kk'}^{(1,2)+}$ is determined by the following series expansion:

$$G_{kk'}^{(1,2)+} = \tilde{G}_k^{(1,2)+}\delta_{kk'} + \tilde{G}_k^{(1,2)+}V_{kk'}^0\tilde{G}_{k'}^{(1,2)+} + \tilde{G}_k^{(1,2)+}\sum_{k_1} V_{kk_1}^0\tilde{G}_{k_1}^{(1,2)+}V_{k_1k'}^0\tilde{G}_{k'}^{(1,2)+} + \ldots, \tag{13}$$

where $\tilde{G}_k^{(1,2)+}$ is the effective-medium retarded Green function (propagator)

$$\tilde{G}_k^{(1,2)+} = \tilde{G}_{kk}^{(1,2)+} = \frac{2}{i\hbar\left(v_1 + v_2 + i\frac{2}{\hbar}\Sigma^{0+}\right)} = \frac{1}{[G_0^{(1,2)+}(k)]^{-1} - \Sigma^{0+}},$$

$$G_0^{(1,2)+}(k) = \frac{2}{i\hbar(v_1 + v_2)}, \tag{14}$$

diagonal in k space and describing the electron specular transmission through an interface with translationally invariant impurity potential $\Sigma^{0+}=n_i^0\sigma^{0+}$ [thus, we define the nonhermitian potential in Eq. (5) as σ^{0+}], and $G_0^{(1,2)+}(k)$ is the unperturbed (retarded) Green function corresponding to the case of a perfect interface.

In the real space the introduced Green function may be represented in the following way:

$$G^{(1,2)+}(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{A}\sum_{\mathbf{k}_\parallel,\mathbf{k}_\parallel'} G_{\mathbf{k}_\parallel\mathbf{k}_\parallel'}^{(1,2)+}\exp[i(k_2^\perp x_2 + \mathbf{k}_\parallel\rho)] \times\exp[-i(k_1^\perp x_1 + \mathbf{k}_\parallel'\rho')], \tag{15}$$

where $\mathbf{r}_i=(x_i,\rho)$, x_i denotes the perpendicular to an interface coordinates in the ith metal ($i=1,2$) and ρ is a two dimensional vector in the plane of the interface. The summation includes both propagating and evanescent states.

It is not difficult to rewrite Eq. (13) with the help of a scattering T matrix as

$$G_{kk'}^{(1,2)} = \tilde{G}_k^{(1,2)}\delta_{kk'} + \tilde{G}_k^{(1,2)}T_{kk'}^0\tilde{G}_{k'}^{(1,2)}, \tag{16}$$

where the T^0 matrix (for an interface at $x=0$) is defined as

$$T_{kk'}^0 = V_{kk'}^0 + \sum_{k_1} V_{kk_1}^0\tilde{G}_{k_1}^{(1,2)}V_{k_1k'}^0 + \sum_{k_1k_2} V_{kk_1}^0\tilde{G}_{k_1}^{(1,2)}V_{k_1k_2}^0\tilde{G}_{k_2}^{(1,2)}V_{k_2k'}^0 + \ldots. \tag{17}$$

Actually, we need to determine the electron transmission probability through the interface, which is defined by

$$\langle|G_{kk'}^{(1,2)}|^2\rangle = |\langle G_{kk'}^{(1,2)}\rangle|^2 + \sum_{k_1k_2}|\langle G_{kk_1}^{(1,2)}\rangle|^2 W_{k_1k_2}|\langle G_{k_2k'}^{(1,2)}\rangle|^2, \tag{18}$$

where $\langle\ldots\rangle$ denotes a configurational average over all the interface impurities configurations (over all possible impurity positions ρ_α) and $W_{kk'}$ is the vertex function. Using (16) and taking into consideration that the averaged one-particle Green function $\langle G_{kk'}^{(1,2)}\rangle$ is diagonal (the averaging restores the in-plane translational invariance) and, therefore, the averaged T matrix is also diagonal, Eq. (18) may be rewritten in the following way (compare with Ref. 19)

$$\langle|G_{kk'}^{(1,2)}|^2\rangle = \{|\tilde{G}_k^{(1,2)}|^2 + |\tilde{G}_k^{(1,2)}|^2 2\,\mathrm{Re}[\langle T_{kk}^{0+}\rangle\tilde{G}_k^{(1,2)+}] + |\tilde{G}_k^{(1,2)}|^2|\langle T_{kk}^0\rangle|^2|\tilde{G}_k^{(1,2)}|^2\}\delta_{kk'} + |\tilde{G}_k^{(1,2)}|^2[\langle|T_{kk'}^0|^2\rangle - |\langle T_{kk}^0\rangle|^2\delta_{kk'}]|\tilde{G}_{k'}^{(1,2)}|^2. \tag{19}$$

The result (19) is still exact in the framework of the adopted model. The first (diagonal) term defines the probability of specular scattering while the second one corresponds to the diffuse scattering. It is not difficult to show that at $k=k'$ the scattering matrix T_{kk}^0 is independent of the positions of the interface scatterers [see also Eq. (29) below] and, therefore, $T_{kk}^0=\langle T_{kk}^0\rangle$. Thus, the second term in Eq. (19) describing diffuse scattering (deviation of the T matrix from its average value) is equal to zero at $k=k'$.

By comparing Eqs. (18) and (19), it is seen that the specular scattering may be completely described by the Green's function $\tilde{G}_k^{(1,2)}$ for the effective medium Σ^0 if we choose the coherent potential Σ^0 in such a way that

$$\langle T_{kk}^{0+}(\Sigma^{0+})\rangle = 0. \tag{20}$$

In this self-consistent approach the average Green's function (16) reduces to

$$\langle G_{kk'}^{(1,2)+}\rangle = \tilde{G}_k^{(1,2)+}\delta_{kk'}, \tag{21}$$

and the vertex function, defining diffuse scattering, is

$$W_{kk'} = \langle|T_{kk'}^0|^2\rangle, \quad (k\neq k'). \tag{22}$$

Thus, as it follows from Eqs. (12), (14), (19), and (20) in the self-consistent approximation the transmission probability for a single interface is

$$T_{kk'}^{(1,2)} = \langle|t_{kk'}^{(1,2)}|^2\rangle = T_k^{(1,2)S}\delta_{kk'} + T_{kk'}^{(1,2)D}, \tag{23}$$

where the first term

$$T_k^{(1,2)S} = |\tilde{t}_{kk}^{(1,2)}|^2 = |i\hbar\sqrt{v_1 v_2}\tilde{G}_k^{(1,2)+}|^2 = \frac{4v_1(k)v_2(k)}{\left[v_1(k)+v_2(k)-\frac{2}{\hbar}\,\mathrm{Im}\,\Sigma^0\right]^2+\left(\frac{2}{\hbar}\,\mathrm{Re}\,\Sigma^0\right)^2} \tag{24}$$

fully describes the specular transmission probability through a homogeneous interface with the effective (coherent) potential Σ^0 on each site, and the second term

$$T_{kk'}^{(1,2)D} = \frac{16v_1(k')v_2(k)}{\hbar^2\left|v_1(k)+v_2(k)+i\frac{2}{\hbar}\Sigma^0\right|^2\left|v_1(k')+v_2(k')+i\frac{2}{\hbar}\Sigma^0\right|^2} \times\langle|T_{kk'}^0|^2\rangle, \quad (k\neq k') \tag{25}$$

defines the diffuse scattering caused by the potential fluctuations $\tilde{\gamma}_\alpha^0=\gamma_\alpha^0-\sigma^0$. Here, we restored the velocity dependence on k [$v_1'=v_1(k')$]. It should also be noted, that the second line of Eq. (24) is valid only for those values of k for which all $v_i(k)$ are real quantities (see more below).

We have also used the fact that the coherent potential Σ^0 is a complex quantity, i.e., $\Sigma^{0\pm}=\mathrm{Re}\Sigma^0\pm i\,\mathrm{Im}\,\Sigma^0$. Using analytical properties of Green functions $\tilde{G}_k^{(1,2)\pm}(\Sigma^{0\pm})$, it may be shown that $\mathrm{Im}\,\Sigma^0\leqslant 0$, and, therefore, e.g., $T_k^{(1,2)S}\leqslant 1$, as it is seen from Eq. (24).

As it follows from Eqs. (24) and (25), the transmission probability depends on the transverse wave vector $k=\mathbf{k}_\parallel$ and, therefore, on the angle at which an electron strikes the interface. Equation (24) shows that the interface disorder results in decrease of the specular transmission probability as compared to that for the perfect interface $4v_1v_2/(v_1+v_2)^2$. That decrease is due to an interface translationally invariant scattering (coherent) potential caused by the interface defects (emerging as the result of different atoms intermixing). The real part of the coherent potential $\mathrm{Re}\,\Sigma^0$ is caused (in the first approximation) by the average impurity potential (or the evanescent states localized at an interface) and the imaginary part $\mathrm{Im}\,\Sigma^0$ leads to the emerging of the diffuse scattering (see below).

Now, it is necessary to define more explicitly the coherent potential Σ^0 [fixed by Eq. (20)] and the vertex function (22). Because we defined σ^0 as a single-site translationally invariant potential (independent of the site α and k), the self-consistency condition (20) should also be considered in the single-site approximation. Therefore, the scattering T-matrix $T_{kk'}^0(\Sigma^0)$ in Eq. (20) should be calculated in the single-site approximation, i.e., $T_{kk'}^0$ in this equation [and in Eqs. (22) and (25)] should be replaced with the scattering T matrix in the single-site approximation $T_{kk'}^{0(1)}$. Thus, the equation for determining the coherent potential Σ^0 is

$$\langle T_{kk}^{0(1)+}(\Sigma^{0+})\rangle = 0. \tag{26}$$

The scattering T matrix (17) (in the operator form) may be represented in terms of a single-site scattering matrix T_α as (see, e.g., Ref. 27)

$$T^0 = \sum_\alpha T_\alpha^0 + \sum_\alpha T_\alpha^0\tilde{G}^{(1,2)}\sum_{\beta\neq\alpha} T_\beta^0 + \sum_\alpha T_\alpha^0\tilde{G}^{(1,2)}\sum_{\beta\neq\alpha} T_\beta^0\tilde{G}^{(1,2)}\sum_{\gamma\neq\beta} T_\gamma^0 + \ldots, \tag{27}$$

where a single-site scattering operator is

$$T_\alpha^0 = V_\alpha^0 + V_\alpha^0\tilde{G}^{(1,2)}V_\alpha^0 + V_\alpha^0\tilde{G}^{(1,2)}V_\alpha^0\tilde{G}^{(1,2)}V_\alpha^0 + \ldots = (1-V_\alpha^0\tilde{G}^{(1,2)})^{-1}V_\alpha^0. \tag{28}$$

Taking into account Eq. (6) and diagonality of $\tilde{G}^{(1,2)}$, the matrix element of the scattering matrix (27) in the single-site approximation $T^{0(1)}=\Sigma_\alpha T_\alpha^0$, where T_α^0 is defined by Eq. (28), may be written as

$$T_{kk'}^{0(1)} = \sum_\alpha (T_\alpha^0)_{kk'},$$

$$(T_\alpha^0)_{kk'} = \frac{1}{A}\frac{(\gamma_\alpha^0-\sigma^0)}{1-(\gamma_\alpha^0-\sigma^0)\frac{1}{A}\sum_{k_1}\tilde{G}_{k_1}^{(1,2)}}e^{-i(k-k')\rho_\alpha}. \tag{29}$$

The average (over scatterings' configurations) $\langle(T_\alpha^0)_{kk'}\rangle$ is diagonal in $k=\mathbf{k}_\parallel$ space, equal to $(T_\alpha^0)_{kk}$, and, therefore, does not depend on the positions of imperfections ρ_α. It may be seen explicitly if we adopt, e.g., the following configuration average procedure:

$$\langle f(\rho_1,\ldots,\rho_{N_i})\rangle = \left[\prod_{\alpha=1}^{N_i}\int\frac{d\rho_\alpha}{A}\right]f(\rho_1,\ldots,\rho_{N_i}), \tag{30}$$

where $f(\rho_1,\ldots,\rho_{N_i})$ is some function of the scatterers coordinates. Then, Eq. (26) for the coherent potential Σ^0 reads

$$\sum_\alpha\frac{(\gamma_\alpha^0-\sigma^0)}{1-(\gamma_\alpha^0-\sigma^0)\tilde{G}^{(1,2)+}(0,0)} = 0, \tag{31}$$

where $\tilde{G}^{(1,2)+}(0,0)=(1/A)\Sigma_k\tilde{G}_k^{(1,2)+}$ is the Green function in the real space (at the interface) in accordance with definition (15).

