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Electronic excitation spectra and energy losses of slow ions in solids

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We have calculated the energy distribution $P(\varepsilon)$ of electrons excited by a slowly moving atomic particle in a metal. The particle is represented by an empirical pseudopotential which is known from electronic band structure calculations. The first moment of $P(\varepsilon)$ yields the value of the total energy of excited electrons or, equivalently, the value of the energy losses of the moving particle. The electronic stopping power of Al atoms moving in aluminum calculated by this method is in quantitative agreement with the stopping power obtained by other approaches. The corrections to $P(\varepsilon)$ due to the deviation of real metals from the free-electron model are also estimated. $P(\varepsilon)$ can be used in theories of ion-induced kinetic electron and ion emissions as a source function for calculating the energy spectra of electrons excited in collision cascades.

INTRODUCTION

The detailed information on energy losses suffered by atomic particles moving in condensed matter with very low velocities is of special interest for understanding stopping and other electronic processes in collision cascades. The analysis of low-velocity stopping has been a subject of many papers starting with the work of Fermi and Teller[1] and Lindhard.[2] It was further extended by Ritchie,[3] Trubnikov and Yavlinski,[4] and Lindhard and Scharff.[5] An attempt to include the effect of an electron bound to the projectile was performed by Ferrell and Ritchie,[6] and the proper treatment of the scattering potential by the density-functional formalism has been subsequently carried out by Echenique, Nieminen, and Ritchie.[7,8] Parallel with these developments, Firsov[9] has worked out a theory based on an intuitive model of semiclassical quasimolecules. Though originally designed for analysis of single-collision ion energy losses, the Firsov theory has been mostly used to interpret stropping data. Overall agreement between his theory and experimental results is about as good as with the Lindhard and Scharff formula.[5]

In this contribution we analyze in detail electronic energy losses of slow particles in collision cascade in metals with an emphasis on the analysis of energy spectra of electrons excited during these stopping processes. We assume that the collisions are of such low energies that the localized inner shells are not perturbed and do not cross Fermi energies.[10] Very low-energy collisions may indeed prevail in later temporal stages of collision cascades. Thus, for these processes, we can use the concept of pseudopotentials to describe the scattering centers. Pseudopotentials, either empirical or theoretically estimated from first principles, are commonly used for very precise calculations of valence-band structure of solids and have several useful features.[11] In particular, it is the relative independence on the atomic ordering and, to some extent, also to the electronic surrounding which make pseudopotentials suitable for calculation of electronic excitation in collision cascades.

In contrast to previous treatments of the problem we shall first calculate, using the perturbation theory, the energy distribution $P(\varepsilon)$ of electrons excited by the moving particle per unit time. The detailed knowledge of $P(\varepsilon)$ is the prerequisite for the calculation of the space-time evaluation of electronic excitations in the collision-cascade region and for the estimation of their role in other physical processes like ionization of sputter particles and electron emission. The first momentum of $P(\varepsilon)$ yields the total energy transferred to the electronic system per unit time which is equivalent to the energy losses of the moving particle per unit time. These energy losses are compared with the results obtained by other authors.[5,6,9]

The described approach allows to use the correct form of electron wave functions in solids and to investigate the role of the form of the wave function (i.e., the degree of delocalization) on the energy spectrum of excited electrons. The experience with pseudopotentials in semiconductors enables also to generalize the method by going beyond the Born approximation and to calculate correct forms of scattering T-matrices for materials with energy band gaps.

THEORY

As mentioned in the Introduction the basic assumption of our approach is that the particle moves in the solid with a very low velocity, so that only valence electrons of the solid are perturbed and the particle can be well represented by the corresponding empirical pseudopotential $V(r)$. Furthermore we assume that because of low velocity the effective charge of the particle and thus also the scattering potential $V(r)$ are the same as if the particle were at rest. The corrections to $V(r)$ due to the self-consistency are expected to be small because our interest is mainly in the electronic excitations in collision cascades where the moving particles are usually of the same type as the host lattice. We shall assume that the Born approximation is adequate in metals. It is clear that this approximation may not be suitable for semiconductors or insulators. New states created by the moving particle in and near the band gap and neglected in the Born approximation have narrow linewidth and thus can contribute significantly to the transfer of electrons[10] across the band gap.

