# First-principles calculation of the cross sections for nuclear excitation by electron capture of channeled nuclei

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The time-dependent fields experienced by a nucleus as it passes through a crystal can cause transitions to excited nuclear states. The transition rate is especially large when the speed of the nucleus satisfies a resonance condition. Previous estimates of the nuclear excitation rates have been based on symmetry arguments and experimental data for related processes. We present here a calculation of the nuclear excitation rate which does not rely on these simplifying approximations. Using nonrelativistic quantum mechanics, the excitation cross sections of highly stripped nuclei channeled along the Si $\langle 110 \rangle$  crystal axis have been calculated. The results are smaller than those given by previous estimates by several orders of magnitude. We note that there are similarly large discrepancies between different theoretical and experimental results for other phenomena involving coupled electronic and nuclear transitions. The reason for these disagreements is not clear.

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### I. INTRODUCTION

As early as 1976, Goldanskii and Namiot [1] suggested the possibility of observing inverse internal conversion of the 26-min 73-eV isomeric state of <sup>235</sup>U in a lasergenerated plasma environment, and they estimated the excitation probability for this nuclear level. Recently, the inverse process of internal conversion has attracted attention, and it was suggested as a useful technique for pumping the population of specific nuclear levels, which is important for the development of gamma-ray lasers. In 1989, Cue, Poizat, and Remillieux [2,3] suggested that the same process, which they called nuclear excitation by (target) electron capture (NEEC), is observable when a highly stripped ion is channeled in a single crystal. They estimated the NEEC cross sections of several nuclei. Following that, Kimball, Bittle, and Cu [4] obtained similar results by estimating the NEEC cross sections of the same nuclei by using the experimental nuclear data, rather than the atomic data used by Cue, Poizat, and Remillieux.

We present here a more theoretical calculation of several NEEC cross sections. Following Refs. [2-4], we consider the following situations: The bare nuclei (ions) channel through single crystals, and the target electrons in the channel are captured into the K-shell atomic orbital of an incident nucleus. To conserve energy, the nucleus is simultaneously excited. Although we consider the same model, our results are *not* in good agreement with the estimates obtained in Refs. [2-4]. We have incorporated approximations in our calculations which could introduce some error, but it seems to us unlikely that these could be responsible for the large discrepancies between our results and the earlier estimates. These approximation include using nonrelativistic wave functions for the electrons, assuming a point nucleus, and ignoring various many-particle effects. We will first present our results in Secs. II and III in enough detail so that the reader can see what has been done. The concluding section will discuss the serious discrepancy between the results and will relate this discrepancy to a similar unsatisfactory situation for the case of nuclear excitation for bound-bound electron transitions (NEET's).

### **II. FORMALISM**

### A. Initial wave function of the nucleus-electron system

The initial state of the nucleus-electron system in the NEEC process consists of a ground-state nucleus and a free (target) electron, whose wave function is

$$\Psi' = \phi_{IM} \xi_m e^{ikz} , \qquad (1)$$

where  $\phi_{IM}$  and  $\xi_m$  are the spin wave functions of the nucleus and electron and  $e^{ikz}$  describes a free electron whose momentum is  $\hbar k$ . We assume the highly stripped ion (nucleus) moves along the central z-axis of a crystal channel. The coordinate system is chosen to move with the nucleus, with the origin at the nucleus. Energy is conserved in NEEC, and so only electrons with a suitable velocity with respect to the nucleus can excite the nucleus. We expand  $e^{ikz}$  in spherical harmonics:

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$$e^{ikz} = \exp[ikr\cos(\theta)] = \sum_{l=0}^{\infty} i^{l}\sqrt{4\pi(2l+1)}j_{l}(kr)Y_{l0}(\hat{\mathbf{r}}) , \qquad (2)$$

where r and  $\hat{\mathbf{r}}$  are radial and angular coordinates of the electron and  $j_l(kr)$  and  $Y_{l0}(\hat{\mathbf{r}})$  are Bessel and spherical-harmonic functions.