For the binary alloy type interface with $n_1^0=N_1^0/A$ density of the type 1 atoms and that of type 2 atoms $n_2^0=N_2^0/A$, ($N_1^0+N_2^0=N_i^0$) Eq. (31) may be rewritten as

$$\frac{n_1^0(\gamma_1^0-\sigma^0)}{1-(\gamma_1^0-\sigma^0)\tilde{G}^{(1,2)+}(0,0)}+\frac{n_2^0(\gamma_2^0-\sigma^0)}{1-(\gamma_2^0-\sigma^0)\tilde{G}^{(1,2)+}(0,0)} = 0, \tag{32}$$

where γ_1^0 and γ_2^0 are the scattering strengths for the atoms of the first and second materials mixed at the interface, respectively. In this case, evidently, $\gamma_{1,2}^0=\pm\gamma_0$, where the scattering strength $\gamma_0=\frac{1}{2}|U_1-U_2|(a/2)^3$ is defined by the difference of the on-site potentials in the neighboring materials [the energies are defined relatively to the average energy $\frac{1}{2}(U_1+U_2)$].

Accordingly, for the vertex function (22) in the self-consistent single-site approximation we have from Eq. (29) the following result:

$$W_{kk'} = \langle |T^{0(1)}_{kk'}|^2 \rangle = \sum_{\alpha} \frac{[(\gamma^0_\alpha - \sigma^0)/A]^2}{|1-(\gamma^0_\alpha - \sigma^0)\widetilde{G}^{(1,2)+}(0,0)|^2},$$

$$W_{kk'} = \frac{n^0_1(\gamma^0_1 - \sigma^0)^2/A}{|1-(\gamma^0_1 - \sigma^0)\widetilde{G}^{(1,2)+}(0,0)|^2} + \frac{n^0_2(\gamma^0_2 - \sigma^0)^2/A}{|1-(\gamma^0_2 - \sigma^0)\widetilde{G}^{(1,2)+}(0,0)|^2}, \quad (33)$$

where the second line is written for a binary alloy type interface.

It is important to again underline that in the considered single-site approximation for the coherent potential, when the scattering by clusters (of two and more) of the interface scatterers [which may lead to the interference effects like the (weak) Anderson localization[28]] is disregarded, the vertex function (as well as the self-energy Σ^0) does not depend on the incoming (k') and outcoming (k) transverse electron wave vectors. Thus, the results (24) and (25) for transmission probability correspond to the expressions obtained in Ref. 21 in the semiclassical approximation, but now the self-energy Σ^0 of the effective-medium Green function $\widetilde{G}^{(1,2)}_k$ is fixed by the self-consistency equation (31). Disregarding the mentioned phase coherence at the electron scattering by clusters may be justified, e.g., when the concentration of the interface defects is small enough.

In a similar way the reflection (from the interface) probability may be considered. The continuity relation for the wave function (8) at the interface may also be expressed through the Green function (12)

$$r^{(1,2)}_{kk'} = i\hbar\sqrt{v_1 v'_1}\, G^{(1,2)+}_{kk'} - \delta_{kk'}. \quad (34)$$

Proceeding in accordance with the outlined way above, we arrive at the following reflection (to the first substance from the interface between the first and second materials) probability in the CPA

$$R^{(1,2)} = \langle |r^{(1,2)}_{kk'}|^2 \rangle = R^{(1,2)S}_k \delta_{kk'} + R^{(1,2)D}_{kk'}. \quad (35)$$

Here, the first term

$$R^{(1,2)S}_k = |\tilde{r}^{(1,2)}_{kk}|^2 = |i\hbar v_1 \widetilde{G}^{(1,2)+}_k - 1|^2 = \left| \frac{v_1 - v_2 - i\frac{2}{\hbar}\Sigma^{0+}}{v_1 + v_2 + i\frac{2}{\hbar}\Sigma^{0+}} \right|^2 = \frac{\left[v_1(k) - v_2(k) + \frac{2}{\hbar}\,\mathrm{Im}\,\Sigma^0\right]^2 + \left[\frac{2}{\hbar}\,\mathrm{Re}\,\Sigma^0\right]^2}{\left[v_1(k) + v_2(k) - \frac{2}{\hbar}\,\mathrm{Im}\,\Sigma^0\right]^2 + \left[\frac{2}{\hbar}\,\mathrm{Re}\,\Sigma^0\right]^2} \quad (36)$$

defines the specular reflection from the "perfect" interface with the homogeneous coherent potential σ^0, while the second term

$$R^{(1,2)D}_{kk'} = \hbar^2 v_1 v'_1 |\widetilde{G}^{+}_k|^2 \langle |\widetilde{T}^{0(1)}_{kk'}|^2 \rangle |\widetilde{G}^{+}_{k'}|^2 = \frac{16 v_1(k) v_1(k')}{\hbar^2 \left| v_1(k) + v_2(k) + i\frac{2}{\hbar}\Sigma^{0+} \right|^2 \left| v_1(k') + v_2(k') + i\frac{2}{\hbar}\Sigma^{0+} \right|^2} \times \langle |T^{0(1)+}_{kk'}|^2 \rangle \quad (37)$$

is due to the diffuse scattering by fluctuations $\tilde{\gamma}_\alpha$. Here, the scattering T-matrix $T^{0(1)+}_{kk'}$ is given by Eq. (29) and, therefore, depends on the coherent potential Σ^0, which is defined by Eqs. (26) and (31) [or (32)]. The third line of Eq. (36) is valid for real velocities v_i.

It is important to underline here that the self-consistency condition (20) allows for obtaining the self-energy Σ^{0+}, which completely defines (in the adopted single-site approximation) the specular part of the transmission and reflection probabilities (compare with Ref. 21).

Again, due to inequality $\mathrm{Im}\,\Sigma^0 \leqslant 0$, the specular reflection probability does not exceed unity, as it follows from Eq. (36). Scattering at the interface imperfections leads to the change of the specular reflection probability from the perfect interface $(v_1 - v_2)^2/(v_1 + v_2)^2$ [compare with Eq. (36)] and to the emerging of the diffuse reflection (37). In the presence of a disordered interface the specular reflection probability (36) is no longer symmetric with regard to changing left and right materials ($v_1 \rightleftarrows v_2$), while the specular transmission probability (24) is. It is interesting to note from Eq. (36) that the random disorder at an interface results in a specularly reflected beam even for a symmetric case ($v_1 = v_2$) with a probability $|(1/\hbar)\Sigma^0|^2/|v_1 + i(1/\hbar)\Sigma^0|^2$, i.e., when there is no reflected beam ($R^{(1,2)S}_k = 0$) from a perfect interface (see also Ref. 19).

Summing the specular transmission and reflection probabilities (24) and (36), we find that the flux removed from specular scattering by diffuse scattering is (v_1 and v_2 are real)

$$1 - [T^{(1,2)S}_k + R^{(1,2)S}_k] = -4v_1 \frac{\frac{2}{\hbar}\,\mathrm{Im}\,\Sigma^0}{\left(v_1 + v_2 - \frac{2}{\hbar}\,\mathrm{Im}\,\Sigma^0\right)^2 + \left(\frac{2}{\hbar}\,\mathrm{Re}\,\Sigma^0\right)^2}. \quad (38)$$

We see that the diffuse scattering emerges due to the imaginary part ($\mathrm{Im}\,\Sigma^0 \leqslant 0$) of the self-energy (coherent potential) Σ^0. This fact is the consequence of the current conservation, which dictates that

$$\sum_{k}^{k \leqslant k^F_2} T^{(1,2)}_{kk'} + \sum_{k}^{k \leqslant k^F_1} R^{(1,2)}_{kk'} = 1, \quad (39)$$

where the summations are only over the propagating modes and

$$k_i^F = \sqrt{\frac{2m_i}{\hbar^2}(E_F - U_i)} \tag{40}$$

are the maximum transverse wave vectors corresponding to propagating modes in the first ($i=1$) and second ($i=2$) metals. Combined with the continuity relation (34), the current conservation (39) results in a special case of the optical theorem[21] relating the transmission probabilities $T_{kk'}^{(1,2)} = |t_{kk'}^{(1,2)}|^2$ and transmission amplitudes $t_{kk'}^{(1,2)}$, i.e., relating (in our case) the vertex function $W_{kk'}$ (defining the diffuse scattering) and the self-energy Σ^0 (defining the specular scattering by imperfections). In the symmetric case, $v_1=v_2=v$, i.e., $U_1=U_2=U$, $m_1=m_2=m$ [actually, we assume that, the differences of potential profiles and electronic masses in the neighboring layers are small, $|U_1-U_2|/E_F \ll 1$ and $|m_1-m_2|/(m_1+m_2) \ll 1$, which is a good approximation for the transition metal heterostructures like the Co/Cu based ones] Eq. (39) takes the following simple form

$$\sum_{k}^{k \leqslant k^F} T_{kk'}^{(1,2)} = \mathrm{Re}\, \tilde{t}_{k'k'}^{(1,2)}, \tag{41}$$

where $k^F = \sqrt{(2m/\hbar^2)(E_F - U)}$. Using Eqs. (41), (10), and (24), one can obtain the contribution of the diffuse scattering into the transmission probability

$$\sum_{k \neq k'}^{k \leqslant k^F} T_{kk'}^{(1,2)D} = \mathrm{Re}\, \tilde{t}_{k'k'}^{(1,2)} - T_{k'k'}^{(1,2)S} = -v' \frac{\frac{1}{\hbar}\,\mathrm{Im}\,\Sigma^0}{\left(v' - \frac{1}{\hbar}\,\mathrm{Im}\,\Sigma^0\right)^2 + \left(\frac{1}{\hbar}\,\mathrm{Re}\,\Sigma^0\right)^2}, \tag{42}$$

where $v'=v(k')$ is the velocity of an electron incoming at an interface.

The current conservation also implies that $R_{k'k'}^{(1,2)S} + \Sigma_{k \neq k'} R_{kk'}^{(1,2)D} = 1 - \mathrm{Re}\, \tilde{t}_{k'k'}^{(1,2)}$. Then, from Eqs. (10) and (36) [or from Eqs. (38) and (42)] it follows that the diffuse scattering contribution into reflection probability is equal to that for transmission probability (42) (in the considered symmetric case, when $v_1=v_2=v$).

The relative contributions of the specular scattering into the transmission and reflection probabilities are

$$\frac{T_{k'k'}^{(1,2)S}}{\sum_k T_{kk'}^{(1,2)}} = \frac{v'}{v' - \frac{1}{\hbar}\,\mathrm{Im}\,\Sigma^0},$$

$$\frac{R_{k'k'}^{(1,2)S}}{\sum_k R_{kk'}^{(1,2)}} = \frac{\left|\frac{1}{\hbar}\Sigma^0\right|^2}{\left|\frac{1}{\hbar}\Sigma^0\right|^2 - v'\frac{1}{\hbar}\,\mathrm{Im}\,\Sigma^0}. \tag{43}$$

The first equation (43) is also given in Ref. 21.

From the first equation (43) one can conclude ($\mathrm{Im}\,\Sigma^0 \leqslant 0$) that the relative contribution of diffuse scattering into transmission probability *increases* for larger incoming angles (smaller v'). On the contrary, the second equation (43) predicts that the relative contribution of diffuse scattering into the reflection probability *decreases* for small perpendicular (to an interface) velocity of an incident electron, i.e., for large (measured from the interface normal) incoming angles the reflection from the disordered interface tends to the practically specular one with the probability equal to unity (see above). The latter conclusion (see also below) is important for GMR in the CIP geometry and the interlayer coupling.[29] Thus, while, according to Eqs. (24), (25), (37), (38), and (42), the specular and diffuse transmission probabilities as well as the diffusive part of the reflection probability *decrease* with the increase of the angle of an electron incidence at the interface [and, according to the first equation (43) the specular transmission probability decreases faster than the diffusive one], the specular part of the reflection probability *increases* (up to unity) with the decrease of the electron's perpendicular velocity [see Eq. (36)] in accordance with the current conservation (39).