Within the described approximations the relevant time-dependent matrix element for the transition from the filled state $|k'\rangle$ (below the Fermi energy ε_F) with the energy $\varepsilon_{k'}$ into the empty state $|k\rangle$ with the energy ε_k is given by

$$\langle\psi_{\mathbf{k}}|V(\mathbf{r}-\mathbf{R}(t))|\psi_{\mathbf{k}'}\rangle\ , \tag{1}$$

where $\mathbf{R}(t)$ is the time-dependent vector indicating the position of the moving particle in the solid. The probability of transition from the states of energies between $\varepsilon_{k'}$ and $\varepsilon_{k'}+d\varepsilon_{k'}$ into states of energies between ε_k and $\varepsilon_k+d\varepsilon_k$ is given by

$$W(\varepsilon_k,\varepsilon_{k'})\rho(\varepsilon_k)\rho(\varepsilon_{k'})d\varepsilon_k d\varepsilon_{k'}=\frac{1}{2\hbar^2}\int_0^{4\pi}\frac{d\Omega_k}{4\pi}\int_0^{4\pi}\frac{d\Omega_{k'}}{4\pi}\left|\int_{-\infty}^{+\infty}dt\langle\psi_k|V(\mathbf{r}-\mathbf{R}(t))|\psi_{k'}\rangle\exp\left[i\frac{\varepsilon_k-\varepsilon_{k'}}{\hbar}t\right]\right|^2 \times\rho(\varepsilon_k)\rho(\varepsilon_{k'})d\varepsilon_k d\varepsilon_{k'}\ , \tag{2}$$

where $\rho(\varepsilon)$ is the density of states at the energy ε. The factor of $\frac{1}{2}$ comes from the assumption that spins of electrons do not change orientation during the excitation.

The total energy transferred into the electronic system or, equivalently, the energy ΔE lost by the particle in the excitation process is

$$\Delta E=\int_{\varepsilon_F}^{\infty}d\varepsilon_k\int_{-\infty}^{\varepsilon_F}d\varepsilon_{k'}\,W(\varepsilon_k,\varepsilon_{k'})(\varepsilon_k-\varepsilon_{k'})\times\rho(\varepsilon_k)\rho(\varepsilon_{k'})\ . \tag{3}$$

If the wave functions $\psi_{\mathbf{k}}$ and $\psi_{\mathbf{k}'}$ of the solid and the pseudopotential V of the moving particle are known the formulas (2) and (3) allow to evaluate $W(\varepsilon_k,\varepsilon_{k'})$ and ΔE for any trajectory $R(t)$. Equation (2) includes also contributions to $W(\varepsilon_k,\varepsilon_{k'})$ which are caused by nonstationarity of the particle motion.

For the calculation of stopping power we can simplify the calculation by considering the particle motion along the straight line in the z direction with a constant velocity v. We shall take the electron wave functions to be equal, in the first approximation, to the free-electron wave functions. Then the matrix element (1) becomes

$$\int\exp(-i\mathbf{k}\cdot\mathbf{r})V(\mathbf{r}-vt\mathbf{z}_0)\exp(i\mathbf{k}'\cdot\mathbf{r})d^3r\ , \tag{4}$$

where $\mathbf{z}_0$ is the unit vector in the z direction and the integration is over the whole volume. We substitute

$$\mathbf{r}-vt\mathbf{z}_0=\mathbf{r}' \tag{5}$$

and transform Eq. (4) into

$$\exp(-ikvt\cos\theta)\exp(ik'vt\cos\theta')\times\int\exp(-i\mathbf{k}\cdot\mathbf{r}')V(\mathbf{r}')\exp(i\mathbf{k}'\cdot\mathbf{r}')d^3r'\ , \tag{6}$$

where θ and θ' are the polar angles of $\mathbf{k}$ and $\mathbf{k}'$, respectively.

