216--16

CONF-8909210--10

DE90 008570

RADIATIVE ELECTRON CAPTURE BY CHANNELED IONS

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Abstract

Considerable experimental data have been accumulated relative to the emission of photons accompanying electron capture by swift, highly stripped atoms penetrating crystalline matter under channeling conditions. Recent data suggest that the photon energies may be less than that expected from simple considerations of transitions from the valence band of the solid to hydrogenic states on the moving ion. We have studied theoretically the impact parameter dependence of the radiative electron capture (REC) process, the effect of the ion's wake and the effect of capture from inner shells of the solid on the photon emission probabilitiy, using a statistical approach. Numerical comparisons of our results with experiment are made.

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1. *Introduction*

Many processes can give rise to X-ray production when energetic heavy ions interact with solids. Radiative electron capture (REC) is said to occur when an ion captures an electron into one of its shells and emits a photon[1].

This process contributes only in a very small way to the total production of radiation; however, it becomes more important and amenable to interpretation when the bombarding ions are channeled through the solid, since in these conditions the ions never approach closer than 0.1 or 0.2Å to target atoms, so that the yield of characteristic X-rays, one of the most important contributions to the total production of radiation, is very much smaller than that observed when the beam is incident on the crystal in a random direction. Furthermore, it has been shown that stripped, incident channeled ions have "frozen" charge states, and although nonradiative electron capture is the dominant mechanism for charge transfer, in ion channeling the inhibition of close collisions makes the radiative process relatively more important[2].

The REC process has the possibility of becoming a significant tool in the study of the momentum distribution of target electrons, so that some experimental data[3-7] have been accumulated. Indeed, recent data[7] suggest that the photon energies may be less than that expected from simple considerations of transitions from the valence band of the solid to hydrogenic states on the moving ion.

The purpose of this paper is to extend previous[5,8,9] theoretical approaches, and to study theoretically the impact parameter dependence of the REC process and the effect of capture from inner shells of the solid.

2.- Theory

We consider a solid through which a swift, heavy, stripped ion of charge Z_1 and velocity v passes and captures an electron accompanied by the emission of a single photon. The nonrelativistic Hamiltonian of the system may be written as

$$H = H_0 + H_{rad} + H' , \qquad (1)$$

where H_0 and H_{rad} are the hamiltonians of the electron-ion system and the free radiation field, respectively, and

$$H' = -\frac{i}{c}\, A \,.\, \nabla \qquad (2)$$

is the interaction hamiltonian between them, with

$$A = \frac{1}{i}\sum_{k\,\lambda}\left(\frac{2\pi c^2}{\omega_k V}\right)^{1/2} e_{k\,\lambda}\, e^{i\,k.r}\left(a_{k\,\lambda} + a^{+}_{-k\,\lambda}\right) . \qquad (3)$$

$a_{k\,\lambda}$ and $e_{k\,\lambda}$ are, respectively, the annihilation operator and the polarization vector of a photon with wave vector **k** and polarization index $\lambda(\lambda= 1,2)$, which in free space is perpendicular to the direction of propagation, ω_k=ck is the frequency of a photon of wave vector **k**, and V is the normalization volume of the radiation field. The movement of the ion relative to the center of mass of the system has been neglected, as well as a term in H' which is quadratic in the potential vector. Unless otherwise stated, atomic units are used throughout.

The transition probability for a target electron to be captured into a k-shell orbital of the moving ion, emitting a photon, may be written in first order perturbation theory as follows:

$$\gamma_{fi} = \left|\int_{-\infty}^{+\infty} d\,t\, e^{i\,\omega_k t} < H'_{fi}\,(t) >\right|^2 , \qquad (4)$$

where $< H'_{fi}\,(\,t\,) >$ represents the time-dependent matrix element of the matter-radiation interaction:

$$< H'_{f\,i}\,(\,t\,) > = < 0 \,|\, a_k < \varphi_f\,(\,\mathbf{r}, t\,) \,|\, H' \,|\, \varphi_i\,(\mathbf{r}, t\,) > |\, 0 > , \qquad (5)$$

where $\varphi_f\,(\,\mathbf{r}, t\,)$ is the final wave function corresponding to a k orbital of the swift ion:

$$\varphi_f\,(\,\mathbf{r}, t\,) = \left(\frac{Z_1^2}{\pi}\right)^{1/2} e^{-Z_1\,|\,\mathbf{r}\,-\,\mathbf{b}\,-\,\mathbf{v}t\,|}\; e^{-\,i\,\mathbf{v}.\mathbf{r}}\; e^{-\,i\,(-E_B + E_1)\,t} . \qquad (6)$$