As it follows from Eqs. (24), (25), (36), and (37), the conventional perturbation theory[19] based on the "bare" Green function $G_0^{(1,2)}(k)$ [instead of the effective-medium Green function $\tilde{G}_k^{(1,2)}$ (14)] in the expansion (16), (17) may be only used for the problem under consideration if

$$\frac{2}{\hbar}\frac{|\Sigma^0|}{|v_1(k) \pm v_2(k)|} \ll 1. \tag{44}$$

For transmission probability it is the case when an electron strikes an interface with a small value of transverse momentum k (with a large perpendicular to the interface component of velocity) and for reflection probability $|v_1(k)-v_2(k)|$ should be big enough [see Eq. (45)]. Thus, if relation (44) holds, then equations for transmission and reflection probabilities may be expanded in the series in the small parameter (44). In the first approximation in the small parameter (44) the specular transmission and reflection probabilities are (at $\mathrm{Re}\,\Sigma^0 \sim \mathrm{Im}\,\Sigma^0$)

$$T_k^{(1,2)S} \approx \frac{4v_1(k)v_2(k)}{[v_1(k)+v_2(k)]^2}\left[1 + \frac{4}{\hbar}\frac{\mathrm{Im}\,\Sigma^0}{v_1(k)+v_2(k)}\right],$$

$$R_k^{(1,2)S} \approx \frac{[v_1(k)-v_2(k)]^2}{[v_1(k)+v_2(k)]^2}\left[1 + \frac{8}{\hbar}v_1(k)\frac{\mathrm{Im}\,\Sigma^0}{v_1^2(k)-v_2^2(k)}\right]. \tag{45}$$

As it is seen from Eq. (45), in this case the real part of self-energy [at $\bar{\gamma}_0=(1/N_i)\Sigma_\alpha \gamma_\alpha^0=0$ defined by the evanescent modes] is not important (for more details see below). The diffuse parts may be easily obtained in this approximation from Eqs. (25) and (37) by neglecting Σ^0 in the denominators and taking the scattering matrix in the corresponding approximation. If scattering is weak, Σ^0 practically coincides with the diagonal part of the scattering matrix $\langle T^{0(1)} \rangle$ (29), which is independent of k. In the second (Born) approxima-

tion for $\langle T^{0(1)}\rangle$ the formulas (45) coincide with those obtained and discussed in the paper.[19]

However, if relation (44) does not hold, the convergence of the perturbation expansion in this parameter is poor, and one should use the self-consistent approach (like that developed in this paper) with the introduction of a self-energy Σ^0, but not a nonself-consistent method based on the use of a bare Green's function $G_0^{(1,2)}$ (14) (instead of the Green function for an effective medium $\tilde{G}^{(1,2)}$) and the scattering T-matrix (instead of a self-energy).

Note, that for the practically used multilayers exhibiting large GMR effect, the band in one spin channel of magnetic metal should match closely an electronic band in a nonmagnetic spacer. Thus, in this case $v_1 \approx v_2$ and condition (44) is not satisfied.

Since the self-energy plays an important role, let us consider it in more detail. Equation (32) (for a binary-alloy-type interface with $\gamma_\alpha = \pm\gamma_0$) may be rewritten as follows:

$$\sigma^0 = \frac{\bar{\gamma}_0 + \gamma_0^2 \frac{1}{A}\sum_k \tilde{G}_k^{(1,2)+}}{1 + \sigma^0 \frac{1}{A}\sum_k \tilde{G}_k^{(1,2)+}}, \tag{46}$$

where $\bar{\gamma}_0 = (1/N_i^0)\Sigma_\alpha \gamma_\alpha^0 = (c_1 - c_2)\gamma_0$, $\gamma_0 = \frac{1}{2}|U_1 - U_2|(a/2)^3$, $c_{1,2} = N_{1,2}^0/N_i^0$ are the concentrations of the first and second materials mixed at the interface ($c_1 + c_2 = 1$), $\tilde{G}_k^{(1,2)+}$ is defined by Eq. (14) and summation (integration) over the parallel (to an interface) wave vector includes both propagating and evanescent intermediate states. The evanescent states come from integration over the range $k > k_i^F$ (40), where the electron velocity $v_i(k)$ is purely imaginary. The summation over evanescent states should be cutoff at a wave vector αk_i^F ($\alpha \geqslant 1$) to account for the finite range of the scattering potential and to avoid an ultraviolet divergence which is a consequence of using the δ-like impurity potentials (5). If $\bar{\gamma}_0 \neq 0$, ($c_1 \neq c_2$), the expression for the coherent potential σ^0 may be obtained by iterating Eq. (46). In the first approximation $\sigma^0 = \bar{\gamma}_0$ and, therefore, $\Sigma^0 = \mathrm{Re}\,\Sigma^0 = n_i^0 \bar{\gamma}_0$. In this approximation $\mathrm{Im}\,\Sigma^0 = 0$ and the diffuse scattering is absent, as it follows from Eq. (38). In the next approximation

$$\Sigma^0 = n_i^0 \bar{\gamma}_0 + n_i^0 [\gamma_0^2 - (\bar{\gamma}_0)^2] \frac{1}{A}\sum_k \bar{G}_k^{(1,2)+}. \tag{47}$$

Here, $\bar{G}_k^{(1,2)+}$ is defined by Eq. (14), where Σ^{0+} is substituted with $n_i^0 \bar{\gamma}_0$ and $\gamma_0^2 = \overline{\gamma_0^2} = \Sigma_\alpha (\gamma_\alpha^0)^2 / N_i^0$. The self-energy (coherent potential) is now complex [the second term in Eq. (47) has both the real and imaginary parts]. If $\bar{\gamma}_0 \neq 0$, then, the fluctuations of the scattering potential are small, i.e., $([\gamma_0^2 - (\bar{\gamma}_0)^2]/(\bar{\gamma}_0)^2)|\bar{\gamma}_0 (1/A)\Sigma_k \bar{G}_k^{(1,2)+}| \ll 1$, when $[\gamma_0^2 - (\bar{\gamma}_0)^2]/(\bar{\gamma}_0)^2 = 4c_1c_2/(1-4c_1c_2) \lesssim 1$, because the perturbative expansion (47) presumes that $|\bar{\gamma}_0 \bar{G}^{(1,2)+}| = |\bar{\gamma}_0 (1/A)\Sigma_k \bar{G}_k^{(1,2)+}| \ll 1$. It can be easily shown, that, if the self-energy is small, $|(2/\hbar)\Sigma^0|/v^F \approx (2/\hbar) n_i^0 |\bar{\gamma}_0|/v^F = (2|\bar{\gamma}_0| m/\hbar^2)(n_i^0/k^F) \ll 1 (v^F = \hbar k^F/m)$, then, $|\bar{\gamma}_0 \bar{G}^{(1,2)+}| \approx |\bar{\gamma}_0| m k^F / 2\pi\hbar^2$ (for evaluation of the integral over k, we neglected for simplicity the difference in the potential profiles and effective masses in different layers). Thus, the condition $(2\bar{\gamma}_0 m/\hbar^2)(n_i^0/k^F) \approx 2\bar{\gamma}_0 m k^F/\hbar^2 \ll 1$ (we put $n_i^0 \approx 1/a^2 \approx k^{F^2}$) leads to the needed smallness of the perturbative parameters $|\bar{\gamma}_0 \bar{G}^{(1,2)+}| \ll 1$ and, therefore, the weak-scattering parameter $\bar{\gamma}_0 m k^F/2\pi\hbar^2 \ll 1$ (see also Ref. 21) is equivalent to the condition for the self-energy smallness $|(2/\hbar)\Sigma^0|/v^F \ll 1$. In this case of weak scattering and when $c_1 c_2 \leqslant 1/8$, $|\mathrm{Re}\,\Sigma^0| \approx |n_i^0 \bar{\gamma}_0| \gg |\mathrm{Im}\,\Sigma^0|$, because $\mathrm{Im}\,\Sigma^0$ (defined by the scattering potential fluctuations) is of the next order of the perturbation expansion [in $|(2/\hbar)\Sigma^0|/v^F$].

However, as it follows from Eqs. (43), in the considered case of weak scattering regime, when $|(2/\hbar)\Sigma^0|/v^F \ll 1$, $\bar{\gamma}_0 \neq 0$, $c_1 c_2 \leqslant 1/8$ and, therefore, $|\mathrm{Re}\,\Sigma^0| \gg |\mathrm{Im}\,\Sigma^0|$, both specular transmission and reflection dominate if the fluctuations of scattering strength are small, $[\gamma_0^2 - (\bar{\gamma}_0)^2]/(\bar{\gamma}_0)^2 = 4c_1c_2/(1-4c_1c_2) \ll 1$, i.e., $c_1 c_2 \ll 1/8$, and the incoming electron velocity v' is close to v^F (close to normal incidence at the interface). The specular transmission is much larger than the diffusive one, when $v' \gg |(1/\hbar)\mathrm{Im}\,\Sigma^0|$, and it is definitely realized for $v' \approx v^F \gg |(2/\hbar)\Sigma^0|$. The specular reflection dominates when $|(1/\hbar)\Sigma^0|^2 \gg |v'(1/\hbar)\mathrm{Im}\,\Sigma^0|$ and, for the case under consideration and $v' \approx v^F$, this condition reduces to $|\mathrm{Im}\,\Sigma^0|/|\mathrm{Re}\,\Sigma^0| \approx ([\gamma_0^2 - (\bar{\gamma}_0)^2]/(\bar{\gamma}_0)^2)|\bar{\gamma}_0 \bar{G}^{(1,2)+}| \ll (1/\hbar)|\mathrm{Re}\,\Sigma^0|/v_F \approx |\bar{\gamma}_0 \bar{G}^{(1,2)+}| \ll 1$, which leads to the above-mentioned criterion $c_1 c_2 \ll 1/8$.

If $\bar{\gamma}_0 = 0$ ($c_1 = c_2$), then, according to Eqs. (46) and (14), in the first approximation in the small parameter $2\Sigma^0/\hbar v^F \approx (2/\hbar v^F) n_i^0 \gamma_0^2 (1/A)\Sigma_k G_0^{(1,2)+}(k) \approx (1/\pi)(\gamma_0 m k^F/\hbar^2)^2 \ll 1$, $\mathrm{Re}\,\Sigma^0 \sim \mathrm{Im}\,\Sigma^0 \sim n_i^0 \gamma_0^2 (1/A)\Sigma_k G_0^{(1,2)+}(k)$, and in this case $\mathrm{Re}\,\Sigma^0$ is due to the contribution of evanescent states into the sum over k. Thus, the approximate formulas (45) rather correspond to this situation ($\bar{\gamma}_0 = 0$).

To numerically model the dependence of specular transmission and reflection probabilities on k (on the angle of incidence of electron at an interface) and to identify the parameters governing this dependence, it is convenient to present Eqs. (24) and (36) in terms of the following dimensionless parameters:

$$\tilde{k} = k/k_1^F, \quad a = k_2^F/k_1^F, \quad b = m_1/m_2,$$

$$\gamma_0' = (2/\hbar)\mathrm{Re}\,\Sigma^0/v_1^F, \quad \gamma_0'' = (2/\hbar)\mathrm{Im}\,\Sigma^0/v_1^F, \tag{48}$$

where $v_i^F = \hbar k_i^F/m_i$ ($i = 1, 2$) and k_i^F is given by Eq. (40). It is worth reminding that $\mathrm{Im}\,\Sigma^0 \leqslant 0$ ($\gamma_0'' \leqslant 0$). Thus, the dimensionless parameter of the perturbation theory in the scattering strength is $(2/\hbar)|\Sigma^0|/v_1^F$ (as it has been already noted above).