The free-electron wave function is distorted by the Coulomb field of the nucleus. The electron's distorted radial wave function is obtained by replacing  $j_l(kr)$  in (2) by  $\exp(i\sigma_l)F_l(kr)/(kr)$ . Here  $F_l(kr)$  is a Coulomb distorted wave function and  $\sigma_l = \arg[\Gamma(l+1+i\eta)]$  is the Coulomb phase shift, with  $\eta_{mZe}^2/(\hbar^2k)$ , Ze is the charge of the nucleus, and m is the electron mass. Thus the initial wave function of the nucleus-electron system is

$$\Phi = \phi_{IM} \xi_m \sum_{l=0}^{\infty} i^l \sqrt{4\pi (2l+1)} Y_{l0}(\hat{\mathbf{r}}) \exp(i\sigma_l) F_l(kr) / (kr)$$

$$= \phi_{IM} \sum_{l=0}^{\infty} \sum_{j=l\pm 1/2} i^l \sqrt{4\pi (2l+1)} \langle l0\frac{1}{2}m|jm \rangle \overline{Y}_{ljm} \exp(i\sigma_l) F_l(kr) / (kr)$$

$$= \sum_{l=0}^{\infty} \sum_{j=l\pm 1/2} \sum_{J=|j-I|}^{j+I} i^l \sqrt{4\pi (2l+1)} \langle l0\frac{1}{2}m|jm \rangle \langle jmIm_I|JM \rangle \Phi((lj,I)JM) \exp(i\sigma_l) F_l(kr) / (kr) , \qquad (3)$$

where  $\overline{Y}_{ljm}$  is a total-spin wave function of the electron,  $\Phi((lj, I)JM)$  is a channel total-spin wave function of the initial state of the spin-*I* ground-state nucleus coupled to the angular momentum *j* of the initial electron which gives the total spin *J* and projection *M*, and  $\langle j_1m_1j_2m_2|jm \rangle$  are Clebsch-Gorden coefficients.

#### B. Final wave function of the nucleus-electron system

In the NEEC process, the final wave function of the nucleus-electron system is

$$\widetilde{\Phi} = \widetilde{R}(r) \Phi((\widetilde{l}\widetilde{j}, \widetilde{I}) \widetilde{J} \widetilde{M}) , \qquad (4)$$

where  $\tilde{R}(r)$  is a radial wave function of a bound electron state and  $\Phi((\tilde{l} \ \tilde{j}, \tilde{I}) \tilde{J} \tilde{M})$  is the channel wave function of final state with total spin  $\tilde{J}$  and projection  $\tilde{M}$ . (For notational convenience, we will consistently apply the tilde to final-state wave functions and quantum numbers.)

#### C. Interaction Hamiltonian of the nucleus-electron system

Noting that NEEC is a direct interaction process (virtual photon process) [2] and assuming a nonrelativistic, nonscreening point-nucleus model, the interaction Hamiltonian for an electric  $2^L$ -pole transition is [5]

$$\mathcal{H}^{(\mathrm{EL})} = \overline{\mathbf{y}}_{L}(N) \cdot \overline{\mathbf{y}}(e)$$
$$\equiv \sum_{\mu} (-1)^{\mu} y_{L\mu}(N) y_{L-\mu}(e) , \qquad (5)$$

where

$$y_{L\mu}(N) = \sum_{t} e_t r_t Y_{L\mu}(\hat{\mathbf{r}}_t)$$
(6)

is the nuclear electric  $2^{L}$ -pole transition operator (t indexes the protons in one nucleus) and

$$y_{L\mu}(e) = -\frac{4\pi e}{2L+1} \frac{1}{r^{L+1}} Y_{L\mu}(\hat{\mathbf{r}})$$
(7)

is related to the  $2^{L}$ -multipole field at the origin produced by the electron.

The interaction Hamiltonian from a nuclear magnetic moment  $\bar{\mu}_I$  with the magnetic field produced by the electron at the origin (the position of nucleus) is

$$\mathcal{H}^{(M1)} = \vec{\mu}_I \cdot \vec{\mathbf{B}}^{(M1)} + \vec{\mu}_I \cdot \vec{\mathbf{B}}_I , \qquad (8)$$

where

$$\vec{\mathbf{B}}^{(M1)} = \frac{2\mu_B}{r^3} \left[ \frac{3(\vec{\mathbf{r}} \cdot \vec{\mathbf{S}})}{r^2} \vec{\mathbf{r}} - \vec{\mathbf{S}} \right]$$
(9)

is the magnetic dipole field produced by the electron [S is the electron-spin operator, and  $\mu_B = e\hbar/(2mc)$  is the Bohr magneton] and

