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FRACTAL DESCRIPTION OF ELECTRON SCATTERING IN SOLIDS: SEVERAL NEW RESULTS AND A SIMPLE MODELIZATION OF THE FRACTAL DIMENSION

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Abstract

The fractal behaviour of electron scattering in solids is studied with electron trajectories simulated by Monte Carlo simulations. More precisely, the Hausdorff-Besicovitch dimension is determined for several electrons trajectories simulated in solids of different compositions. Then, a simple model to compute the fractal dimension of electron trajectories in solids is presented, a model which raises a question concerning the maximum value of the backscattering coefficient. Results of Monte Carlo simulations of electron trajectories in several elements with total randomness for the polar and azimuthal angles of scattering are presented as a tentative answer to this question. Finally, the multifractal behaviour of the energy distribution of backscattered electrons is presented.

Key Words : Fractal dimension, electron scattering, Monte Carlo simulations, multifractals, backscattering electrons.

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Introduction

The determination of the fractal behaviour of the trajectories of incident electrons in a solid is important in a fundamental point of view as in a technological point of view concerning scanning electron microscopy and electron beam lithography.

Since the work of Mandelbrot (1982), it is well known that continuous curves or surfaces having no derivatives are fully characterized by their Hausdorff-Besicovitch dimension, or box counting dimension, and such curves (or surfaces) are called fractal curves (or fractal surfaces). Numerous examples of curves and surfaces having a fractal behaviour have been found. These include the coast of countries (Mandelbrot, 1967), fracture surfaces (Mandelbrot et al., 1984), earth's relief (Mandelbrot, 1975) and dendrites in solidified alloys (Uwaha and Saito, 1990). Also, the fractal behaviour of ions which cascade in solids has been characterized theoretically and measured from Monte Carlo simulations (Rossi et al., 1989). Gauvin and Drouin (1992) have undertaken studies concerning the fractal behaviour of the trajectories of incident electrons in solids when they scatter in a specimen analyzed in the scanning electron microscope. In this paper, other results concerning the fractal behaviour of electron scattering in solids are presented.

The first part of this paper briefly presents the Monte Carlo model used to simulate electron scattering in solids. The second part presents the determination of the Hausdorff-Besicovitch dimension using the box counting method for one electron trajectory simulated in C, Cu, Ag and Au with initial energy, E_0, equals to 10 keV. Then, this dimension is determined for 30 trajectories simulated in the same systems with E_0 equals to 10 and 30 keV. Finally, the Hausdorff-Besicovitch dimension is determined for 1000 electron trajectories simulated in gold with E_0 equal to 30 keV. The third part of this paper presents a

simple model to compute the fractal dimension of electron trajectories in solids. A correlation between the fractal dimension computed with this model and backscattering coefficients of several elements raise a question concerning the maximum value of the backscattering coefficient, and results of Monte Carlo simulations of electron trajectories in several elements with total randomness for the polar and azimuthal angles are presented as a tentative answer to this question. Finally, the last part of this paper presents the multifractal behaviour of the energy distribution of backscattered electrons for several elements.

Monte Carlo Simulations of Electron Trajectories

Figure 1 shows the sequence of events which are assumed when an electron diffuses into a solid in Monte Carlo simulations. At the point P_i, the electron with an energy equal to E_i suffers an elastic collision since the scattering of primary electrons in solids is mostly caused by elastic collisions, except for light elements when inelastic scattering dominates (Newbury et al., 1986). Its trajectory is changed by a polar angle θ_i, and an azimuthal angle ϕ_i, and this electron travels a distance L_i to the next point P_{i+1} when it suffers another collision.

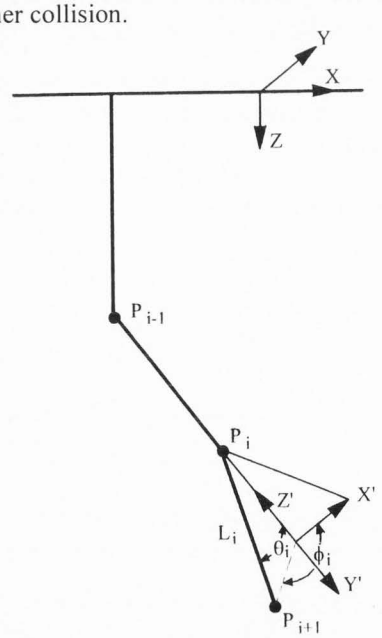

Figure 1. Geometry used to compute the trajectory of an electron when it travels from point P_i to point P_{i+1} separated by a distance L_i. θ_i and ϕ_i are the polar and azimuthal angles of collision at point P_i.