We will plot Eqs. (24) and (36) in the range, where $\tilde{k}$ changes from $\tilde{k} = 0$ (perpendicular to an interface electron incidence from metal 1) up to $\tilde{k} = 1$ (parallel incidence). If $k_2^F \geqslant k_1^F$ ($a \geqslant 1$), there is no contribution of the evanescent states to Eqs. (24) and (36). If $k_2^F < k_1^F$ ($a < 1$), then $\tilde{k}$ also takes the values $1 \geqslant \tilde{k}^2 > a^2$ that corresponds to evanescent states in material 2 to which an electron transmits to or reflects from. Note, that when $\tilde{k} \to 1$ ($v_1 \to 0$), the specular

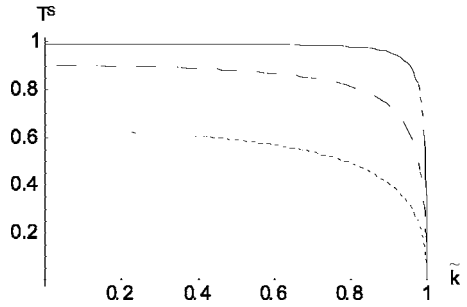

FIG. 1. Specular transmission probability $T^{(1,2)S}(\tilde{k})$ for Co(majority)/Cu interface ($a=\sqrt{2.746/2.230}$, $b=1$, $\tilde{k}=k_x/k_1^F$, $k_1^F=k_{\mathrm{Co}(maj)}^F$). Solid line—no intermixing ($\gamma_0'=0$, $\gamma_0''=0$); dashed line—an intermixed interface with the predominance of specular scattering ($\gamma_0'=0.5$, $\gamma_0''=-0.05$); dotted line—an intermixed interface with more contribution of diffuse scattering ($\gamma_0'=0.5$, $\gamma_0''=-0.5$).

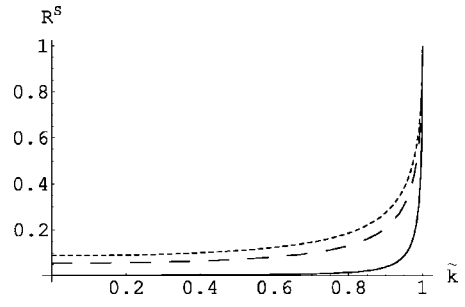

FIG. 2. Specular reflection probability $R^{(1,2)S}(\tilde{k})$ for Co(majority)/Cu interface ($a=\sqrt{2.746/2.230}$,$b=1$,$\tilde{k}=k_x/k_1^F$,$k_1^F=k_{\mathrm{Co}(maj)}^F$). Solid line—no intermixing ($\gamma_0'=0$,$\gamma_0''=0$); dashed line—an intermixed interface with prevailing specular scattering ($\gamma_0'=0.5$,$\gamma_0''=-0.05$); dotted line—an intermixed interface with more contribution of the diffuse scattering ($\gamma_0'=0.5$,$\gamma_0''=-0.5$).

transmission (24) and reflection probabilities (36) tend to zero and unity, correspondingly.

When $\tilde{k}^2 \geqslant a^2$ ($a \leqslant 1$) the velocity v_2 in the transmission $\tilde{t}_{kk}^{(1,2)}$ (10) and reflection $\tilde{r}_{kk}^{(1,2)}$ (36) amplitudes should be replaced with $iV=b(\hbar/m_1)k_2^{\perp}$, where $k_2^{\perp}=ik_1^F\sqrt{\tilde{k}^2-a^2}=iK$ ($1 \geqslant \tilde{k} \geqslant a, a \leqslant 1$). In this range of k the transmitted waves are evanescent [in Eq. (8) $k_2^{\perp}=iK$ is imaginary] and the specular transmission and reflection probability take the form (see also Sec. III C below)

$$T_k^{(1,2)S}=\frac{4v_1V}{\left(v_1-\frac{2}{\hbar}\,\mathrm{Im}\,\Sigma^0\right)^2+\left(V+\frac{2}{\hbar}\,\mathrm{Re}\,\Sigma^0\right)^2}e^{-2Kd},$$

$$R_k^{(1,2)S}=\frac{\left(v_1+\frac{2}{\hbar}\,\mathrm{Im}\,\Sigma^0\right)^2+\left(V+\frac{2}{\hbar}\,\mathrm{Re}\,\Sigma^0\right)^2}{\left(v_1-\frac{2}{\hbar}\,\mathrm{Im}\,\Sigma^0\right)^2+\left(V+\frac{2}{\hbar}\,\mathrm{Re}\,\Sigma^0\right)^2},$$

$$1 \geqslant \tilde{k} \geqslant a, \quad a \leqslant 1. \tag{49}$$

It is interesting to note, that the specular reflection probability (49) from a potential barrier is less than unity if $\mathrm{Im}\,\Sigma^0 \neq 0$ ($\mathrm{Im}\,\Sigma^0 < 0$). This is due to the diffuse scattering. However, when $v_1(k)$ tends to zero ($\tilde{k} \to 1$) and the diffuse scattering vanishes [see Eq. (38)], then $R_k^{(1,2)S} \to 1$. In the absence of disorder at the interface ($\Sigma^0=0$), $R_k^{(1,2)S}=1$ for $1 \geqslant \tilde{k} \geqslant a, a \leqslant 1$ as it should be (total reflection).

The specular transmission (24) and reflection (36) and (49) probabilities are plotted in Figs. 1, 2, and 3 as the functions of $\tilde{k}=k/k_1^F$ for different potential profiles (a) and scattering strength (γ_0', γ_0'').

Specular transmission and reflection probabilities are plotted in Figs. 1 and 2 for Co(majority)/Cu interface for which a potential step $a=\sqrt{2.746/2.230}>1$ is estimated via the on-site energies of majority d electrons of Co ($E^F-U_{\mathrm{Co}}^{maj}=2.230$ eV) and d electrons of Cu ($E^F-U_{\mathrm{Cu}}=2.746$ eV). The majority channel was chosen because it has only one Bloch state for most $k=\mathbf{k}_{\parallel}$ in both Co and Cu and, therefore, in this case the adopted parabolic effective-mass approximation for the electronic spectrum with $m_1=m_2$ ($b=1$) is expected to be reasonable. For a perfect interface the transmission probability is high and the reflection is low (solid lines) for most values of k due to close matching $[(U_{\mathrm{Co}}^{maj}-U_{\mathrm{Cu}})/E^F \ll 1]$ of the bands for majority Co and Cu. The dashed lines represent the situation when the real part of the coherent potential Σ^0 is essentially bigger than the imaginary part ($\gamma_0' \gg |\gamma_0''|$), i.e., the fluctuations of the interface potential are small. In this situation the diffuse scattering is small [see Eq. (38)], and the specular transmission and reflection probabilities are mostly affected (in addition to the interface potential step) by the specular interface scattering caused by intermixing. Figures 1 and 2 show, that the interface intermixing affects the specular transmission and reflection probabilities more strongly for large values of k (small perpendicular velocities). The specular transmission probability *decreases* due to additional scattering caused by an alloylike Co/Cu interface for all k and drops as the momentum parallel to the interface increases. On the other hand, in this situation ($v_2 > v_1$) the intermixed interface scattering leads to the *increase* of the specular reflection as compared to the perfect interface.

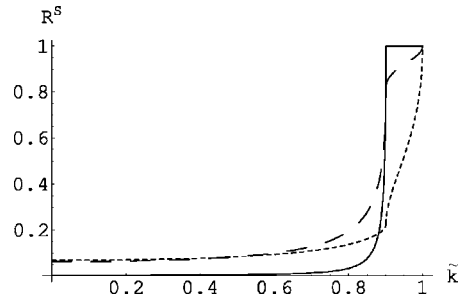

FIG. 3. Specular reflection probability $R^{(1,2)S}(\tilde{k})$ for Cu/Co(majority) inverted intermixed interface ($a=\sqrt{2.230/2.746}<1$,$b=1$,$\tilde{k}=k_x/k_1^F$,$k_1^F=k_{\mathrm{Cu}}^F$). Solid line—no intermixing ($\gamma_0'=0$,$\gamma_0''=0$); dashed line ($\gamma_0'=0.5$,$\gamma_0''=-0.05$) and dotted line ($\gamma_0'=0.5$,$\gamma_0''=-0.5$)—influence of specular and diffuse scattering caused by intermixing.

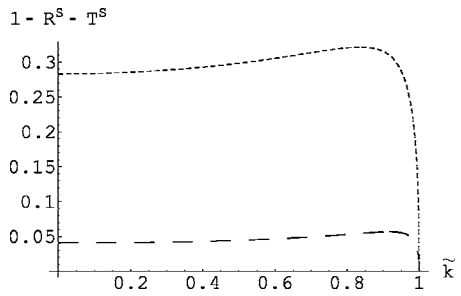

FIG. 4. Dependence of the diffuse scattering on the angle of electron incidence [Eq. (38)] for Co(majority)/Cu interface ($a=\sqrt{2.746/2.230}>1, b=1$, $\tilde{k}=k_x/k_1^F, k_1^F=k_{\mathrm{Co}(maj)}^F$). Dashed line—intermixed interface with small interface potential fluctuations ($\gamma_0'=0.5, \gamma_0''=-0.05$); dotted line—intermixed interface with essential interface potential fluctuations ($\gamma_0'=0.5, \gamma_0''=-0.5$).

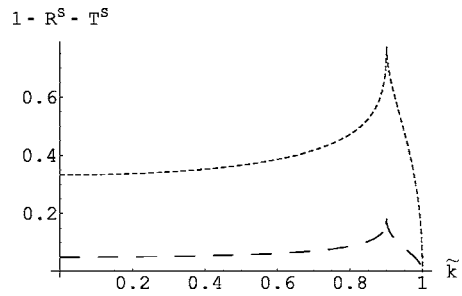

FIG. 5. Dependence of the diffuse scattering on the angle of electron incidence [Eqs. (38) and (50)] for Cu/Co (majority) interface ($a=\sqrt{2.230/2.746}<1, b=1, \tilde{k}=k_x/k_1^F, k_1^F=k_{\mathrm{Cu}}^F$). Dashed line—intermixed interface with small interface potential fluctuations ($\gamma_0'=0.5, \gamma_0''=-0.05$); dotted line—intermixed interface with essential interface potential fluctuations ($\gamma_0'=0.5, \gamma_0''=-0.5$).

These results are in accordance with the first-principles calculations made in Ref. 19 for Co/Cu interface. The dotted lines in Figs. 1 and 2 show that the increased diffuse scattering more essentially influences the specular transmission probability (leads to its further decrease) than the specular reflection, which increases slightly [in the considered case ($a>1$, i.e., $v_2>v_1$)]. This fact may be important for CIP GMR and the interlayer coupling.[29]

Figure 3 shows the specular reflection probability from the inverted Cu/Co(majority) interface, i.e., for the case when an electron comes to the interface from Cu (in Figs. 1 and 2 an electron comes to an interface from Co), where its velocity is larger than in Co ($a=\sqrt{2.230/2.746}<1$, i.e., $v_1>v_2$). In this case ($v_1>v_2$) at $\tilde{k}\geqslant a=\sqrt{2.230/2.746}$ ($V\geqslant 0$) and in the absence of the diffuse scattering ($\gamma_0''=0$) an electron would experience a total reflection, $R^{(1,2)S}(\tilde{k})=1$ [see Eq. (49)]. But the diffuse scattering in the range $a\leqslant\tilde{k}<1$ results in *decrease* of the specular reflection (the more diffuse scattering the more essential decrease) and, therefore, allows for scattering of an electron with an incident $\mathbf{k}_\parallel$ (on the larger Fermi surface) into the values of $\tilde{k}$ that are not accessible to specular transmission and reflection. In any case ($a>1$ and $a<1$) the specular reflection tends to unity at $\tilde{k}=1$ indicating that the diffuse scattering contribution *decreases* as the electron perpendicular velocity becomes small (in accordance with that, the transmission probability vanishes).