$$\vec{\mathbf{B}}_l = \frac{2\mu_B}{r^3} \vec{l} \tag{10}$$

is the magnetic field produced by the orbital motion of the electron with orbital angular momentum  $\vec{l}$ . We note that because we accept the point-nucleus model, the normal delta-function term does not appear in Eq. (9) [6]. It is easy to verify [7] that

$$\frac{3(\vec{\mathbf{r}}\cdot\vec{\mathbf{S}})}{r^{2}}r_{\nu}-S_{\nu}$$

$$=-\sqrt{8\pi}(Y_{2}S)_{1\nu}$$

$$\equiv-\sqrt{8\pi}\sum_{\mu}\langle 1-\mu 2\mu+\nu|1\nu\rangle Y_{2\mu+\nu}(\hat{\mathbf{r}})S_{-\mu}.$$
(11)

# **D.** NEEC cross section of electric $2^{L}$ -pole transition

Staring from the golden rule, the NEEC transition probability is

$$T = \frac{2\pi}{\hbar} |\langle \tilde{\Phi} | H_{\rm int} | \Phi \rangle|^2 \rho , \qquad (12)$$

where  $H_{int}$  contains a summation over all multipole or-

ders of electric and magnetic transition.

For an electric  $2^L$ -pole transition operator  $\mathcal{H}^{(EL)}$ , the NEEC probability is

$$T_{j}^{(\mathrm{EL})} = \frac{2\pi}{\hbar} |\langle \tilde{\Psi} | \mathcal{H}^{(\mathrm{EL})} | \Psi \rangle|^{2} \rho .$$
(13)

For a nonpolarized incident nucleus and target electron, the NEEC cross section for the electric  $2^L$ -pole transition is

$$\sigma_J^{(\text{EL})} = \frac{1}{n_{\ell'}} \frac{1}{2(2I+1)} \sum_{mm_I \tilde{M}} T_J^{(\text{EL})} , \qquad (14)$$

where n is the density of the target electrons, and v is the velocity of the electron (with respect to nucleus).

Substituting Eqs. (1), (4), and (5) into Eqs. (13) and (14) and using conservation of angular momentum, (14) can be written as

$$\sigma_{\tilde{J}}^{(\text{EL})} = \frac{1}{n \, e^{\nu}} \frac{\rho}{2(2I+1)} \sum_{mm_{I}M} \frac{2\pi}{\tilde{n}} \left| \langle \tilde{R}(r) \tilde{\Phi}((\tilde{l}\tilde{j},\tilde{I})\tilde{J}\tilde{M}) | \bar{\mathbf{y}}_{L}(N) \cdot \bar{\mathbf{y}}_{L}(e) \right| \\ \times \sum_{ljJ} i^{l} \sqrt{4\pi(2l+1)} \langle l0\frac{1}{2}m|jm \rangle \langle jmIm_{I}|JM \rangle \Phi((lj,I)JM) \exp(i\sigma_{l})F_{l}(kr)/(kr) \right|^{2} \delta_{J\tilde{J}} .$$
(15)

Because the symbols of the interference terms between different partial waves may be positive or negative, which cancel each other, we ignore these interference terms for summation over l. Now Eq. (15) becomes

$$\sigma_{J}^{(\mathrm{EL})} = \frac{8\pi^{2}\rho}{2(2I+1)n\,\omega^{*}\hbar} \sum_{mm_{l}\tilde{M}} \sum_{ljJ} \langle l0\frac{1}{2}m|jm\rangle^{2} \langle jm\,\mathrm{Im}_{I}|JM\rangle^{2} \\ \times (2l+1) \left| \langle \tilde{R}(r)\Phi((\tilde{l}\tilde{j},\tilde{I})\tilde{J}\tilde{M})|\bar{\mathbf{y}}_{L}(N)\cdot\bar{\mathbf{y}}_{L}(e)|\Phi((lj,I)JM)F_{l}(kr)/(kr)\rangle \right|^{2} \delta_{J\tilde{J}} \\ = \frac{8\pi^{2}\rho}{2(2I+1)n\,\omega^{*}\hbar} \sum_{mm_{l}\tilde{M}} \sum_{lj} \langle l0\frac{1}{2}m|jm\rangle^{2} \langle jmIm_{I}|\tilde{J}\tilde{M}\rangle^{2} (2l+1)|H^{(\mathrm{EL})}|^{2} , \qquad (16)$$