The polar angle of collision, θ_i, is obtained by generating a random number uniformly distributed between 0 and 1, R_1, and by solving this equation :

$$R_1 = \frac{\int_0^{\theta_i} \left(\frac{d\sigma_{el}}{d\Omega}\right)_{E_i} \sin\theta \, d\theta}{\int_0^{\pi} \left(\frac{d\sigma_{el}}{d\Omega}\right)_{E_i} \sin\theta \, d\theta} \qquad (1)$$

where $\left(\frac{d\sigma_{ei}}{d\Omega}\right)_{E_i}$ is the partial elastic cross-section at energy E_i as a function of the solid angle $d\Omega$. The azimuthal angle of collision is uniformly distributed between 0 and 2π, and it is obtained by solving this equation :

$$\phi_i = 2\pi R_2 . \qquad (2)$$

where R_2 is another random number uniformly generated between 0 and 1.

The distance between collisions is computed by generating another random number uniformly distributed between 0 and 1, R_3, and by solving this relation :

$$L_i = \frac{-1}{2\pi\rho \int_0^{\pi} \left(\frac{d\sigma_{el}}{d\Omega}\right)_{E_i} \sin\theta \, d\theta} ln\left(R_3\right) \qquad (3)$$

where ρ is the atomic density of the solid. This equation is valid when specimen composition is homogeneous. In this work, the partial elastic cross-section of Rutherford is used with the screening parameter of Nigam et al. (1959) giving analytical expressions for equations (1) and (3) (Murata et al., 1973). When an electron travels from the point P_i from the point P_{i+1}, it is assumed in conventional Monte Carlo simulations that the electron travels in a straight line, which is certainly not the case in reality because the strong coulombic field between the incident electron and the atoms of the specimen certainly gives a curvature to its trajectory. Also, it is assumed that the electron looses energy continuously when it travels from P_i to P_{i+1} because of the inelastic collisions. The energy at the point P_{i+1}, E_{i+1}, is obtained by solving this relation :

$$E_{i+1} = E_i + \left(\frac{dE}{dS}\right)_{E_i} \cdot L_i \qquad (4)$$

where $\left(\frac{dE}{dS}\right)_{E_i}$ is the rate of energy loss at energy E_i, and the relativistic expression of Livingston and Bethe (1937) is used in this work :

$$\frac{dE}{dS} = -\frac{4\pi e^4}{m_0 c^2 \beta_i^2} N_0 \rho \frac{Z}{A}$$

$$\left\{ ln\left(\frac{297{,}91\ \beta_i^2}{J}\right) - ln\left(1-\beta_i^2\right) - \beta_i^2 \right\} \qquad (5)$$

where ρ is the mass density of the solid $e_v = e_v^2 / (4\pi\varepsilon_o)$, e_V is the electronic charge, ε_O is the permittivity of free space, Z, A and J are the atomic number, atomic weight and mean ionization of the solid, respectively, c is the speed of light, m_O is the rest mass of the electron and β_i is the ratio of the speed of the electron, of energy E_i, to that of the speed of light. In this work, values of J recommended by Murata et al. (1973) are used.

The trajectory of an incident electron, specified by its initial direction and energy in a solid, is thus simulated by the successive summation of the events described above until it escapes the specimen, which gives a backscattered electron, or when its energy becomes equal to the mean energy of the conduction electrons of the solid (because of the failure of equation (5) at low energy, the computation of the trajectory of the electron is stopped when $E \leq 5J$ in our simulations). This gives the single scattering approach to simulate electron trajectories. In our simulations, random numbers are generated using the algorithm of Press et al. (1986).

The Hausdorff-Besicovitch Dimension of Electron Trajectories in Solids

The Hausdorff-Besicovitch dimension D of a curve is related to the number of square (or cube) boxes $N(\delta)$ of length δ which cut the curve by :

$$N(\delta) = k\,\delta^{-D} \qquad (6)$$

where k will be defined later. As tentatively defined by Mandelbrot (1982), a fractal is by definition a set for which the Hausdorff-Besicovitch dimension strictly exceeds the topological dimension. Since this definition involves formal mathematics, Mandelbrot has proposed another definition (Feder, 1988) : a fractal is a shape made of parts similar to the whole in some way.