Here $\varphi_i\,(\,\mathbf{r}, t\,)$ is the wave function of the electron in the initial state, and $|\,0>$ is the vacuum state of the radiation field. In eq. (6) **b** represents the impact parameter, E_B represents the binding energy of the captured electron in the K orbital:

$$E_B = \frac{1}{2} Z_1^2 - \frac{\pi Z_1 \omega_p}{2\,v} \quad , \tag{7}$$

and

$$E_1 = \frac{1}{2} v^2 \; . \tag{8}$$

with v the velocity of the ion. The effect of the ion's wake has been considered including in eq. (7) the potential of the polarized medium at the site of the ion[10]. We should mention, however, that for typical REC experiments this potential is approximately 15eV, in such a way that this correction turns out to be not greater than a 1 or 2% of the total REC energy.

REC processes can proceed by capture of free, as well as bound electrons. In particular, with the aim of understanding how the emission probability corresponding to capture of bound electrons depends on the impact parameter, one can write, on very general grounds, the initial wave function of the target electron as follows:

$$\varphi_i(\mathbf{r}, t) = \left(\frac{\alpha^3}{\pi}\right)^{1/2} e^{-\alpha r}\, e^{-i\omega_i t} , \tag{9}$$

and find, after having introduced (6) and (9) into (5) and (5) into (4) the following expression for the transition probability per unit energy and solid angle to any one of a group of final states with wave vector nearly equal to **k**:

$$\frac{d^3 \gamma_{fi}}{d\,\omega_k d\,\Omega} = \frac{2^6 Z_1^5 \alpha^5}{\pi^4 c^3}\,\omega_k \left| \int \frac{d\mathbf{q}\, e^{i\,\mathbf{q}.\mathbf{b}}\, \mathbf{e}_k \cdot \mathbf{p}}{(Z_1^2+p^2)^2(\alpha^2+q^2)^2}\; \delta\,(\mathbf{q}.\mathbf{v}+\omega_{fi}+E_1+\omega_k) \right|^2 \tag{10}$$

where

$$\mathbf{p} = \mathbf{q} + \mathbf{k} + \mathbf{v} \quad , \tag{11}$$

$$\omega_{fi} = \omega_f - \omega_i \quad , \tag{12}$$

and $d\Omega$ is the infinitesimal element of solid angle in the direction of emission. The spectrum obtained in this way has been found to be very much wider than that for capture from the electron gas; moreover, it has been found to be wider as the impact parameter increases, as is obvious from figure 1, where the REC peak widths obtained with eq. (10) are plotted against the impact parameter when photons are emitted parallel to the beam direction.

In order to study in detail the effect of capture from inner shells of the solid on the photon emission probability, a knowledge of the many-electron wave function of the solid is required; however, in order to simplify we adopt a statistical approximation[5], assuming that the response of an infinitesimal element of volume in the solid at position **r**, where the total density is n(**r**), is the same as that of an electron gas at that density. Thus, we define the local Fermi energy to be

$$E_F(\mathbf{r}) = \frac{\left[3\,\pi^2 n\,(\mathbf{r})\right]^{2/3}}{2} \quad . \tag{13}$$

when capture occurs from the vicinity of **r** .

Assuming in this approximation that the wave functions of electrons in a given part of the solid are plane waves:

$$\varphi_i\,(\,\mathbf{r}, t\,) = \frac{1}{\sqrt{V}}\; e^{\,i\,\mathbf{q}_i\cdot\mathbf{r}}\; e^{-i\frac{1}{2}(q_i^2 - q_F^2)\,t} \quad , \tag{14}$$

where $\mathbf{q}_i$ represents the initial momentum of the electron and q_F is the Fermi momentum ($q_F=1.92/r_s$), the REC probability per unit energy and solid angle of the emitted radiation is[11]

$$\frac{d^3\gamma_{fi}}{d\omega_k\,d\Omega} = \frac{2^3 Z_1^5\,\omega_k}{\pi^3 c^3} \int d\,\mathbf{q}_i\, \frac{(\mathbf{e}_k\cdot\mathbf{q}_i)^2}{(Z_1^2 + q_i'^2)^4}\;\delta\,(\omega), \tag{15}$$

where

$$\mathbf{q}'_i = \mathbf{q}_i - \mathbf{k} - \mathbf{v}\,, \tag{16}$$

and

$$\omega = -\,E_B - \frac{1}{2}\,(\,\mathbf{q}_i - \mathbf{v})^2 + \frac{1}{2}q_F^2 - \mathbf{k}\,.\,\mathbf{v} + \omega_k \tag{17}$$