As only electrons around the Fermi energy are perturbed we can set

$$|\mathbf{k}|=|\mathbf{k}'|=|\mathbf{k}_F|,\quad \rho(\varepsilon_k)=\rho(\varepsilon_{k'})=\rho(\varepsilon_F)=\rho\ , \tag{7}$$

where $\mathbf{k}_F$ is the wave vector at the Fermi energy and we denote

$$\int\exp(-i\mathbf{k}_F\cdot\mathbf{r})V(\mathbf{r})\exp(i\mathbf{k}_F'\cdot\mathbf{r})d^3r=c(\phi,\theta,\phi',\theta')\ . \tag{8}$$

The matrix element c is also function of azimuthal angles ϕ and ϕ' as indicated in (8).

Thus Eq. (2) can be written

$$W(\varepsilon_k,\varepsilon_{k'})\rho^2 d\,\varepsilon_k d\varepsilon_{k'}=\frac{2\pi\rho^2}{2\hbar^2(4\pi)^2}\int_0^{4\pi}d\Omega_k\int_0^{4\pi}d\Omega_{k'}|c(\phi,\theta,\phi',\theta')|^2\delta^2\left[k_f v\cos\theta-k_F v\cos\theta'-\frac{\varepsilon_k-\varepsilon_{k'}}{\hbar}\right]d\varepsilon_k d\varepsilon_{k'}\ . \tag{9}$$

From Eq. (9) the probability per unit time that an electron will be transferred from a state around $\varepsilon_{k'}$ to a state around ε_k is given by

$$\omega(\varepsilon_k,\varepsilon_{k'})=\frac{2\pi}{2(4\pi)^2\hbar^2}\int_0^{4\pi}d\Omega_k\int_0^{4\pi}d\Omega_{k'}|c(\phi,\theta,\phi',\theta')|^2\delta\left[k_F v\cos\theta-k_F v\cos\theta'-\frac{\varepsilon_k-\varepsilon_{k'}}{\hbar}\right]\ . \tag{10}$$

Our main task is to calculate $P(\varepsilon_k)\rho\,d\varepsilon_k$, i.e., the probability per unit time that an electron appears in an empty level with energy between ε_k and $\varepsilon_k+d\varepsilon_k$. The quantity $P(\varepsilon_k)$ is obtained by integrating $\omega(\varepsilon_k,\varepsilon_{k'})$ over all occupied states $\varepsilon_{k'}$.

To simplify the notation in the integrals over spherical angles and over the energies we introduce new variables

$$k_F v\cos\theta=y,\quad k_F v\cos\theta'=y',\quad \varepsilon_k-\varepsilon_F=\varepsilon,\quad \varepsilon_F-\varepsilon_{k'}=\varepsilon'\ . \tag{11}$$

Then

$$P(\varepsilon)=\frac{2\pi\rho}{2(4\pi)^2\hbar^2}\int_0^{\infty}d\varepsilon'\int_{-k_Fv}^{+k_Fv}dy\int_{-k_Fv}^{k_Fv}dy'\int_0^{2\pi}d\phi\int_0^{2\pi}d\phi'|c(\phi,y,\phi',y')|^2\delta\left[y'-y-\frac{\varepsilon+\varepsilon'}{\hbar}\right] . \tag{12}$$

The integration over y yields

$$P(\varepsilon)=\frac{2\pi\rho}{2(4\pi)^2\hbar^2(k_Fv)^2}\int_0^{2\hbar k_Fv-\varepsilon}d\varepsilon'\int_{-k_Fv}^{k_Fv-(\varepsilon+\varepsilon'/\hbar)}dy'\int_0^{2\pi}d\phi\int_0^{2\pi}d\phi'\left|c\left[\phi,y'+\frac{\varepsilon+\varepsilon'}{\hbar},\phi',y'\right]\right|^2 . \tag{13}$$

Equation (13) is a general expression for calculating the energy distribution of electrons excited per unit time by a particle moving with a constant velocity through a solid represented by a free-electron gas. The integration can be carried out analytically only in simplest cases such as for s scatters when the matrix element c is angular independent.