The length of a curve could be approximated by multiplying the number of boxes needed to cover the line by their size giving :

$$L(\delta) = k\,\delta^{1-D}. \qquad (7)$$

When a curve is not fractal, D = 1 as it is for a straight line or a circle and the length of this curve remains finite and k is the length of the curve. When a curve is fractal, D exceeds 1 and the length of the curve increases when δ decreases. Thus, the length of a fractal curve is a function of δ and diverges as δ tends to zero. To generalize, the measure M_d is defined in this way :

$$M_d = \Sigma\gamma(d)\delta^d = \gamma(d)\,N(\delta)\,\delta^d \qquad (8)$$

where $\gamma(d)$ is a constant which is related to the shape of the element which cover the whole set. $\gamma(d)$ is a function of d which may be a non-integer value. When a set is covered by lines, square or cubes, $\gamma(d) = 1$. Substituting equation (6) into equation (8) gives :

$$M_d = E\,\delta^{-D}\,\delta^d \qquad (9)$$

where $E = \gamma(d)\,k$. When $d < D$, M_d tends to ∞ and when $d > D$, M_d tends to 0 as δ tends to zero in both cases. Thus, the Hausdorff-Besicovitch dimension D of a set is the critical dimension for which the measure M_d changes from zero to infinity as δ tends to zero. When $d = D$, $M_d = E$ and Mandelbrot (1982) called it tentatively an approximate measure in dimension d.

A plot of log ($N(\delta)$) versus log (δ) gives a slope of -D. Such a plot is shown in Figure 2 for an electron trajectory simulated in silver with an initial energy equal to 10 keV. When δ is greater than the whole electron trajectory, $N(\delta)$ equals 1 and D equals zero. When δ is on the order of the whole electron trajectory, a value of $D \cong 1.7$ is observed. Since D is greater than the topological dimension of the curve, a fractal behaviour is observed. When δ decreases, a value of D equals one is measured because in this range of δ, just one part of the electron trajectory is intercepted by the boxes and the trajectories of electrons are assumed, in Monte Carlo simulations, to be straight lines between elastic collisions. This is also consistent to the fact that the length of electron trajectories in solids are finite because their range is a function of their initial energy and of the rate of energy loss

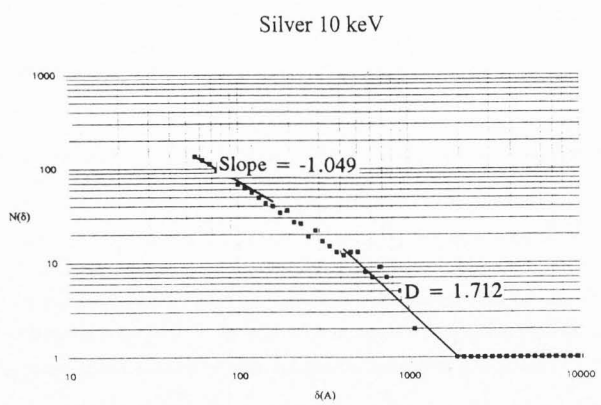

Figure 2. Log(N(δ)) versus log(δ) for an electron trajectory simulated in Ag with an initial energy equal to 10 keV.

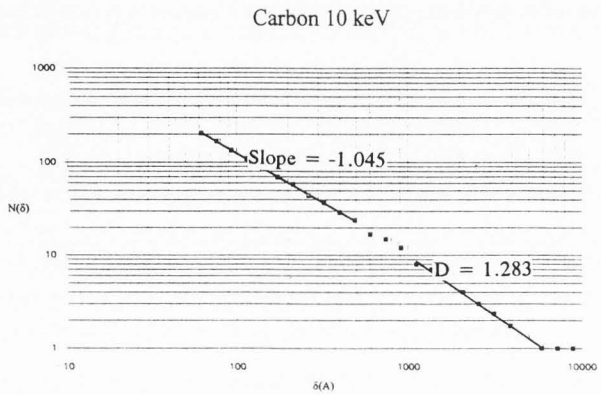

Figure 3. Log(N(δ)) versus log(δ) for an electron trajectory simulated in C with an initial energy equal to 10 keV.