It is also instructive to visualize the dependence of the diffuse scattering contribution (38) as a function of an incidence angle (or $\tilde{k}$). Note, that Eq. (38) is valid at $0\leqslant\tilde{k}\leqslant 1\leqslant a$. For $a\leqslant\tilde{k}\leqslant 1$, $a\leqslant 1$ the diffuse scattering contribution acquires the form [see Eq. (49)]

$$1-[T_k^{(1,2)S}+R_k^{(1,2)S}] = -4v_1\frac{\frac{2}{\hbar}\,\mathrm{Im}\,\Sigma^0}{\left(v_1-\frac{2}{\hbar}\,\mathrm{Im}\,\Sigma^0\right)^2+\left(V+\frac{2}{\hbar}\,\mathrm{Re}\,\Sigma^0\right)^2}. \quad (50)$$

Figure 4 shows, that for the case, when an electron comes to an interface from a material with the smaller Fermi surface ($a>1$) the contribution of the diffuse scattering (38) remains flat for almost all values of incident angles and drops sharply for $\tilde{k}>a\approx 0.9$ after a slight increase. This maximum becomes sharp and has a discontinuous slope for the case of an electron incidence from the side with the bigger Fermi surface ($a<1$), as Fig. 5 shows. The position of this maximum $\tilde{k}=a\approx 0.9$ corresponds to the maximum value of $\tilde{k}$ for which specular transmission is possible (see Fig. 3). For still larger $\tilde{k}>a$ the diffuse transmission is possible, but not specular transmission. In this region the diffuse scattering rapidly (with infinite slope) decreases to zero at $k_x=k_{\mathrm{Cu}}^F$.

III. TRANSMISSION AND REFLECTION FOR A TRILAYER

In this section the self-consistent theory for interfacial scattering by a single interface developed in the preceding section will be generalized to the case of a metallic or insulator spacer sandwiched between two metallic (semiconductor) layers. The spin-dependent scattering of the electrons caused by both a spacer potential well or barrier and the interfacial disorder will be taken into consideration. Thus, in Eq. (1) we have to put

$$m^*(x)=m_1,\quad U(x)=U_1,\quad x<0,$$

$$m^*(x)=m_2,\quad U(x)=U_2,\quad 0<x<d,$$

$$m^*(x)=m_3,\quad U(x)=U_3,\quad x>d \quad (51)$$

and the following scattering potential [compare with Eq. (5)]:

$$V(x,\rho)=\sum_\alpha\sum_{j=0,d}(\tilde{\gamma}_\alpha^j+\sigma^j)\,\delta(x-j)\,\delta(\rho-\rho_\alpha). \quad (52)$$

Here, d is a spacer width, $j=0$ is a location (at the x axis) of the interface between the first and second (spacer) substances, $j=d$ is that between the spacer and third materials, and $\tilde{\gamma}_\alpha^j=\gamma_\alpha^j-\sigma^j$, where γ_α^j and σ^j are the scatterers' strength and coherent potential related to the jth interface (it is not

necessary to introduce different sets of coordinates for the impurity locations ρ_α at each interface because there is no correlation between them and averaging over their locations should be made independently).

As earlier, we consider the electron's transport in a bulk of each material as a ballistic one (no scattering). The matrix element of the scattering potential (52) entering Eq. (3) is given by Eq. (6) where index 0 is substituted with j [i.e., Eq. (6) holds for each interface].

Integration of Eq. (3) with the scattering potential (52) over the close vicinity of each interface yields the discontinuity relation (7) for each interface. However, the longitudinal wave function $c_k(x)$ has now to be written as

$$\begin{aligned} c_k(x) &= \frac{1}{\sqrt{v_1}}\delta_{kk'}e^{ik_1^\perp x} + \frac{1}{\sqrt{v_1}}r_{kk'}^{(1,2)}e^{-ik_1^\perp x}, \quad x<0 \\ &= \frac{1}{\sqrt{v_2}}t_{kk'}^{(1,2)}e^{ik_2^\perp x} + \frac{1}{\sqrt{v_2}}\sum_{k''} r_{kk''}^{(2,3)}e^{-ik_2^\perp x}, \quad 0<x<d \\ &= \frac{1}{\sqrt{v_3}}\sum_{k''} t_{kk''}^{(2,3)}e^{ik_3^\perp (x-d)}, \quad x>d. \end{aligned} \tag{53}$$

Here, the incoming wave with the transverse wave vector $k'=\mathbf{k}_\parallel'$ contributes to the wave of interest with momentum $k=\mathbf{k}_\parallel$ by means of: reflection from the interface between the first and second materials with the amplitude $r_{kk'}^{(1,2)}$ (for $x<0$), transmission to the k-wave in the second substance with the amplitude $t_{kk'}^{(1,2)}$ and reflection into a spacer from the second interface with the amplitude $\Sigma_{k''}r_{kk''}^{(2,3)}$ of all transmitted (from first material) waves (for $0<x<d$), and transmission of all waves from the spacer into the k wave of the third material ($x>d$) with the amplitude $\Sigma_{k''}t_{kk''}^{(2,3)}$ (two latter amplitudes also depend in general on the incoming wave vector k'). The perpendicular to the interfaces velocities and wave vectors are defined similarly to the preceding section [see Eq. (4)] as $v_i=v_i(k)=\hbar k_i^\perp/m_i$ and $k_i^\perp=\sqrt{(k_i^F)^2-k^2}$, where k_i^F is given by Eq. (40).

Matching the wave functions (53) and their derivatives at the interfaces located at $x=0$ and $x=d$ results in the following system of equations:

$$\begin{aligned} &\frac{1}{\sqrt{v_1}}\delta_{kk'} + \frac{1}{\sqrt{v_1}}r_{kk'}^{(1,2)} = \frac{1}{\sqrt{v_2}}t_{kk'}^{(1,2)} + \frac{1}{\sqrt{v_2}}\sum_{k''} r_{kk''}^{(2,3)}, \\ &\frac{1}{\sqrt{v_2}}t_{kk'}^{(1,2)}e^{ik_2^\perp d} + \frac{1}{\sqrt{v_2}}\sum_{k''} r_{kk''}^{(2,3)}e^{-ik_2^\perp d} = \frac{1}{\sqrt{v_3}}\sum_{k''} t_{kk''}^{(2,3)}, \end{aligned} \tag{54}$$

and

$$\begin{aligned} &i\frac{\sqrt{v_2}}{\hbar}\left[t_{kk'}^{(1,2)} - \sum_{k''} r_{kk''}^{(2,3)}\right] - i\frac{\sqrt{v_1}}{\hbar}[\delta_{kk'} - r_{kk'}^{(1,2)}] \\ &\quad = \frac{2}{\hbar^2}\Sigma^0\frac{1}{\sqrt{v_1}}[\delta_{kk'} + r_{kk'}^{(1,2)}] + \frac{2}{\hbar^2}\sum_{k''} V_{kk''}^0 c_{k''}(0), \\ &i\frac{\sqrt{v_3}}{\hbar}\sum_{k''} t_{kk''}^{(2,3)} - i\frac{\sqrt{v_2}}{\hbar}\left[t_{kk'}^{(1,2)}e^{ik_2^\perp d} - \sum_{k''} r_{kk''}^{(2,3)}e^{-ik_2^\perp d}\right] \\ &\quad = \frac{2}{\hbar^2}\Sigma^d\frac{1}{\sqrt{v_3}}\sum_{k''} t_{kk''}^{(2,3)} + \frac{2}{\hbar^2}\sum_{k''} V_{kk''}^d c_{k''}(d), \end{aligned} \tag{55}$$

where Eq. (54) is the continuity relations for the wave function (53) at $x=0$ and $x=d$ and Eqs. (55) resulted from matching the derivatives of Eq. (53) at the interfaces. In these equations $\Sigma^j=n_i^j\sigma^j$, $n_i^j=N_i^j/A$ ($j=0,d$) is the density of scatterers at the interface located at $x=j$ and $V_{kk'}^j$ is the matrix element of potential caused by fluctuations $\tilde{\gamma}_\alpha^j=\gamma_\alpha^j-\sigma^j$ of scattering strength from the coherent potential σ^j at the corresponding interface [see Eq. (6)].

We want to derive the probability amplitude for electron transmission to the third layer, which for the system under consideration may be defined as $t_{kk'}^{(1,3)}=\Sigma_{k''}t_{kk''}^{(2,3)}$ [as it was mentioned earlier, the transmitted to the spacer waves (specified by index k'') and generated by incoming in the first layer wave with momentum k', contribute to the wave k transmitted to the third layer]. To this end, we will solve the system of Eqs. (54) and (55) in several steps.

The first one is to find the amplitude $t_{kk'}^{(1,3)}$ from the sum of the last equation of (54) and the last equation of (55) with $c_{k''}(d)$ defined by the third line of Eq. (53). The result is (in the operator notations)

$$t^{(1,3)} = t^d e^{i\mathbf{k}_2^\perp d}t^{(1,2)}. \tag{56}$$

Here, $e^{i\mathbf{k}_2^\perp d}$ is the operator diagonal in k space with the matrix elements $(e^{i\mathbf{k}_2^\perp d})_{kk'}=e^{ik_2^\perp(k')}\delta_{kk'}$ and t^d is the transmission amplitude through a single interface located at $x=d$ and dividing the layers 2 and 3 [compare with Eq. (9)]

$$t^d = [I + i\Gamma^{(2,3)}]^{-1}\tilde{t}^{(2,3)} \tag{57}$$

with the matrix elements [see Eqs. (10) and (11)]

$$\begin{aligned} \tilde{t}_{kk'}^{(2,3)} &= 2\frac{\sqrt{v_2v_3}}{v_2+v_3+i\frac{2}{\hbar}\Sigma^d}\delta_{kk'}, \\ \Gamma_{kk'}^{(2,3)} &= \frac{2}{\hbar}\frac{\sqrt{v_3}}{\left(v_2+v_3+i\frac{2}{\hbar}\Sigma^d\right)\sqrt{v_3'}}V_{kk'}^d, \\ I_{kk'} &= \delta_{kk'} \end{aligned} \tag{58}$$

where $v_i'=v_i(k')$.

The next step is to sum up the first equations of (53) and (54) taking for $c_{k''}(0)$ the second line of Eq. (53). This results in the following matrix relation:

$$[I + i\Gamma^{(1,2)}]t^{(1,2)} = \tilde{t}^{(1,2)} + [\tilde{r}^{(2,1)} - i\Gamma^{(1,2)}]\tilde{R}, \tag{59}$$

where the matrix elements of $\tilde{t}^{(1,2)}$ and $\Gamma^{(1,2)}$ are defined like Eq. (58) by Eqs. (10) and (11), respectively, $\tilde{R}_{kk'}=\Sigma_{k''}r_{kk''}^{(2,3)}$ (as it was mentioned earlier this sum depends on the incom-

ing wave vector k'), and $\tilde{r}^{(2,1)}$ is defined like Eq. (36) by

$$\tilde{r}^{(2,1)}_{kk'} = \frac{v_2 - v_1 - i\frac{2}{\hbar}\Sigma^0}{v_2 + v_1 + i\frac{2}{\hbar}\Sigma^0}\delta_{kk'}. \tag{60}$$

At last, subtracting the last equation of (55) from the last equation of (54) and using for $c_{k''}(d)$ the second line of Eq. (53), we get the second operator equation relating $t^{(1,2)}$ and $\tilde{R}$

$$[I + i\Gamma^{-(2,3)}]\tilde{R} = [\tilde{r}^{(2,3)}e^{2ik_2^{\perp}d} - i\Gamma^{+(2,3)}]t^{(1,2)}, \tag{61}$$

where

$$\Gamma^{\pm(2,3)}_{kk'} = \frac{2}{\hbar}\frac{\sqrt{v_2}}{\left(v_2 + v_3 + i\frac{2}{\hbar}\Sigma^d\right)\sqrt{v_2'}}V^d_{kk'}e^{i(k_2^{\perp} \pm k_2^{\perp\prime})d},$$

$$\tilde{r}^{(2,3)}_{kk'} = \frac{v_2 - v_3 - i\frac{2}{\hbar}\Sigma^d}{v_2 + v_3 + i\frac{2}{\hbar}\Sigma^d}\delta_{kk'}. \tag{62}$$

Finding $t^{(1,2)}$ from Eqs. (59) and (61) and inserting it in Eq. (56), we obtain the following equation for the transmission amplitude $t^{(1,3)}$:

$$t^{(1,3)} = t^d e^{i\mathbf{k}_2^{\perp}d}\frac{I}{I - r^{(2,1)}r^{(2,3)}}t^0, \tag{63}$$

where t^0 is the transmission amplitude through the interface at $x=0$ (9) and the reflections amplitudes $r^{(2,1)}$ and $r^{(2,3)}$ are defined as

$$r^{(2,1)} = [I + i\Gamma^{(1,2)}]^{-1}[\tilde{r}^{(2,1)} - i\Gamma^{(1,2)}],$$

$$r^{(2,3)} = [I + i\Gamma^{-(2,3)}]^{-1}[\tilde{r}^{(2,3)}e^{2i\mathbf{k}_2^{\perp}d} - i\Gamma^{+(2,3)}]. \tag{64}$$

Equation (63) is the central result of this section and gives the exact amplitude for electron transmission through spacer 2 from layer 1 to layer 3. It describes the process when incoming electron transmits through the interface at $x=0$ with amplitude t^0 (9) and then after multiple reflection in the spacer from the third ($r^{(2,3)}$) and first ($r^{(2,1)}$) layers transmits through the interface at $x=d$ with the amplitude t^d (57). All interference effects are taken into consideration. Different potential profiles $E-U_i$, electron effective masses m_i in different layers ($i=1,2,3$) and different scattering properties of interfaces, Σ^j, V^j, ($j=0,d$), are accounted for.