The integral over $\mathbf{q}_i$ in (15) covers a Fermi sphere of electrons, so that we obtain, after some algebra, the following expression:

$$\frac{d^3\gamma_{fi}}{d\omega_k\, d\Omega} = \frac{Z_1^5\, \omega_k}{2\pi^3 c^3 v} \int_0^{2\pi} d\varphi \int_{q_1}^{q_2} dq\; q^3\, \frac{A^2+B^2}{C^4}, \tag{18}$$

when

$$E_B - E_F + \left(\sqrt{E_1} - \sqrt{E_F}\right)^2 \le \omega'_k \le E_B - E_F + \left(\sqrt{E_1} + \sqrt{E_F}\right)^2 , \tag{19}$$

and zero otherwise. In these expressions,

$$\begin{aligned} A &= \mu \sin\theta - (1-\mu^2)^{1/2} \cos\theta \cos\varphi \\ B &= (1-\mu^2)^{1/2} \sin\varphi \\ C &= E_F + \omega_k \left[1 - \frac{q}{c}\left(\mu \cos\theta + (1-\mu^2)^{1/2} \sin\theta \cos\varphi\right) + \frac{\omega_k^2}{2c^2} \right] \end{aligned} \tag{20}$$

$$q_1 = \sqrt{2}\, \left| \sqrt{\omega'_k - E_B + E_F} - \sqrt{E_1} \right| \tag{21}$$

$$q_2 = \sqrt{2}\ \min\left(\sqrt{E_F}\ ,\ \left| \sqrt{\omega'_k - E_B + E_F} + \sqrt{E_1} \right| \right), \tag{22}$$

$$\mu = \frac{1}{q\,v}\left[E_B + \frac{1}{2} q^2 + \frac{1}{2} v^2 - E_F - \omega'_k \right] \tag{23}$$

and

$$\omega'_k = \omega_k \left(1 - \frac{v}{c} \cos\theta \right) , \tag{24}$$

with θ being the angle formed by the direction of emission and the beam direction. To obtain (18) summation over the directions of e_k in a plane perpendicular to the given direction of the emitted radiation has been performed.

If we define the local Fermi energy to be given by (13) we may calculate, in our approximation, the REC probability per unit energy and solid angle when capture occurs from the vicinity of r, once the total electronic density there is known.

We have employed the electronic density values shown in fig. 2 for silicon, as computed from a relativistic Hartree-Fock program[12] using the Wigner-Seitz boundary condition, and we have found that the peak energy of the emitted radiation decreases strongly when electrons are captured from inner shells of the solid, as is obvious from fig. 3, where REC peak energies for 160 MeV S^{16+} stripped ions channeled through silicon are plotted against r, that is, the position where capture occurs, when photons are emitted at 46,5° to the incident beam.

Notice that the REC peak energy of photons resulting from capture of target electrons at r_{ws}, the Wigner-Seitz radius, is almost equal to

$$E_{REC} = E_B + E_i \tag{25}$$

as may be inferred from considerations of transitions from the valence band of the solid to hidrogenic states on the moving ion, but it deviates when capture occurs from regions of relatively high electron density. This variation may explain the REC "deficit" observed in recent data, as we will see below.

Finally, if we assume that the bombarding channeled ions sample on straight-line trajectories all portions of the WS sphere corresponding to impact parameters greater than a given b_{min}, the statistical average of the REC probabilities per unit energy and solid angle may be written as

$$< \frac{d^3\gamma_{fi}}{d\Omega_\kappa d\Omega} > = \frac{3}{r_{ws}^3} \int_{b_{min}}^{r_{ws}} r\,(r - b_{min}) \frac{d^3\gamma_{fi}}{d\omega_k d\Omega} \left[E_F(r) \right], \tag{26}$$

where

$$\frac{d^3\gamma_{fi}}{d\omega_\kappa d\Omega}$$

is given by (18), and $E_F(r)$ by (13), as discussed above.

On the other hand, if one assume that each electron undergoing capture from the solid experiences the full Coulomb field of the projectile, neglecting screening by other electrons of the solid, essentially the same dependence of the REC probabilities on projectile velocity is predicted[5,13].