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when they diffuse into a solid, and since they have a finite amount of initial energy, their range is finite. From this argument, the Hausdorff-Besicovitch dimension of an electron trajectory should be equal to one as δ tends to zero. Therefore, the shape of electron trajectories simulated in solids has a fractal behaviour in a specific range of δ when δ is on the order of the whole electron trajectory. Such behaviour is confirmed in Figures 3 to 5 which show plots of log (N(δ)) versus log (δ) for electron trajectories simulated in carbon, copper and gold with initial electron energy equal to 10 keV. The fractal behaviour of the electron trajectories simulated in these elements with E_0 equal to 10 keV is similar to the results of Gauvin and Drouin (1992) obtained for the same elements at 30 keV.

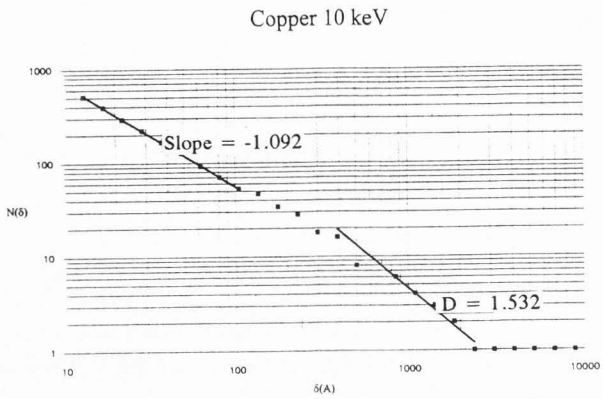

Figure 4. Log(N(δ)) versus log(δ) for an electron trajectory simulated in Cu with an initial energy equal to 10 keV.

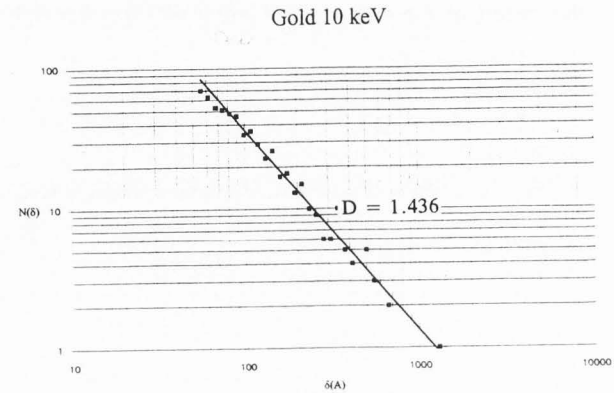

Figure 5. Log(N(δ)) versus log(δ) for an electron trajectory simulated in Au with an initial energy equal to 10 keV.

Also, Gauvin and Drouin (1992) were able to show that the shape of an electron trajectory simulated in a solid from a plot of an electron trajectory looks the same with different magnifications. This observation of self-similarity was qualitative, and it can be made quantitative following Normant and Tricot (1991). A curve is self-similar if, for all t and τ :

$$q(t - \tau, t + \tau) \sim P(t - \tau, t + \tau) \qquad (10)$$

where t is the parameter of a curve K and $\tau \leq t$. $q(t, \tau)$ and $P(t, \tau)$ are the size and the deviation, respectively, of the smallest convex body enclosing a subarc of K. Thus, equation (10) will certainly help in the near future to assess quantitatively the

self-similarity of the shape of electron trajectories in solids.