where

$$H^{(\mathrm{EL})} \equiv \langle \widetilde{R}(r) \Phi((\widetilde{l}\widetilde{j},\widetilde{I})\widetilde{J}\widetilde{M}) | \overline{\mathbf{y}}_{L}(N) \cdot \overline{\mathbf{y}}_{L}(e) | \Phi((lj,I)JM)F_{l}(kr)/(kr) \rangle$$

$$= (-1)^{l+l+2\widetilde{l}+1/2+L+\widetilde{J}} e^{\left[\frac{4\pi(2\widetilde{j}+1)(2j+1)(2l+1)}{2L+1}\right]^{1/2}} \langle l0L0|\widetilde{l}0 \rangle$$

$$\times W(Ij\widetilde{l}\widetilde{j};\widetilde{J}L)W(lj\widetilde{l}\widetilde{j};\frac{1}{2}L) \langle \widetilde{I} || \overline{\mathbf{y}}_{L}(N) || I \rangle \int \widetilde{R}(r)F_{l}(kr)/(kr^{L})dr . \qquad (17)$$

In (17) the W's are Wigner 6j coefficients and  $\langle I_f || \overline{\mathbf{y}}_L(N) || I_i \rangle$  is the reduced matrix element of the electric 2<sup>L</sup>-pole transition operator of the nucleus. The Wigner-Echart theorem and the explicit expression for the reduced matrix elements of tensor products [8] were combined with Eqs. (5) and (7) to obtain Eq. (17). Substituting Eq. (17) into (16) and noting that

$$\sum_{mm_I\tilde{M}} \langle l0\frac{1}{2}m|jm\rangle^2 \langle jmIm_I|\tilde{J}\tilde{M}\rangle^2 = \frac{2\tilde{J}+1}{2l+1} , \qquad (18)$$

we have

$$\sigma_{\tilde{J}}^{(\text{EL})} = \frac{32\pi^{3}e^{2}\rho}{2(2I+1)n\,e^{\tilde{R}}} \left| \langle \tilde{I} \| \bar{\mathbf{y}}_{L}(N) \| I \rangle \right|^{2} \\ \times \sum_{lj} \frac{(2\tilde{J}+1)(2\tilde{j}+1)(2j+1)}{2L+1} \left[ \langle l0L0 | \tilde{l}0 \rangle W(Ij\tilde{l}\tilde{j};\tilde{J}L) W(lj\tilde{l}\tilde{j};\frac{1}{2}L) \right]^{2} \left| \int \tilde{R}(r)F_{l}(kr)/(kr^{L})dr \right|^{2}.$$
(19)

For fixed  $\tilde{I}$  and  $(\tilde{l}, \tilde{j})$ , the NEEC cross section of the electric 2<sup>L</sup>-pole transition is obtained from a sum over all available  $\tilde{J}$ ,

$$\sigma^{(\mathrm{EL})} = \sum_{j} \sigma_{j}^{(\mathrm{EL})} \,. \tag{20}$$

### E. Momentum distribution of the target electrons

In Sec. IV we considered a single target electron. In fact, there are many electrons in the path of the channeling nucleus which can play the role of the target electron. The electrons have a distribution of momenta. We take the Thomas-Fermi approximation to deal with these effects [4]. That is, the target electrons are assumed to form a Fermi sphere of a low-temperature electron gas whose density  $\bar{n}$  is the same as the density of the electrons in the channel. In momentum space this Fermi sphere is centered at  $\vec{p}_0 = m\vec{v}_0$  (with respect to the incident nucleus), where  $-v_0$  is the velocity of the incident nucleus. Let f(p) be the probability of finding an electron in a state with momentum p (with respect to the incident nucleus) and  $f(\vec{p})V/h^2$  be the probability density in momentum space (h is Planck's constant and V is a unit volume in the coordinate space):

$$f(\vec{p}) = \begin{cases} 1 & \text{for } |\vec{p} - \vec{p}_0| \le p_F , \\ 0 & \text{for } |\vec{p} - \vec{p}_0| > p_F , \end{cases}$$
(21)

where  $p_F$  is the Fermi momentum, which can be determined by the standard formula

$$p_F^3 = 3\pi^2 \hbar^3 \bar{n} \ . \tag{22}$$

Here the electron density *n* has been replaced by  $\overline{n}$ , which is the average density along the path of the channeling nucleus. For the real crystal, we can calculate  $\overline{n}$  [9]. For example, along the Si $\langle 110 \rangle$  direction the calculated result is  $\overline{n} = 4.347 \times 10^{-17}$  (fm<sup>-3</sup>).