3. Results

Figure 4 exhibits plots of the REC probabilities per unit energy and unit solid angle for a target electron to be captured accompanied by emission of radiation at θ as obtained from eq. (26) for 160 MeV S^{16+} ($\theta = 46.5^0$) ions channeled through silicon with b_{min}=0.3Å . Figure 5 shows the dependence of the peak energy positions so obtained on the minimum impact parameter, together with the REC energies calculated from (25), and the experimentally measured REC energies [7].

Notice that the agreement with experiment is good when the minimun impact parameter is 0.3Å, showing that capture from regions of relatively high electron density in the channel explains the experimentally observed REC deficit. The origin of the REC deficit is obvious, too, from figure 6, where measured and calculated REC peak positions for bare sulfur ions channeled through silicon are shown as a function of incident ion energy, for different values of the minimun impact parameter.

This work has been sponsored by the Universidad del Pais Vasco / Euskal Herriko Unibertsitatea, by the office of Health and Environmental Research, U.S. Department of Energy, under contract DE-AC05-840R21400 with Martin Marietta Energy Systems, Inc., and by the US-Japan Cooperative Science Program of the National Science Foundation, Joint Research Project No. 87-16311/MPCR-168.

Note: The authors are preparing a revised and more accurate version of the theory described above in which the REC probability is calculated using wave functions that describe the electron and the ion in relative and center-of-mass coordinates.

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Figure Captions

Fig. 1 REC linewidths calculated from eq. (10), as a function of impact parameter.

Fig. 2 Relativistic Hartree-Fock calculations of the total electronic density in the Wigner-Seitz sphere, for silicon[12].

Fig. 3 REC positions for 160 MeV bare sulfur ions channeled through silicon, as obtained from eq. (18), as a function of the distance r from the captured target electron to the nearest atom in the crystal.

Fig. 4 REC probability per unit energy and solid angle, as obtained from eq. (26) when photons are emitted at $\theta = 46{,}5^{0}$ with respect to the beam direction, for 160 MeV S^{16+} ions channeled through silicon .

Fig. 5 Calculated REC peak positions for 160 MeV bare sulfur channeled through Si, with $\theta = 46.5^{o}$, as a function of minimun impact parameter. Also shown are the REC energies calculated from eq. (25) and the experimentaly measured ones of ref. 7.

Fig. 6 Measured[7] and calculated REC peak positions for bare sulfur ions channeled through silicon, as a function of the incident energy of the ions, for b_{min}= 0.1 and 0.3 Å. Also shown are the REC energies obtained from eq. (25).

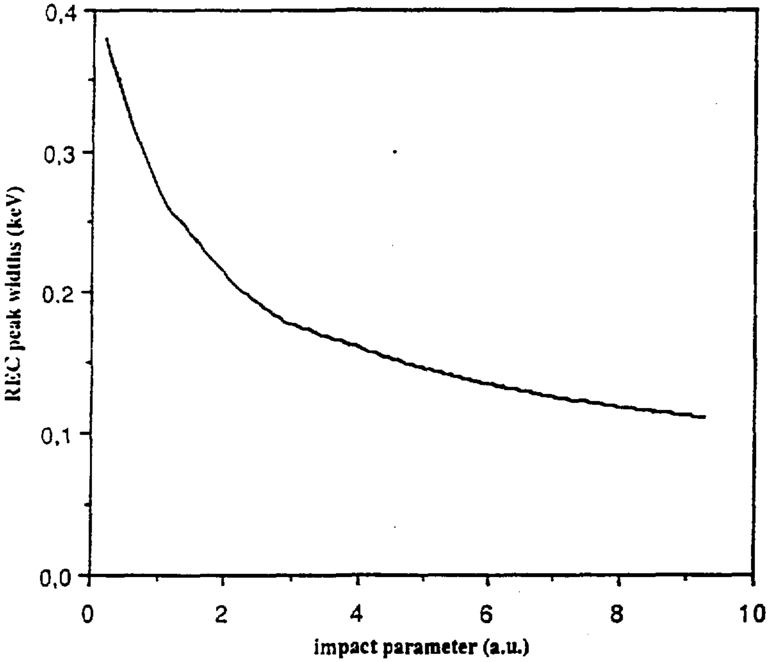
0,4
0,3
0,2
0,1
0,0
REC peak widths (keV)
0
2
4
6
8
10
impact parameter (a.u.)