Table 1 presents the results of D and E as a function of the atomic number of the target, of the initial energy of incident electrons and of the number of electron trajectories. Figures 6 and 7 show plots of log(N(δ)) versus log(δ) for 30 and 1000 electron trajectories, respectively, simulated in gold with E_0 equal to 30 keV. From these results, it is difficult to make a relation between D and E_0 and Z. This is even worse for E, for which the physical meaning is not obvious to define. When the number of electrons used to compute D and E increases, both D and E increase, as confirmed for gold at 30 keV for 1, 30 and 1000 electrons. This is also confirmed by the results shown in Table 2. This table presents values of D and E measured independently for 5 electron trajectories simulated in gold at 10 keV. Each value of D and E is for one specific electron trajectory. D is not the same for different electron trajectories. This is certainly related to the statistical nature of the shape of electron trajectories in solids and to the imprecision in the linear regression used to find D since few points are available. All these values obtained for five single electron trajectories are smaller than the values obtained for 30 and 1000 electron trajectories for Au at 10 keV. This could be related to the fact that when measuring N(δ) for several electron trajectories, the effect of the cumulative trajectories on N(δ) mask the net value of a single trajectory. Since Gauvin and Drouin (1992) have stated that D is between 1 and 2 for electron trajectories in a solid from a physical argument, when the number of trajectory increases in the measure of N(δ), the "random walk" part of electron trajectories dominates and D becomes closer to 2, which is the value of a random walk process. Also, for the measurements using 1000 electron trajectories in gold, and 30 electron trajectories in Cu, values of D greater than 2 have no physical sense, and they are related to an early saturation behaviour of the number of counts in boxes of size δ when several electron trajectories are used in the box counting method. Thus, the fractal dimension of electron trajectory in solids must be measured independently for several electron trajectories alone, and the mean should be taken rather than measure N(δ) for all the trajectories included together when the box counting method is used. Also, more accurate methods, to measure D have been proposed. Normant and Tricot (1991) review these methods, and they present a new one which is known to be more accurate than the box counting method.

Table 1. Values of D and E as a function of the atomic number of the target, the initial energy of incident electrons and of the number of electron trajectories.

Element	E_0 (keV)	# of Electron trajectories	D	E $(Å)^D$
C	10	1	1.28	-
Cu	10	1	1.53	177828.
Ag	10	1	1.71	417000.
Au	10	1	1.43	26900.
C	10	30	1.35	2.63×10^6
Cu	10	30	2.23	9.33×10^9
Au	10	30	1.82	2.45×10^6
C	30	30	1.8	2.18×10^9
Ag	30	30	1.93	1.2×10^7
Au	30	30	1.80	5.75×10^7
Au	30	1000	2.25	6.3×10^9

Table 2. Values of D and E for five different single electron trajectories simulated in gold with E_0 = 10 keV.

Trajectory number	D	E $(Å)^D$
1	1.23	26900
2	1.50	42660
3	1.37	16980
4	1.19	3310
5	1.41	89125
Mean	1.38	35795

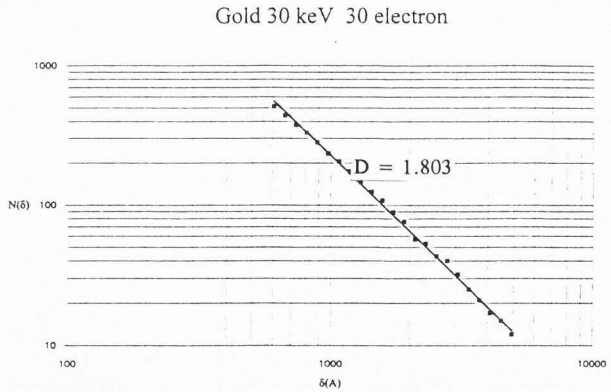

Figure 6. Log(N(δ)) versus log(δ) for 30 electron trajectories simulated in Au with an initial energy equal to 30 keV.

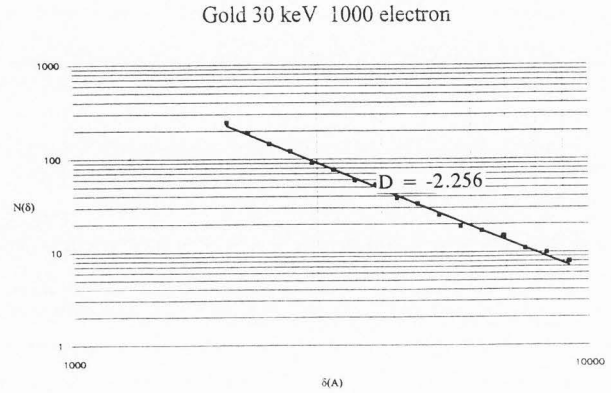

Figure 7. Log(N(δ)) versus log(δ) for 1000 electron trajectories simulated in Au with an initial energy equal to 30 keV.