Then Eq. (13) yields

$$P(\varepsilon)=\frac{\pi\rho|c|^2}{8\hbar^3(k_Fv)^2}(2\hbar k_Fv-\varepsilon)^2 \quad \text{for } 2\hbar k_Fv>\varepsilon>0 ,$$
$$P(\varepsilon)=0 \quad \text{for } \varepsilon>2\hbar k_Fv . \tag{14}$$

The spectrum (14) is shown in Fig. 1 by a dashed line.

Next problem is to calculate with the use of (14) the average energy losses dE/dt per unit time. Because the excitations above and below the Fermi energy are symmetrical we can use, instead of (3), the relation

$$\frac{dE}{dt}=2\int_0^{\infty}P(\varepsilon)\varepsilon\rho\,d\varepsilon . \tag{15}$$

By substituting (14) into (15) we get

$$\frac{dE}{dt}=\frac{\hbar}{3}\pi\rho^2|c|^2k_F^2v^2=\frac{2\pi\hbar}{3M}\rho^2|c|^2k_F^2E_k , \tag{16}$$

where E_k and M are the kinetic energy and the mass of the moving particle, respectively.

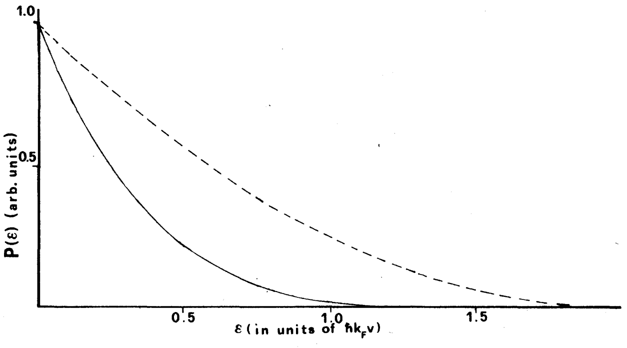

FIG. 1. The shapes of energy distributions $P(\varepsilon)$ of electrons excited above the Fermi energy in a metal by a slow-moving particle. The energies ε are in units of $\hbar k_Fv$, where k_F is the electron wave vector at the Fermi level and v is the velocity of the particle. The energy $\varepsilon=0$ corresponds to the Fermi energy of the metal. The distribution $P(\varepsilon)$ produced by an s scattering potential in free-electron metals is shown by the dashed line and the distribution produced by the realistic pseudopotential of an Al atom in Al metal is shown by the solid line. The amplitudes of $P(\varepsilon)$ are arbitrary in the figure but are normalized to have the same amplitudes at $\varepsilon=0$.

The electronic stopping power is proportional to dE/dt and is equal to

$$\frac{dE}{dx}=\frac{I}{v}\frac{dE}{dt}=\frac{\pi\hbar}{3}\rho^2|c|^2k_F^2v . \tag{17}$$

If the matrix c is angular dependent, the evaluation (13) of $P(\varepsilon)$ and consequently also of dE/dx must be carried out numerically. However, it turns out that the numerical values of dE/dx can be exactly reproduced by Eq. (17) if the value of $|c|^2$ in Eq. (17) is replaced by $|c_t|^2$, i.e.,

$$\frac{dE}{dx}=\frac{\pi\hbar}{3}\rho^2|c_t|^2k_F^2v , \tag{18}$$

where

$$|c_t|^2=\tfrac{1}{2}\int|c(\beta)|^2(1-\cos\beta)\sin\beta\,d\beta \tag{19}$$

and β is the angle between $\mathbf{k}_F$ and $\mathbf{k}'_F$. By definition

$$\cos\beta=\cos\theta\cos\theta'+\sin\theta\sin\theta'\cos(\phi-\phi') . \tag{20}$$

The integration (19) is similar to the one transforming the differential cross section $\sigma(\beta)$ into the transport cross section σ_t. This result is not unexpected since Eq. (17) resembles the expression for electronic stopping power obtained in previous studies[4,6] and, by comparison, $|c|^2$ should be proportional to the scattering transport cross section. To see this explicitly we relate $|c(\beta)|^2$ to the scattering cross section,[12]

$$|c(\beta)|^2=\sigma(\beta)\frac{4\pi^2\hbar^4}{m^2} , \tag{21}$$

where m is the electron mass.