Fig. 1

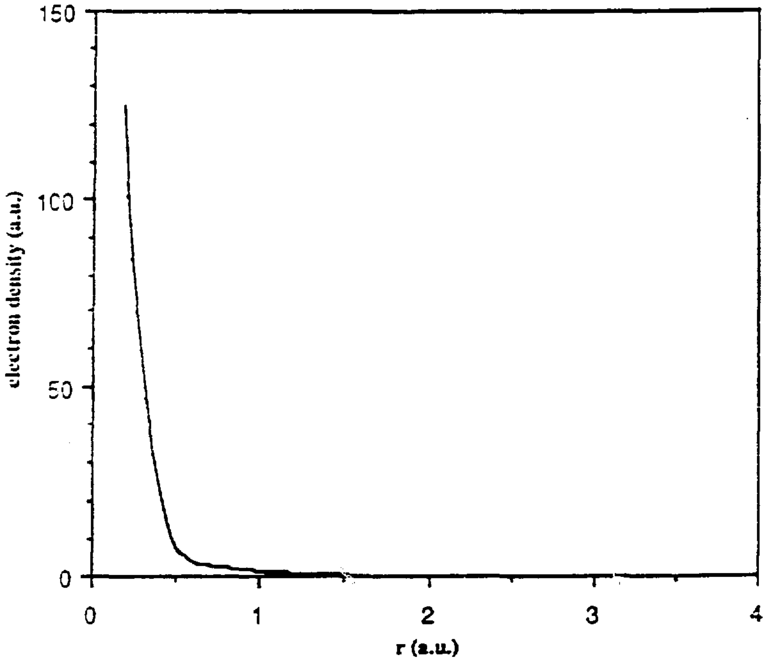

Fig. 2

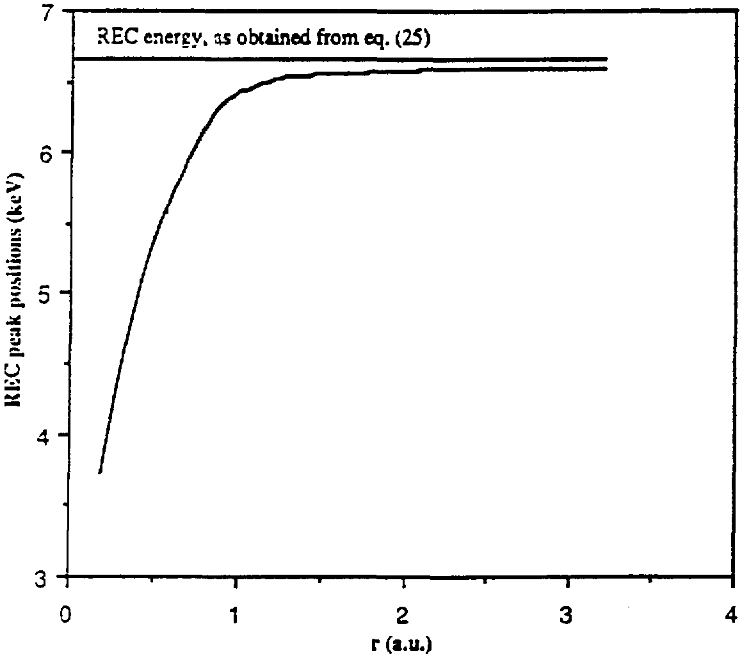
REC energy, as obtained from eq. (25)
REC peak positions (keV)
r (a.u.)
3
4
5
6
7
0
1
2
3
4