The obtained transmission amplitude (63) is important for consideration of GMR and TMR in the layered systems. The corresponding transmission probability is defined by the averaged (over scatterers arrangements) square modulus of the amplitude (63), $T^{(1,3)}_{kk'} = \langle |t^{(1,3)}_{kk'}|^2 \rangle$.

It is not difficult to show that the transmission and reflection amplitudes considered in this section are related to the Green functions in the following way [compare with Eqs. (12) and (34)]

$$t^0_{kk'} = i\hbar\sqrt{v_2 v_1'}G^{(1,2)+}_{kk'},$$

$$t^d_{kk'} = i\hbar\sqrt{v_3 v_2'}G^{(2,3)+}_{kk'},$$

$$r^{(2,1)}_{kk'} = i\hbar\sqrt{v_2 v_2'}G^{(1,2)+}_{kk'} - \delta_{kk'},$$

$$r^{(2,3)}_{kk'} = i\hbar\sqrt{v_2 v_2'}G^{(2,3)+}_{kk'}e^{i(k_2^{\perp} + k_2'^{\perp})d} - \delta_{kk'}e^{2ik_2^{\perp}d}, \tag{65}$$

where the Green function $G^{(1,2)+}_{kk'}$ is defined by Eqs. (13) and (14) and the Green function (propagator) $G^{(2,3)+}_{kk'}$, which describes the scattering by the interface with the scatterers (of strength $\tilde{\gamma}^d_\alpha + \sigma^d_\alpha$) located at $x=d$, is given by the same series (13) with

$$\tilde{G}^{(2,3)+}_k = \tilde{G}^{(2,3)+}_{kk} = \frac{2}{i\hbar\left(v_2 + v_3 + i\frac{2}{\hbar}\Sigma^{d+}\right)}$$

$$= \frac{1}{[G^{(2,3)+}_0(k)]^{-1} - \Sigma^{d+}},$$

$$G^{(2,3)+}_0(k) = \frac{2}{i\hbar(v_2 + v_3)}, \tag{66}$$

and $V^d_{kk'}$. Using the representation of the Green functions in terms of the scattering T matrix [see Eq. (16)] and following the procedure outlined above [see Eqs. (17)–(19)], we can reach the situation when the specular scattering is fully defined by the Green functions $\tilde{G}^{(1,2)+}_k, \tilde{G}^{(2,3)+}_k$ for the translationally invariant effective medium Σ^j, if the coherent potential Σ^j is determined from Eq. (20) (for each interface). This equation in the explicit form is given by Eq. (31) [or Eq. (32)] with the parameters corresponding to the interface under consideration (0 or d).

Thus, the specular transmission and reflection amplitudes in the CPA are

$$t^{0S}_k = \tilde{t}^{(1,2)}_{kk} = i\hbar\sqrt{v_1 v_2}\tilde{G}^{(1,2)+}_k,$$

$$r^{(2,1)S}_k = \tilde{r}^{(2,1)}_{kk} = i\hbar v_2\tilde{G}^{(1,2)+}_k - 1,$$

$$t^{dS}_k = \tilde{t}^{(2,3)}_{kk} = i\hbar\sqrt{v_2 v_3}\tilde{G}^{(2,3)+}_k,$$

$$r^{(2,3)S}_k = \tilde{r}^{(2,3)}_{kk}e^{2ik_2^{\perp}d} = [i\hbar v_2\tilde{G}^{(2,3)+}_k - 1]e^{2ik_2^{\perp}d}. \tag{67}$$

In the CPA the transmission and reflection probabilities (for a single scattering at the interface) are defined by the square modulus of these amplitudes (in accordance with the results of the previous section). They are diagonal in k space, independent of random variables $\gamma^j_\alpha - \sigma^j$, and, therefore, no averaging is needed for calculation of the corresponding specular transmission and reflection probabilities.

The diffuse single scattering is defined by the following transmission and reflection amplitudes

$$t^{0D}_{kk'} = i\hbar\sqrt{v_2 v_1'}\tilde{G}^{(1,2)+}_k T^0_{kk'}\tilde{G}^{(1,2)+}_{k'},$$

$$r_{kk'}^{(2,1)D} = i\hbar\sqrt{v_2 v_2'}\,\tilde{G}_k^{(1,2)+} T_{kk'}^0 \tilde{G}_{k'}^{(1,2)+},$$

$$t_{kk'}^{dD} = i\hbar\sqrt{v_3 v_2'}\,\tilde{G}_k^{(2,3)+} T_{kk'}^d \tilde{G}_{k'}^{(2,3)+},$$

$$r_{kk'}^{(2,3)D} = i\hbar\sqrt{v_2 v_2'}\,\tilde{G}_k^{(2,3)+} T_{kk'}^d \tilde{G}_{k'}^{(2,3)+} e^{i(k_2^{\perp}+k_2'^{\perp})d}, \qquad (68)$$

where the T^j matrix is given by the series (17) with the appropriate superscript ($j=0,d$). Therefore, in the CPA the diffuse single scattering probabilities are defined by the average square modulus of $T_{kk'}^j$, [see Eqs. (25) and (37)].

A. Metallic spacer

In this case all k_i^F (40) are real. Let us consider the specular part of transmission probability $T_k^{(1,3)S}$ from the 1st to the 3rd metal, the amplitude of which is given by Eq. (63). This part of transmission probability may be obtained by disregarding $\Gamma_{kk'}^{(1,2)}$, $\Gamma_{kk'}^{(2,3)}$, and $\Gamma_{kk'}^{\pm(2,3)}$ (which describe the diffuse scattering at the interfaces) in the amplitude (63). The remaining part of the amplitude, $t_{kk}^{(1,3)S}$, is diagonal in k space and does not depend on the impurity configurations at the interfaces (it is defined by the translationally invariant coherent potentials Σ^j). Thus, the specular transmission probability may be written as

$$T_k^{(1,3)S} = |t_{kk}^{(1,3)S}|^2 = \frac{T_k^{0S} T_k^{dS}}{|1 - e^{2ik_2^{\perp}d}\tilde{r}_{kk}^{(2,1)}\tilde{r}_{kk}^{(2,3)}|^2}$$

$$= T_k^{0S} T_k^{dS} \sum_{n,m=0}^{\infty} \exp[2ik_2^{\perp}d(n-m)] \times [\tilde{r}_{kk}^{(2,1)}\tilde{r}_{kk}^{(2,3)}]^n [\tilde{r}_{kk}^{*(2,1)}\tilde{r}_{kk}^{*(2,3)}]^m, \qquad (69)$$

where $T_k^{0S}=|t_k^{0S}|^2$ and $T_k^{dS}=|t_k^{dS}|^2$ are the specular transmission probabilities for the first (at $x=0$) and second ($x=d$) interfaces, respectively, and t_k^{0S}, t_k^{dS}, $\tilde{r}_{kk}^{(2,1)}$, and $\tilde{r}_{kk}^{(2,3)}$ are defined by Eq. (67). Working through some algebra, we get

$$T_k^{(1,3)S} = 4v_1 v_2^2 v_3 \{[(\tilde{v}_1+\tilde{v}_3)^2 + (\mathrm{Re}\,\Gamma^0 + \mathrm{Re}\,\Gamma^d)^2]v_2^2 + \sin^2(k_2^{\perp}d)[(\tilde{v}_1^2 - v_2^2 + \mathrm{Re}^2\,\Gamma^0)(\tilde{v}_3^2 - v_2^2 + \mathrm{Re}^2\,\Gamma^d) - 4v_2^2\,\mathrm{Re}\,\Gamma^0\,\mathrm{Re}\,\Gamma^d] + \sin(2k_2^{\perp}d)v_2[(\tilde{v}_1^2 - v_2^2)\mathrm{Re}\,\Gamma^d + (\tilde{v}_3^2 - v_2^2)\mathrm{Re}\,\Gamma^0 + \mathrm{Re}\,\Gamma^0\,\mathrm{Re}\,\Gamma^d(\mathrm{Re}\,\Gamma^0 + \mathrm{Re}\,\Gamma^d)]\}^{-1}, \qquad (70)$$

where $\tilde{v}_1=v_1-\mathrm{Im}\,\Gamma^0$, $\tilde{v}_3=v_3-\mathrm{Im}\,\Gamma^d$, $\Gamma^0=(2/\hbar)\Sigma^{0+}$, $\Gamma^d=(2/\hbar)\Sigma^{d+}$. Equation (70) is valid for $0\leqslant k\leqslant k_i^F$ ($i=1-3$), i.e., for the range of k where all v_i are real (all waves are propagating).

Equation (70) describes the specular part of transmission probability for a metallic trilayer with disordered interfaces and generalizes the expression for the transmission probability obtained in the paper[23] for the case of perfect interfaces. One can see that the real part of the coherent potential $\mathrm{Re}\,\Gamma^j$ ($j=0,d$) leads to the appearance of a new oscillating term, proportional to $\sin(2k_2^{\perp}d)$. In the case of perfect interfaces ($\Gamma^j=0$) the transmission probability contains only conventional oscillating term with $\sin^2(k_2^{\perp}d)$ (see Refs. 24 and 23).

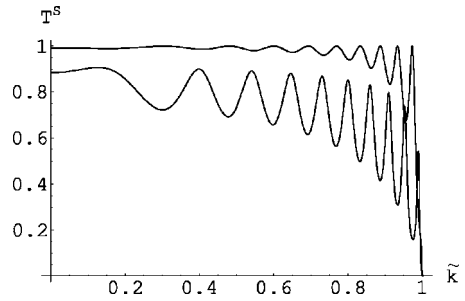

FIG. 6. Specular transmission probability (71) for symmetric [like Co(majority)/Cu/Co(majority)] trilayer vs the angle of electron incidence ($a=a'=\sqrt{2.746/2.230}, b=b'=1, k_1^F d=15\pi, \tilde{k}=k_x/k_1^F$, $k_1^F=k_{\mathrm{Co}(maj)}^F$). Upper line—perfect interfaces ($\gamma_0'=\gamma_d'=0, \gamma_0''=\gamma_d''=0$); bottom line—intermixed interfaces ($\gamma_0'=\gamma_d'=0.5, \gamma_0''=\gamma_d''=-0.05$).