Modelization of the Fractal Dimension of Electron Trajectories in Solids

The Hausdorff-Besicovitch dimension, D, describes the shape of a curve in $\Re^3$ (or in $\Re^2$). We have characterized such curves in the section III. These curves here are called K curves. If we plot the position of the electron, R, as a function of time, there is another curve describing the scattering of an electron in a solid. We use the term J curves for these curves. The position of the electron is computed using this relation :

$$R = \sqrt{(X_i - X_0)^2 + (Y_i - Y_0)^2 + (Z_i - Z_0)^2} \qquad (11)$$

where (X_O, Y_O, Z_O) is the initial position of the incident electron in the solids. As a result, J curves are in $\Re^2$. The time at each collision can be computed knowing E_i and L_i between each collision. Thus, it is easy to obtain a J curve from a K curve from the data of Monte Carlo simulations.

Voss (1985) has shown that the Hausdorff-Besicovitch dimension D_B of a J curve in $\Re^2$ is related to the Hölder exponent H by this relation:

$$D_B = 2 - H \qquad (12)$$

where H can take any value between 0 and 1. When H equals 1/2, the position of the electron as a function of time is described by a random walk process. When H is between 1/2 and 1, the J curve is described by a persistent process which means that the direction of the electron from point P_i to P_{i+1} is the same as it was from P_{i-1} to P_i. When H is between 0 and 1/2, the J curve is described by an antipersistent process, that the direction of the electron from P_i to P_{i+1} is contrary to that of P_{i-1} to P_i.

The Hausdorff-Besicovitch dimension D of the K curve is related to the Hölder exponent of the J curve by this relation :

$$D = \frac{1}{H} \qquad (13)$$

Therefore, for a random walk process, D is equal to 2.

Gauvin and Drouin (1992) have shown from the J curve of an electron trajectory simulated in Au when E_O equals 100 keV that the first part of an electron trajectory scattering into a solid is described by a persistent process and the last part is described by a random walk process. Since an electron trajectory which is described by a perfect persistent process will give a straight line with D = 1 and that an electron trajectory which is entirely described by a random walk process will have D = 2, the Hausdorff-Besicovitch dimension of the K curve of an electron trajectory is expected to lie between 1 and 2. The same result can be obtained quantitatively as follows : since the azimuthal angle is equally distributed between 0 and 2π, the persistence of an electron trajectory is the result of the initial low value of the mean polar angle. H can be given by the probability of going from P_i to P_{i+1} in the same direction as from P_{i-1} to P_i . By considering the effect of the polar angle only, H is obtained by solving this equation :

$$H = \frac{\int_0^{\pi/2} \left(\frac{d\sigma}{d\Omega}\right) \sin\theta \, d\theta}{\int_0^{\pi} \left(\frac{d\sigma}{d\Omega}\right) \sin\theta \, d\theta} \qquad (14)$$

which gives, using screened Rutherford cross-sections :

$$H = \frac{1+\alpha}{2\alpha+1} \qquad (15)$$

where α is the screening parameter given by (Nigam et al., 1959) :

$$\alpha = \frac{5.34 \times 10^{-3} Z^{2/3}}{E}, \qquad (16)$$

E is the energy of the electron, in keV, and Z is the atomic number of the solid where the electrons scatter. When α tends to zero, which is the case for high value of E and low value of Z, H tends to 1 and a persistent process is predicted. When α increases, which is the case for low values of E and high values of Z, H tends to 1/2. Thus, H lies between 1/2 and 1, and D, of the K curve, lies between 1 and 2. For a given element with high enough initial value of E, when the electron scatters into the solid, it loses energy, thus, α increases, and H goes to 1/2. As a result a shift from a persistent process to a random walk process when an electron scatter into a solid is predicted by equation (15). Also, equation (15) predicts that D, of the K curve, should increase with Z. However, for electron scattering in gold, equations (15) and (16) predict a value of H equal to about 0.95 for E equals 2 keV. Thus, electron scattering in gold when E equals 2 keV should be described by a persistent process, which is in flagrant contradiction with the observation of Gauvin and Drouin (1992) of the shift of a persistent to a random walk process, for an electron scattering in Au with E_0 = 100 keV, which occurs for E equal to around 95 keV. Since equation (14) does not include the effect of the azimuthal angle on H, the shift of a persistent to a random walk process for the scattering of electrons in solids is certainly caused by the net effect of the azimuthal angle, with uniform probability distribution and mean value equal to π, on the trajectory of the electron in as a function of time. It follows that equation (15) is not appropriate to compute the fractal dimension of electron trajectories in solids.