Integration of (21) over β according to Eq. (19) yields $|c_t|^2$ in terms of σ_t, which substituted in Eq. (18) gives

$$\frac{dE}{dx}=\frac{\pi^2\hbar^3}{3}\rho^2v_F^2\sigma_tv , \tag{22}$$

where v_F is the velocity of electrons at the Fermi level. Inserting for ρ and v_F the expressions for the free-electron gas[13] we indeed recover the well-known expression[4,6] for low-velocity electronic stopping power in the free-electron gas, i.e.,

$$\frac{dE}{dx}=mn\sigma_tv_Fv , \tag{23}$$

where n is the number of electrons per unit volume in the metal.

Provided the pseudopotential is known so that $|c(\beta)|^2$ and $|c_t|^2$ can be evaluated, Eqs. (18) and (16) represent rather precise descriptions of electronic losses in metals in terms of the electronic density of states ρ at ε_F and the Fermi $\mathbf{k}_F$ vector. In the next section we shall illustrate the use of the pseudopotentials for the calculation of electronic excitations produced by the motion of an aluminum atom in aluminum.

APPLICATION TO Al

The empirical pseudopotentials of almost all atoms are provided in the paper of Cohen and Heine[11] in the form of their spatial Fourier transform $V(q)$. When they are numerically converted into real space they can be conveniently expressed in terms of a series of Gaussian functions. As has been shown by Kane,[14] in silicon only a few Gaussians are needed for a pseudopotential which describes quite precisely the structure of the silicon valence and conduction bands. For Al we have found adequate a pseudopotential similar to that of Si and containing only two Gaussians

$$V_{\mathrm{Al}}(r)=A\exp(-ar^2)-B\exp(-br^2)\ , \tag{24}$$

where $A=131.6$ eV, $B=88.3$ eV, $a=2.96$ Å^{-2}, and $b=1.286$ Å^{-2}.

The Fourier transform (8) of (24) is then equal to

$$c(\beta)=\left[\frac{\pi}{a}\right]^{3/2}A\exp\left[-\frac{k_F^2}{2a}(1-\cos\beta)\right]+\left[\frac{\pi}{b}\right]^{3/2}B\exp\left[-\frac{k_F^2}{2b}(1-\cos\beta)\right]\ , \tag{25}$$

where β is defined by (20).

The calculation of $|c_t|^2$ using Eqs. (25) and (19) is straightforward and gives in units of eV^2 Å^{-6} the value of 1300. Inserted into (16) together with the values of k_F, M for Al and ρ, deduced from the specific-heat measurements on aluminum, yields

$$\frac{dE}{dt}=2.32\times10^{12}E_K\quad(\text{in eV sec})\ . \tag{26}$$

The value should be compared with $dE/dt=2.5\times10^{12}E_k$ obtained from Lindhard and Scharff formula[5] for Al. Since the Lindhard-Scharff formula is known to agree well with experiments, the close agreement between the two numerical values gives credibility to our approach.

Finally, we can insert (25) into (13) and calculate numerically the energy distribution $P(\varepsilon)$ of electron produced by the moving-Al atom in aluminum. The spectrum $P(\varepsilon)$ is shown in Fig. 1 by a solid line and is clearly substantially narrower than $P(\varepsilon)$ produced by the s scattering only.