As it follows from Eqs. (38) and (50), the diffuse part of interfacial scattering is defined by the imaginary part of coherent potential $\mathrm{Im}\,\Sigma^j$ and depends on the angle of electron incoming to an interface (perpendicular velocity). If the average interface scattering potential $\bar{\gamma}_j=(1/N_i^j)\Sigma_\alpha \gamma_\alpha^j \neq 0$, the real part of coherent potential $\mathrm{Re}\,\Sigma^j$ is essential and such is a contribution of the specular transmission (70) (at $c_1c_2 \ll 1/8$, weak scattering and close to normal to an interface electron incidence, as was pointed above). If $\bar{\gamma}_j=0$ ($c_1=c_2$) the real part of the coherent potential $\mathrm{Re}\,\Sigma^j \sim \mathrm{Im}\,\Sigma^j$ and is caused by the evanescent intermediate states [see Eq. (47)].

Equation (70) acquires much simpler form for the case of the electron transmission between two identical metals (labeled 1) through a metallic spacer (2), when $v_1=v_3$, $\Gamma^0=\Gamma^d=\Gamma^1$ (i.e., $\tilde{v}_1=\tilde{v}_3$). In this case Eq. (70) reads

$$T_k^{(1,1)S} = \frac{v_1^2}{\tilde{v}_1^2}\left\{1 + \frac{1}{4\tilde{v}_1^2 v_2^2}[2v_2\,\mathrm{Re}\,\Gamma^1\cos(k_2^{\perp}d) + (\tilde{v}_1^2 - v_2^2 + \mathrm{Re}^2\,\Gamma^1)\sin(k_2^{\perp}d)]^2\right\}^{-1}. \qquad (71)$$

Remembering that $\tilde{v}_1=v_1-\mathrm{Im}\,\Gamma^1 \geqslant v_1$ ($\mathrm{Im}\,\Gamma^1 \leqslant 0$), we see that $T_k^{(1,1)S} \leqslant 1$. If we put $\Gamma^1=0$, Eq. (71) reduces to the expression for the transmission probability over a potential well with perfect interfaces, well known from the textbooks (see, e.g., Ref. 24). However, it is interesting to note, that whenever $\mathrm{Re}\,\Gamma^1 \neq 0$ (as it should be for a real alloylike interface) Eq. (71) contains an additional [to conventional $\sin(k_2^{\perp}d)$ term causing the resonant well states] oscillating $\cos(k_2^{\perp}d)$ term.

In order to plot the dependence of Eq. (70) [or Eq. (71)] on the angle of electron incidence $\tilde{k}=k/k_1^F$, it is convenient to present these equations in terms of the dimensionless parameters (48) and parameters $\gamma_d'=\mathrm{Re}\,\Gamma^d/v_1^F$, $\gamma_d''=\mathrm{Im}\,\Gamma^d/v_1^F$, $a'=k_3^F/k_1^F$, $b'=m_1/m_3$, $k_1^F d$ ($k_2^{\perp}d=k_1^F d\sqrt{a^2-\tilde{k}^2}$), where $0\leqslant\tilde{k}\leqslant\min(1,a,a')$ (all waves are propagating). Figures 6 and 7 show the dependencies of the specular transmission coefficient (70) on the angle of electron incidence ($\tilde{k}$).

From these figures one may see that interfacial scattering at the intermixed interfaces leads to decrease of the transmis-

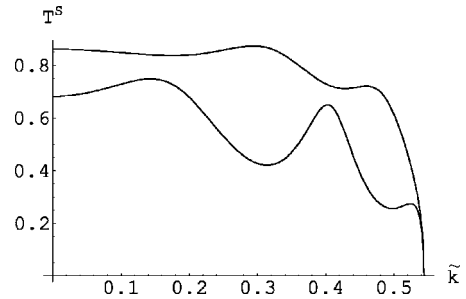

FIG. 7. Specular transmission probability for an asymmetric [like Co(majority)/Cu/Co(minority)] trilayer (70) vs the angle of electron incidence ($a=\sqrt{2.746/2.230}, a'=\sqrt{0.660/2.230}, b=b'=1$, $k_1^F d=15\pi, \tilde{k}=k_x/k_1^F, k_1^F=k_{\mathrm{Co}(maj)}^F$). Upper line—perfect interfaces ($\gamma_0'=\gamma_d'=0, \gamma_0''=\gamma_d''=0$); bottom line—intermixed interfaces with different strengths of scattering ($\gamma_0'=0.5, \gamma_d'=0.8, \gamma_0''=-0.05$, $\gamma_d''=-0.08$).

sion (through a trilayer) probability. An interesting feature is that the specular transmission probability exhibits oscillations caused by defects located at the interfaces. They are due to additional oscillating terms in Eqs. (70) and (71) proportional to the real part of the coherent interfacial scattering potential. For the parameters corresponding to Figs. 6 and 7 (small potential steps and essential real part of the coherent potential) the oscillations caused by $\cos(k_2^{\perp} d)$ term prevail [one can see that the phases of oscillations in Figs. 6 and 7 are opposite to those caused by the conventional $\sin(k_2^{\perp} d)$ term, which leads to the quantum well states].

Generally, Eq. (70) can be used for evaluation of the specular scattering contribution to GMR in magnetic trilayers (it provides the main contribution under the conditions specified above). For this purpose one should include into consideration the electron's spin. Considering for simplicity a trilayer made of two identical metallic magnetic layers separated by a nonmagnetic metallic spacer, we can relate all electron characteristics in the first and second magnetic layers (identified by indexes 1 and 3) to the corresponding values in one of the two current channels with a given projection of electron spin η on the magnetization direction of the magnetic layer (e.g., $v_1=v^{\eta}$, $v_3=v^{\eta'}$). Accordingly, Γ^j ($j=0,d$) may be attributed to the spin-dependent coherent potential Γ^{η} at the interfaces between a nonmagnetic layer and magnetic layers with different orientation of magnetization ($\Gamma^j=\Gamma^{\eta}$).

Then, the conventional magnetoresistance ratio (MR), defining the GMR, may be expressed in terms of the conductances for ferromagnetic (parallel) and antiferromagnetic (antiparallel) configurations of magnetic layers as

$$R=(G^{\uparrow\uparrow}+G^{\downarrow\downarrow}-G^{\uparrow\downarrow}-G^{\downarrow\uparrow})/(G^{\uparrow\downarrow}+G^{\downarrow\uparrow}). \tag{72}$$

In the two-current model and CPP geometry the conductance between channels η and η', $G^{\eta\eta'}$, is given by

$$G^{\eta\eta'}=\frac{e^2}{h}\sum_{kk'}\langle T_{kk'}^{(\eta,\eta')}\rangle, \tag{73}$$

where $\langle T_{kk'}^{(\eta,\eta')}\rangle$ is the average (over the defects configurations at the interfaces) probability for an electron to transmit through a nonmagnetic spacer from one magnetic layer, where it is in the transverse mode k' with the projection $\eta'=(\uparrow,\downarrow)$ of a spin on the direction of magnetization vector, to mode k with the electron spin projection on the direction of magnetization $\eta=(\uparrow,\downarrow)$ in another magnetic layer (no spin-flip processes are allowed). The specular part of $\langle T_{kk'}^{(\eta,\eta')}\rangle = T_k^{(\eta,\eta')S}$ is given by Eq. (70) with the indexes 1, 3, and j substituted with $\eta, \eta'(=\uparrow,\downarrow)$, as was pointed above.

B. Semiclassical approximation for a metallic trilayer with rough interfaces

There may be two types of imperfections at interfaces: long-range and short-range as compared to the electron mean free path l. The short-range defects break the in-plane translational invariance and may be attributed to intermixing, which is modeled here by a substitutional alloy of the short-range scattering centers (atoms) located in the interface plane. In this case the in-plane components of the wave vector k are not conserved leading to the appearance of the diffuse scattering. The effects of interface roughness may be associated with the long-range deviations of either the thickness of layers or the crystallographic orientations of layers.

The formula for the specular transmission probability in the case of smoothly varying thickness of each layer, when the thickness of an interlayer (spacer) remains practically constant within the electron mean free path, may be obtained by averaging Eq. (69) over the thickness of a spacer. The result is [the surviving terms with $m=n$ in Eq. (69)]

$$T_k^{(1,3)S}=\frac{T_k^{0S}T_k^{dS}}{1-|\tilde{r}_{kk}^{(2,1)}|^2|\tilde{r}_{kk}^{(3,2)}|^2}. \tag{74}$$

This result corresponds to the semiclassical approximation for a multilayer considered in Ref. 21 (see also Refs. 30 and 31). Making use of Eqs. (10), (58), (60), and (62), we obtain for transmission probability (74)

$$T_k^{(1,3)S}=\frac{4v_1v_2v_3}{\tilde{v}_1(\tilde{v}_3^2+v_2^2+\mathrm{Re}^2\,\Gamma^d)+\tilde{v}_3(\tilde{v}_1^2+v_2^2+\mathrm{Re}^2\,\Gamma^0)}, \tag{75}$$

where $\tilde{v}_1$, $\tilde{v}_3$, Γ^0, and Γ^d are defined in the text after Eq. (70) and $0\leqslant k\leqslant k_i^F$ ($i=1-3$), i.e., all v_i are real (all waves are propagating).

Figure 8 shows that the semiclassical transmission probability exhibits no oscillations [Eq. (75) does not depend on the spacer thickness d] and follows the average value of the corresponding lines of Fig. 6. Increased diffuse scattering (essential defect potential fluctuations) leads naturally to diminished specular transmission (dotted line in Fig. 8).

C. Insulating spacer

For the case of insulating spacer, we have $E_F<U_s$ and $k_s^F=i\sqrt{(2m_s/\hbar^2)(U_s-E_F)}=iK_s^F$, where U_s is a potential barrier height. Therefore, the electron perpendicular wave vector $k_s^{\perp}=i\sqrt{(K_s^F)^2+k^2}=iK(k)$ and velocity $v^s=i(\hbar/m_s)K=iV$ in a spacer are purely imaginary. Thus, in all formulas we have to

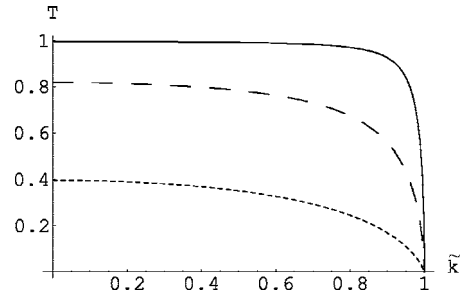

FIG. 8. Specular transmission probability (75) for symmetric [like Co(majority)/Cu/Co(majority)] trilayer vs the angle of electron incidence ($a=a'=\sqrt{2.746/2.230}, b=b'=1, \tilde{k}=k_x/k_1^F, k_1^F=k_{\mathrm{Co}(maj)}^F$). Solid line—perfect interfaces ($\gamma_0'=\gamma_d'=0, \gamma_0''=\gamma_d''=0$); dashed line—intermixed interfaces with small coherent potentials fluctuations ($\gamma_0'=\gamma_d'=0.5, \gamma_0''=\gamma_d''=-0.05$); dotted line—intermixed interfaces with essential coherent potentials fluctuations ($\gamma_0'=\gamma_d'=0.5, \gamma_0''=\gamma_d''=-0.5$).

substitute the electron perpendicular wave vector ($k_2^{\perp}$) and velocity (v_2) in the spacer by the introduced imaginary values. If the insulating spacer is sandwiched between two identical metallic magnetic layers, we may represent the specular transmission probability (69) for different (parallel and antiparallel) orientations of magnetic layers as

$$T_k^{(\eta,\eta')S}=\frac{T_k^{\eta S}T_k^{\eta' S}e^{-2Kd}}{\left|1-e^{-2Kd}\tilde{r}_k^{\eta}\tilde{r}_k^{\eta'}\right|^2},\ \eta,\eta'=\uparrow,\downarrow, \tag{76}$$

where

$$T_k^{\eta S}=\frac{4v^{\eta}V}{\tilde{v}^{\eta 2}+V_+^{\eta 2}},\quad \tilde{r}_k^{\eta}=\frac{iV_-^{\eta}-\tilde{v}^{\eta}}{iV_+^{\eta}+\tilde{v}^{\eta}},$$

$$\tilde{v}^{\eta}=v^{\eta}-\mathrm{Im}\,\Gamma^{\eta},\quad V_{\pm}^{\eta}=V\pm\mathrm{Re}\,\Gamma^{\eta}. \tag{77}$$

Making use of Eq. (77), the transmission probability (76) may be rewritten as

$$T_k^{(\eta,\eta')S}=\frac{16v^{\eta}v^{\eta'}V^2e^{-2Kd}}{\left|(\tilde{v}^{\eta}+iV_+^{\eta})(\tilde{v}^{\eta'}+iV_+^{\eta'})-e^{-2Kd}(\tilde{v}^{\eta}-iV_-^{\eta})(\tilde{v}^{\eta'}-iV_-^{\eta'})\right|^2}. \tag{78}$$

For the spacer with perfect interfaces, when $\Gamma^{\eta}=0$ ($\tilde{v}^{\eta}=v^{\eta}$, $V_{\pm}^{\eta}=V$), the transmission probability (78) reduces to the expression

$$T_k^{(\eta,\eta')S}=\frac{16v^{\eta}v^{\eta'}V^2e^{-2Kd}}{(1-e^{-2Kd})^2(v^{\eta 2}+V^2)(v^{\eta' 2}+V^2)+4e^{-2Kd}(v^{\eta}+v^{\eta'})^2V^2} \tag{79}$$

obtained and used in Ref. 25 for numerical study of the tunneling magnetoresistance ratio R_{TMR} (72).