The total NEEC transition probability is obtained by summing over all the target electrons. This gives an integral of the NEEC probability in momentum space, which is limited by the energy-conservation condition. The modified NEEC probability of the electric  $2^L$ -pole transition becomes

$$T_{J(\text{mo})}^{(\text{EL})} = \frac{2\pi}{\hbar} \int |\langle \tilde{\Psi} | \mathcal{H}^{(\text{EL})} | \Psi(p) \rangle|^2 \\ \times \frac{2f(\vec{p})V}{h^3} \delta(\tilde{E} - E) dp , \qquad (23)$$

where

$$\delta(\tilde{E}-E) = \delta\left[\frac{p^2}{2m} + u - U\right] = \frac{m}{p_E}\delta(|p|-p_E), \quad (24)$$

 $p^2/(2m)$  is the electron's kinetic energy, u is its binding energy in a captured orbital, and U is the nuclear excitation energy. The energy-conservation condition is satisfied when the magnitude of the electron's momentum is  $p_E$  (that is, a NEEC resonance occurs when  $|p_0| = p_E$ ), defined by

$$\frac{p_E^2}{2m} = U - u \quad . \tag{25}$$

Substituting Eq. (24) into (23) and noting that  $\langle \tilde{\Psi} | \mathcal{H}^{(EL)} | \Psi(p) \rangle$  depends only on the magnitude of  $\vec{p}$ , the modified NEEC probability of the electric 2<sup>L</sup>-pole transition is

$$T_{\tilde{j}(\mathrm{mo})}^{(\mathrm{EL})} = \frac{2\pi}{\hbar} |\langle \tilde{\Psi} | \mathcal{H}^{(\mathrm{EL})} | \Psi(p_0) \rangle|^2 \frac{m p_F^2 V}{4\pi^2 p \hbar^3}$$
$$= \frac{m p_F^2 V}{4\pi^2 p \hbar^3 \rho} T_{\tilde{j}}^{(\mathrm{EL})} .$$
(26)

In the first step of (26), because  $p_E \gg p_F$ , we replaced the intersection of the Fermi sphere with the surface of  $|p| = p_E$  by the intersections of the Fermi sphere with the plane  $P_Z = P_E$  (with  $p_Z$  along the direction of  $p_0$ ).

Finally, the modified NEEC cross section of the electric  $2^L$ -pole transition is

$$\sigma_{\rm mo}^{\rm (EL)} = \frac{m p_F^2 V}{4\pi^2 p_E \hbar^3 \rho} \sigma^{\rm (EL)} .$$
<sup>(27)</sup>

### F. NEEC cross section for the magnetic dipole transition

The basic theory for magnetic multipole transitions is similar to that for electric multipole transitions. Starting from Eq. (12) and using Eqs. (8)–(11), the modified NEEC cross section for the magnetic dipole transition is

$$\begin{split} \sigma_{\rm mo}^{(M1)} &= \frac{mp_F^2 V}{4\pi^2 p_E \hbar^3 \rho} \sigma^{(M1)} = \frac{mp_F^2 V}{4\pi^2 p_E \hbar^3 \rho} \frac{4\pi}{2(2I+1)n \, \nu \cdot \hbar} \left| \langle \tilde{I} || \bar{\mu}_I || I \rangle \right|^2 \\ & \times \sum_{\tilde{J}} \sum_{lj} (2\tilde{J}+1)(2\tilde{J}+1)(2\tilde{I}+1)[W(Ij\tilde{I}\tilde{J};\tilde{J}1)]^2 (2\mu_B)^2 \\ & \times \left| \delta_{l\tilde{l}}(-1)^{3/2-l-j} \sqrt{l(l+1)(2l+1)(2l+1)}W(lj\tilde{l}\tilde{J};\frac{1}{2}1) \right. \\ & \left. + 3\sqrt{5} \sqrt{(2l+1)(2j+1)} \langle l020|\tilde{l}0\rangle \left[ \frac{\tilde{l}}{l} - \frac{1}{2} - \tilde{j} \\ \left. l + \frac{1}{2} - \tilde{l} \right] \right|^2 \\ & \times \left| \int \tilde{R}_f(r) F_l(kr) / (kr^2) dr \right|^2 \,, \end{split}$$

(28)



(31)



FIG. 1. Momentum-space diagram illustrating the dynamics of NEEC. The nucleus can be excited if it is struck with an electron whose momentum lies on the surface of the energy-conserving sphere of radius  $p_F$ . The Fermi sphere is displaced from the origin by a momentum  $p_0$ , which represents the motion of the nucleus with respect to the electron gas. When  $p_0 = p_{E'}$ , a resonance NEEC process occurs.

where

is the 9*j* symbol [7] and  $\langle \tilde{I} || \bar{\mu}_I || I \rangle$  is the reduced matrix element of the nuclear magnetic moment.