The extension of the $P(\varepsilon)$ calculation beyond the free-electron approximation is straightforward. One uses in (1) instead of $\psi_{\mathbf{k}}=\exp(i\mathbf{k}\cdot\mathbf{r})$ the real wave functions of the metal. The real wave functions are linear combinations of $\exp(i\mathbf{k}\cdot\mathbf{r})$ and $\exp[i(\mathbf{k}+\mathbf{K})\cdot\mathbf{r}]$, where $\mathbf{K}$ are the reciprocal lattice vectors of the solid. The potential that mixes the wave functions is the sum of the same pseudopotential used as a dynamic perturbation in (1) over all lattice points. As the mixing is expected to be rather weak in metals like aluminum, we can approximate the real wave function by[15]

$$\psi_{\mathbf{k}}=\exp(i\mathbf{k}\cdot\mathbf{r})+\sum_{\mathbf{K}}A(\mathbf{K},\mathbf{k})\exp[i(\mathbf{k}+\mathbf{K})\cdot\mathbf{r}]\ , \tag{27}$$

where

$$A(\mathbf{K},\mathbf{k})=\frac{1}{\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}+\mathbf{K}}}\int\exp(-i\mathbf{K}\cdot\mathbf{r})\sum_i V(\mathbf{r}-\mathbf{R}_i)d^3r \tag{28}$$

and $\sum_i$ is the sum over all lattice sites. Substituting Eq. (27) in Eq. (4) and performing the same calculations as before, we obtain a generalization of $P(\varepsilon)$. In the particular case that only s scattering is considered, there are additional terms to $P(\varepsilon)$ which have the same general form as (14) but extend from zero to $2\hbar k_F v+\hbar K v\cos\theta_0+\hbar K' v\cos\theta_0'$. θ_0 and θ_0' are the angles between the z axis and $\mathbf{K}$ and $\mathbf{K}'$, respectively. For the reciprocal lattice vectors $\mathbf{K}$ and $\mathbf{K}'$ oriented along the z axis, the maximum transferred energy can have the value

$$2\hbar k_F v+\hbar|\mathbf{K}|v+\hbar|\mathbf{K}'|v\ .$$

Since the reciprocal lattice vectors are roughly multiples of $2k_F$ the spectrum of excitations can extend to substantially larger energies than only $\varepsilon=2\pi k_F v$ in (14). However, these additional contributions to $P(\varepsilon)$ are considerably reduced in amplitude compared to (14) since they are proportional to $|A(\mathbf{K},k_F)A(\mathbf{K}',\mathbf{k}_F')|^2$. As the coefficients $A(\mathbf{K},\mathbf{k}_F)$ are of the order of 10^{-1} in typical metals like Al, the extended contributions to $P(\varepsilon)$ would have very small amplitudes. Further reduction is due to smaller matrix elements $|c|^2$ for larger k vectors. Thus, in most applications the corrections to $P(\varepsilon)$ can be neglected.

CONCLUSIONS

We have calculated the energy distribution $P(\varepsilon)$ of electrons excited in metals by slow-moving particles. The particle is represented by the corresponding empirical non-self-consistent pseudopotentials. By this choice we are limited to very slow velocities of the particle as any inner-shell excitations must be avoided. Also the metal should consist of the same kind of atoms in the particle. Because pseudopotentials are generally transferable, the latter limit is probably not very stringent.

The energy distribution $P(\varepsilon)$ has been first calculated with a simplified s scattering potential and then numerically, using the pseudopotential of Al atoms in Al metal. The first momentum of these distributions leads to the expressions of electronic energy losses and electronic stopping powers. In the case of the Al atom moving in the Al metal, the calculated stopping power is in very good agreement with the stopping power calculated from the Lindhard-Scharff formula.[5]

Finally, we have estimated the influence of the corrections of the free-electron plane-wave approximation on the shape of $P(\varepsilon)$. We have found that these corrections lead to an extension of $P(\varepsilon)$ far above the cutoff energy

$2\hbar k_F v$ but the extension has the amplitude by orders of magnitude smaller than is the amplitude of the free-electron $P(\varepsilon)$.

The distribution $P(\varepsilon)$ described in the paper can be used as the source function for the calculation of energy spectra of electrons excited in solids by moving particles. Subsequent modifications of these source function by transport through the solid and possibly also by the electron-electron interaction in the strongly excited areas near the moving particle are of particular interest for the theory of the ion-induced kinetic electron emission and for the ionization theory of particles sputtered from collision cascades.

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