Fig. 3

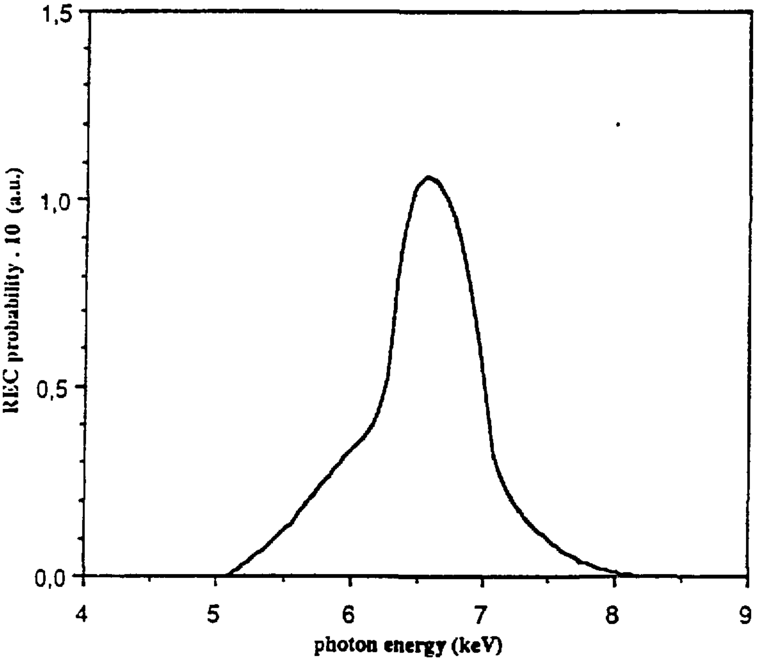

Fig. 4

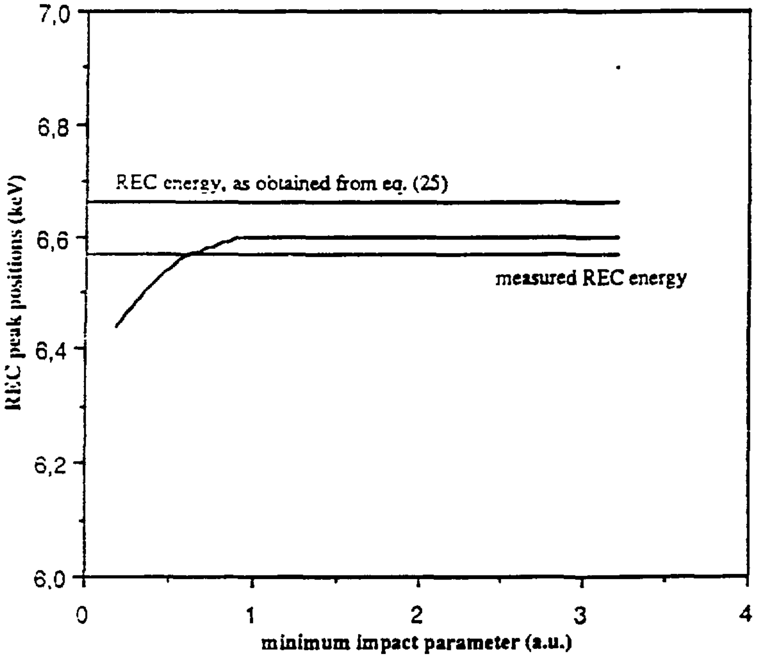
7,0
6,8
6,6
6,4
6,2
6,0
REC peak positions (keV)
REC energy, as obtained from eq. (25)
measured REC energy
0
1
2
3
4
minimum impact parameter (a.u.)

Fig. 5

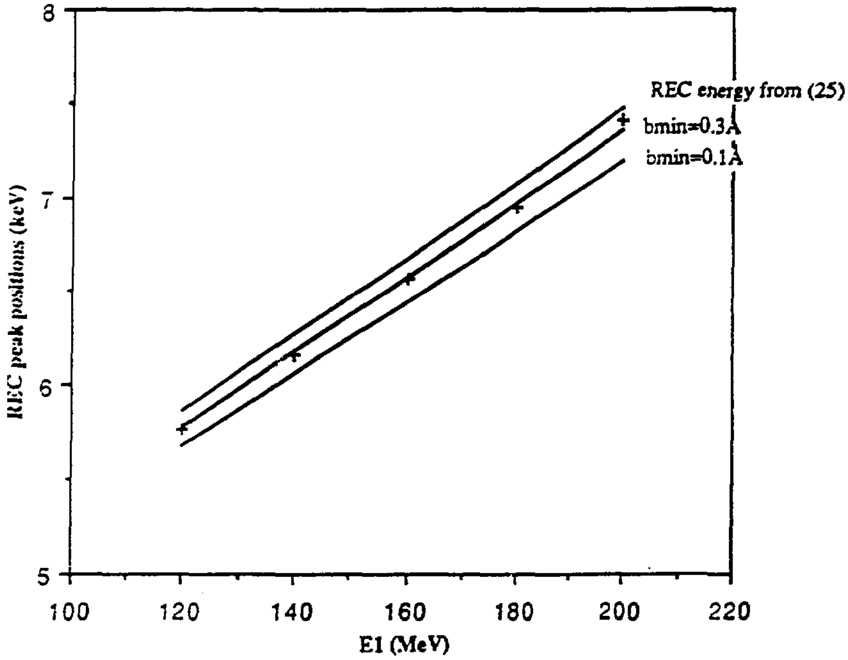
REC energy from (25)
bmin=0.3Å
bmin=0.1Å
REC peak positions (keV)
8
7
6
5
100
120
140
160
180
200
220
El (MeV)

Fig. 6