# **III. CALCULATIONS AND RESULTS**

Using the formulas (27) and (28) deduced above, we calculated the NEEC cross sections of  ${}^{165}_{67}$ Ho,  ${}^{173}_{70}$ Yb,  ${}^{185}_{75}$ Re,  ${}^{187}_{75}$ Re, and  ${}^{195}_{78}$ Pt. In these calculations the initial states of these nuclei are ground states and the final states are first excited states. The nuclear properties ( $J^{\pi}$  of the ground and excited states, excitation energy U, and partial radiative width  $\Gamma_{fi}$ ) are obtained from standard references [10] and are listed in Table I. The resonance energies of the incident nuclei are also given in Table I. They are determined by

$$\mathcal{E} = \frac{M}{m} (U - u) . \tag{29}$$

The resonance widths have been described in Ref. [4]. The final state of the electron is a  $1S_{1/2}$  state with its wave function

$$\widetilde{R}(r) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a} , \qquad (30)$$

where  $a = a_0/Z$ , and  $a_0 = \hbar^2/(me^2)$  is the atomic Bohr radius. The nuclear reduced matrix elements  $\langle \tilde{I} || \bar{\mu}_I || I \rangle$ and  $\langle \tilde{I} || \bar{\mathbf{y}}_L(N) || I \rangle$  are evaluated by using two methods. In the first method, they are deduced from the measured partial radiative width  $\Gamma_{fi}$  [11]. In the second method, they are deduced from the Weisskopf estimates of the reduced transition probabilities, which are related to the reduced matrix elements by the formulas [8]

 $B_{fi}^{(\mathrm{EL})} = \frac{1}{2I+1} |\langle \widetilde{I} \| \overline{\mathbf{y}}_L(N) \| I \rangle|^2$ 

$$B_{f_i}^{(M1)} = \frac{1}{2I+1} |\langle \tilde{I} \| \bar{\mu}_I \| I \rangle|^2 .$$
(32)

The Weisskopf estimates of these reduced transition probabilities are [8]

$$B_{fi}^{(\text{EL})} = \frac{1}{4\pi} \left[ \frac{3}{L+3} \right]^2 R^{2L} \quad (\text{ in } e^2 \,\text{fm}^2)$$
(33)

and

and

$$B_{fi}^{(M1)} = \frac{10}{\pi} \left[ \frac{3}{4} \right]^2 \quad (\text{ in } \mu_N^2) , \qquad (34)$$

where the nuclear radius  $R = r_0 A^{1/3}$  and  $r_0 = 1.20$  fm.

In principle, the NEEC cross sections are sums over all available multiple orders of the electric and magnetic transition operators which conserve parity. In practice, the transition probabilities rapidly decreased with increasing order, and so we need to consider the lowest nonzero terms. On the other hand, the parities of the final nucleus-electron system and initial nucleus in our calculations are fixed and the available l values of the initial electron wave functions are all of odd or even l for parity conservation. This means that the available multipole orders L of transitions are all of odd or even. The above considerations make it possible that we only need to calculate the NEEC cross sections for electric quadrupole and magnetic dipole transitions in our calculations. The results were obtained for the five nuclei listed in

TABLE I.  $J_i^{\Pi}$  and  $J_f^{\Pi}$  of initial and final states of nuclei, nuclear excitation energies U, resonance energies  $\mathscr{E}$ , electronic ionization energies u, nuclear partial radiative width  $\Gamma_{fi}$ , and NEEC cross sections  $\sigma_1$  and  $\sigma_2$  (corresponding nuclear reduced matrix elements deduced from  $\Gamma_{fi}$  and Weisskopf estimates, respectively) are listed for nuclei channeled along the Si $\langle 110 \rangle$  lattice. Earlier estimates of Ref. [4] ( $\sigma^*$ ) are also shown.