If the barrier factor e^{-2Kd} is small enough (a sufficiently thick barrier), we can omit the term proportional to this factor in the denominator of (76) and present the specular part of TMR ratio (72) in terms of velocities $v^{\uparrow(\downarrow)}$ and renormalized velocities $\tilde{v}^{\uparrow(\downarrow)}, V_+^{\uparrow(\downarrow)}$ as

$$R_{TMR}^S=\frac{2\sum_k P_k^2D_k^2e^{-2K(k)d}}{\sum_k(1-P_k^2)D_k^2e^{-2K(k)d}}, \tag{80}$$

where

$$P_k=\frac{T_k^{\uparrow S}-T_k^{\downarrow S}}{T_k^{\uparrow S}+T_k^{\downarrow S}}=\frac{v^{\uparrow}(\tilde{v}^{\downarrow 2}+V_+^{\downarrow 2})-v^{\downarrow}(\tilde{v}^{\uparrow 2}+V_+^{\uparrow 2})}{v^{\uparrow}(\tilde{v}^{\downarrow 2}+V_+^{\downarrow 2})+v^{\downarrow}(\tilde{v}^{\uparrow 2}+V_+^{\uparrow 2})},$$

$$D_k=\frac{1}{4}(T_k^{\uparrow S}+T_k^{\downarrow S})=V\frac{v^{\uparrow}(\tilde{v}^{\downarrow 2}+V_+^{\downarrow 2})+v^{\downarrow}(\tilde{v}^{\uparrow 2}+V_+^{\uparrow 2})}{(\tilde{v}^{\uparrow 2}+V_+^{\uparrow 2})(\tilde{v}^{\downarrow 2}+V_+^{\downarrow 2})}. \tag{81}$$

Note, that K and the factors (81) are dependent on the electron parallel wave vector $k=\mathbf{k}_{\parallel}$.

It is interesting to compare the factors (81) with those introduced by Slonczewski.[10] From Eq. (81) it is seen that the generalized electron polarization is defined by the difference of spin-up and spin-down specular transmission probabilities through (disordered) interface. For the sharp interface ($\Gamma^{\eta}=0$) factors P_k and D_k coincide with the Slonczewski generalized electron polarization and interface factors (see Ref. 10).

For the case $e^{-2Kd}\ll 1$, it is also possible to obtain the Slonczewski-like result and introduce the generalized electron polarization accounting for both the specular and diffuse scattering. In this case the reflection amplitude $r^{(2,3)}$ [defined by Eqs. (62) and (64)] in the transmission amplitude (63) is small and, therefore, the total transmission probability for the case of a thick insulating layer can be written (in an operator form) as

$$T_{kk'}^{(\eta,\eta')}=\left[\langle T^{\eta'}\rangle e^{-2\mathbf{K}d}\langle T^{\eta}\rangle\right]_{kk'}. \tag{82}$$

Here, $(e^{-2\mathbf{K}d})_{kk'}=e^{-2K(k)d}\delta_{kk'}$, the (operator) transmission probability T^{η} from a lead to a spacer for an electron with a spin projection η is given by the modular square of Eq. (9) [or Eq. (57)] with $v_2=iV$, v_1 (or v_3) substituted with v^{η} and, accordingly, Σ^0 (or Σ^d)—with Σ^{η} (all indexes 0 and d are to be changed to $\eta=\uparrow,\downarrow$). The averaging over the interface defects arrangements ($\langle\ldots\rangle$) is applied separately to each of the interfaces [as it is reflected in Eq. (82)] because the locations of imperfections at both interfaces are not correlated. In the self-consistent approximation [defined by Eq. (26)] $\langle T^{\eta}\rangle$ is given by Eq. (23) with the appropriate redefinition of the symbols.

Thus, for a thick barrier the tunneling magnetoresistance ratio R_{TMR} (72) may be presented as

$$R_{TMR}=\frac{\sum_{kk'k_i}[\langle T^{\uparrow}_{kk_i}\rangle e^{-K(k_i)d}-\langle T^{\downarrow}_{kk_i}\rangle e^{-K(k_i)d}][e^{-K(k_i)d}\langle T^{\uparrow}_{k_ik'}\rangle-e^{-K(k_i)d}\langle T^{\downarrow}_{k_ik'}\rangle]}{\sum_{kk'k_i}[\langle T^{\uparrow}_{kk_i}\rangle e^{-2K(k_i)d}\langle T^{\downarrow}_{k_ik'}\rangle+\langle T^{\downarrow}_{kk_i}\rangle e^{-2K(k_i)d}\langle T^{\uparrow}_{k_ik'}\rangle]}. \tag{83}$$

Here, we have taken into consideration that $\langle T^{\eta}_{kk'}\rangle \neq \langle T^{\eta}_{k'k}\rangle$ in the presence of diffuse scattering as it follows from Eqs. (23)–(25). Assuming that the transmission is effective only via the lowest decaying state in the barrier with $k_i=k_0$, we can present the magnetoresistance ratio (83) in the following form:

$$R_{TMR}=\frac{2P_0P_0'}{1-P_0P_0'}, \tag{84}$$

where the average interfacial transmission polarizations P_0 and P_0' are defined as

$$P_0=\frac{\langle T^{\uparrow}\rangle_0-\langle T^{\downarrow}\rangle_0}{\langle T^{\uparrow}\rangle_0+\langle T^{\downarrow}\rangle_0}, \quad P_0'=\frac{\langle T^{\uparrow}\rangle'_0-\langle T^{\downarrow}\rangle'_0}{\langle T^{\uparrow}\rangle'_0+\langle T^{\downarrow}\rangle'_0},$$

$$\langle T^{\uparrow(\downarrow)}\rangle_0=\sum_k\langle T^{\uparrow(\downarrow)}_{kk_0}\rangle, \quad \langle T^{\uparrow(\downarrow)}\rangle'_0=\sum_k\langle T^{\uparrow(\downarrow)}_{k_0k}\rangle. \tag{85}$$

When only the specular scattering is taken into consideration (or it is dominant), the transmission probabilities are diagonal and the expression (84) reduces to Eq. (80) if only the state with the lowest decay rate in the spacer ($k=k_0$) is accounted for in the sums of Eq. (80). In this case $P_0=P_0'$ and is given by Eq. (81) for $k=k_0$.

IV. DISCUSSION

We have developed a fully self-consistent theory of the scattering at the real interfaces in the nanostructures (multilayers and sandwiches) being used in the devices based on the GMR or TMR effects. The real interfaces are characterized by roughness (long-range imperfections as compared to the electron mean free pass l, which do not break the in-plane translational invariance) and intermixing (short-range imperfections breaking the in-plane translational invariance). The interface roughness may be associated with the long-range deviation of either the thickness of layers or the crystallographic orientations of layers, whereas the intermixing of different layers in the interface region may be modeled by a corresponding alloy of short-range scatterers.

Introduction of the translationally invariant interfacial reference medium (a single-site coherent potential) allows to define self-consistently the self-energy Σ of the one-particle effective-medium Green function $\widetilde{G}_k$, which completely describes the specular electron scattering at the disordered interfaces. It has also enabled us to obtain the results, which are applicable for any angle of electron incidence at an interface, any potential difference between layers (potential profile) and any concentrations of different atoms in the interfacial alloy. The results obtained in the previous papers for scattering at a single interface are not valid for all values of the mentioned parameters. Particularly, the conventional perturbation theory [used in Refs. 19 and 22 and based on a bare Green function $G_0(k)$ (14)] does not work at small perpendicular (to an interface) electron velocity and small potential difference (velocity difference) between adjacent layers [see Eq. (44)]. Also, the role of the nonzero average interfacial scattering potential ($\bar{\gamma}_0\neq 0$) has not been considered in these papers and Ref. 21 (this case is realized, e.g., for a binary alloy in the interfacial region with not equal concentrations of components, $c_1\neq c_2$).

The developed self-consistent approach has resulted in the exact (in the single-site approximation for the coherent potential) closed explicit expressions for the specular electron transmission through and reflection from a single disordered interface and for specular transmission through a trilayer with two disordered interfaces. In the adopted effective-mass approximation for the electronic spectra in different layers these results may be regarded as the generalization of the textbook formulas for quantum mechanical transmission through and reflection from perfect potential step/well/barrier on the case of the disordered potential step/well/barrier.

The diffuse scattering at the disordered interfaces are expressed through the effective-medium Green function $\widetilde{G}_k$ and the variance of the scattering T matrix (from its average value). This scattering (arising due to mixing between different transverse electron modes caused by scattering at the interface imperfections) leads to decrease of electron specular transmission probability. On the other hand, the diffuse scattering may lead either to increase (if an electron comes from the side of an interface with smaller Fermi surface) or to decrease (for incident transverse momentum k' on the larger Fermi surface) of the reflection probability. In the latter case an electron is allowed to diffusely transfer into the k region forbidden for the specular scattering (where it experiences a total reflection). The diffuse scattering is defined by the imaginary part of the coherent potential and practically vanishes for grazing electron incidence (with the highest values of transverse momentum k). This fact (the reflection probability is close to unity at large k) is important for the CIP GMR (the channeling effect) and for the interface coupling, which is defined by the electron reflections in the potential well.[29]

Also, it is shown that the specular scattering may dominate, when the electron strikes an interface at an angle close to the perpendicular to an interface one (small k) and when the real part of the coherent potential is much larger than the imaginary one (the fluctuations of the average interfacial

scattering potential are small). The latter may be realized only when the average interfacial potential is not equal to zero (for a binary-alloy-type interface it may happen only when the concentrations of the alloy components are not the same, $c_1 \neq c_2$). This may have important implications for the GMR and TMR effects.

The specular transmission probability for the metallic trilayer exhibits the additional oscillations (to the quantum well ones in a trilayer with perfect interfaces), which are caused by the real part of the coherent potential. These oscillations are of the $\sin(2k_2^{\perp}d)$ or $\cos(k_2^{\perp}d)$ type and different from the conventional $\sin(k_2^{\perp}d)$ type ones typical for a trilayer with perfect interfaces.[24,23]

If the interfaces are rough (in a sense pointed above), these oscillations vanish and the transmission probability does not depend on the spacer width d (semiclassical approximation).

In the case of an insulating spacer the obtained specular transmission probability through a trilayer is expressed via the renormalized (by the coherent potential) electron velocities in the layers and the corresponding tunneling magnetoresistance ratio may be expressed (for a large spacer thickness) in the Slonczewski form with the generalized polarization and interface factors defined by the specular transmission probabilities for the spin-up and spin-down electrons. If the diffuse scattering is also taken into account, the tunneling magnetoresistance ratio may be written (for thick spacer) in terms of the average (over the interface defects configurations) total transmission probabilities.

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