| Nucleus                         | $J_i^{\Pi}$       | $J_f^{\Pi}$       | U (MeV) | $\mathscr{E}$ (MeV/u) | u (MeV) | $\Gamma_{fi}$ ( $\mu eV$ ) | Type of transition | $\sigma_1$ (mb)                                  | $\sigma_2$ (mb)        | $\sigma^*$ (mb) |
|---------------------------------|-------------------|-------------------|---------|-----------------------|---------|----------------------------|--------------------|--|------------------------|-----------------|
| <sup>165</sup> Ho               | $\frac{7}{2}$ -   | $\frac{9}{2}$ -   | 0.0947  | 54.2                  | 0.0611  | 29.9                       | E2<br>M2           | 0.48E-3<br>0.25E-3                               | 0.39E - 8<br>0.14E - 2 | 2.8             |
| $^{173}_{70}$ Yb                | $\frac{5}{2}$ -   | $\frac{7}{2}$ -   | 0.0786  | 12.6                  | 0.0666  | 14.3                       | E2<br>M1           | 0.16E - 2<br>0.44E - 3                           | 0.11E-7<br>0.31E-2     | 20.6            |
| <sup>185</sup> <sub>75</sub> Re | $\frac{5}{2}$ +   | $\frac{7}{2}$ +   | 0.125   | 76.5                  | 0.0765  | 64.5                       | Ē2<br>M1           | 0.42E - 3<br>0.30E - 3                           | 0.70E - 8<br>0.19E - 2 | 3.1             |
| $^{187}_{75}$ Re                | $\frac{5}{2}$ +   | $\frac{7}{2}^{+}$ | 0.134   | 92.7                  | 0.0765  | 58.9                       | Ē2<br>M1           | 0.26E - 3<br>0.21E - 3                           | 0.67E - 8<br>0.18E - 2 | 2.6             |
| <sup>195</sup> <sub>78</sub> Pt | $\frac{1}{2}^{-}$ | $\frac{3}{2}$ -   | 0.0989  | 14.7                  | 0.0827  | 3.90                       | E2<br>M1           | $0.21\overline{E} - 3$<br>$0.48\overline{E} - 4$ | 0.19E - 7<br>0.25E - 2 | 5.1             |

Table I. These are compared with estimated values fromRef. [4] in the last column of Table I.

### IV. CONCLUSIONS AND DISCUSSION

As Table I shows, our calculated NEEC rates for  ${}^{165}_{67}$ Ho  ${}^{173}_{70}$ Yb,  ${}^{185}_{75}$ Re,  ${}^{187}_{75}$ Re, and  ${}^{195}_{78}$ Pt channeled along the Si(110) direction are all several orders of magnitude smaller than earlier estimates [4]. There are no experimental NEEC results.

Our calculations are based on some approximations which may have affected the results. In particular, we applied nonrelativistic quantum mechanics even though characteristic velocities needed for NEEC in the nuclei we studied vary from 0.22c to 0.47c. We also ignored inner-shell screening and the nonzero radius of the nuclei. The nuclear size is important because it will change the Coulomb field of the nucleus and affect the wave functions of the electrons. In addition, the electron will be able to penetrate the nuclear charge and current distributions, and this will change the transition matrix elements. However, it seems unlikely that any of these corrections would change our results by the several orders of magnitude needed to achieve agreement with the earlier estimates. Thus the real magnitude of the NEEC

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process is very much in doubt and in need of experimental verification.

Discrepancies of the same order of magnitude exist for the case of "nuclear excitation by an electron transition," called NEET. In this process the nucleus is excited when an outer bound-state electron makes a transition to a Kshell hole. For this process we are aware of four different calculations: early perturbation estimates by Morita [12], a more careful calculation based on perturbation theory and the golden rule by Ho, Zhang, and Yuan [5], a QED-based approach by Pisk, Kaliman, and Logan [13], and an extension of this latter work by Ljubičić, Kekez, and Logan [14]. These calculations differ by orders of magnitude. There are also five reported experiments [15-19]. Three of these experiments [17-19] measure the 1.26-keV excitation probability for <sup>189</sup>Os, but the experiments also differ by orders of magnitude. For <sup>189</sup>Os, the calculation which agrees best with experiment depends on which experiment one believes. Clearly, our quantitative understanding of combined electronicnuclear transitions leaves much to be desired.

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