A more appropriate equation can be obtained if we assume that D, of the K curve, is given by :

$$D = f_p + 2\left(1 - f_p\right) \qquad (17)$$

where f_p is the fraction of the electron trajectory which is described by a persistent process and in such a case we assume that the fractal dimension is equal to 1. (1 - f_p) is the fraction of the electron trajectory which is described by a random walk process. In this case the fractal dimension is equal to 2. Thus, equation (17) predicts values of D which lie between 1 and 2. Equation (17) also assumes that there is a jump for the local fractal dimension from 1 to 2 where the shift from a persistent to a random walk process occurs which is certainly not the case in reality where a gradual transition should be observed. f_p is equal to the ratio of the diffusion depth to the electron range, Z_d/X_r. Since it is difficult to precisely find f_p from Monte Carlo simulations using the box counting method, an experimental determination of f_p will be useful for a first modelization of D for electron trajectories. Using the expression for Z_d obtained by Cosslett (1964) from experimental measurements in Al, Cu, Ag and Au at 20 keV, f_p is given by :

$$f_p = \frac{12}{Z+8} \qquad (18)$$

Equation (18) describes self-similarity in this way : the fraction of an electron trajectory which is persistent is not a function of E_0; thus when equation (18) is valid, the shape of an electron trajectory in a solid of a given composition is the same for any value of E_0. Therefore, an electron trajectory with initial energy $E_0{}^1$ will look the same (from a statistical point of view) to that having an initial energy equal to the value $E_0{}^2$ if it is magnified by the value $X_r^{E_2}/X_r^{E_1}$ where $X_r^{E_i}$ is the electron range with initial energy E_i.

Inserting equation (18) into equation (17) gives :

$$D = \frac{4+2Z}{Z+8}. \qquad (19)$$

Figure 8 shows the backscattering coefficient, taken from Heinrich (1966), as a function of D, computed using equation (19), for C, Al, Cu, Ag and Au. It is seen that the backscattering coefficient, η, increases with D. This means that

when the fraction of an electron trajectory which is described by a persistent process decreases, the shift from this process to a random walk process occurs at a shorter distance from the top surface of the specimen. As a result, the probability that an electron escapes the specimen increases. As a result, the general behaviour of Figure [8] seems logical but the exact variation depends on the validity of equation (19). Also, since η is a function of E_0 only when E_0 is below 10 keV (Darlington and Cosslett, 1972), D is a function of Z only when E_0 is greater than 10 keV. Therefore, the shape of electron trajectories in solids, for a specific Z, are not self-similar as a function of E_0 when $E_0 \leq 10$ keV. The form of equation (19) is expected to be valid when $E \geq 10$ keV, but the exact coefficients depend on equation (18).

Also, equation (19) depends only on the validity of equation (17) which assumes a discontinuity on the local fractal dimension, as explained above. Therefore, equation (19) is a first attempt to modelize the fractal dimension of the electron trajectories in solids computed using Monte Carlo simulations and from accurate determination of D as a function of E_0 (when $E_0 \leq 10$ keV) and Z. A more precise modelization of D will certainly emerge, but the general form of equation (19) is expected to be valid when $E_0 \geq 10$ keV.

Figure 9 shows a parabolic behaviour of η as a function of D and raises the following question : What is the backscattering coefficient when the scattering of electrons in solids is fully described by a random walk process (when D = 2)? As a this tentative answer to crucial question, from a fundamental point of view, our Monte Carlo

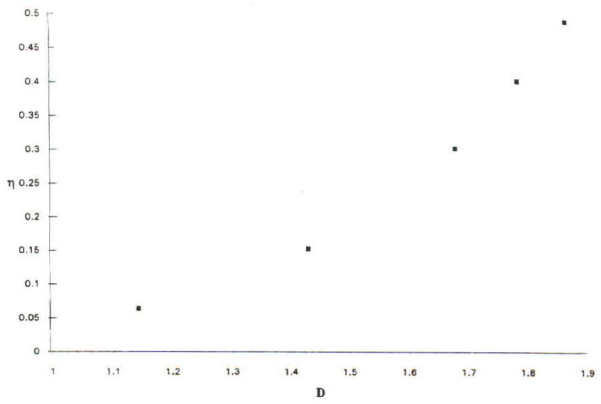

Figure 8. Backscattering coefficient, η, as a function of D, computed using equation (19) for C, Al, Cu, Ag and Au. The values of η were taken from Heinrich (1966).

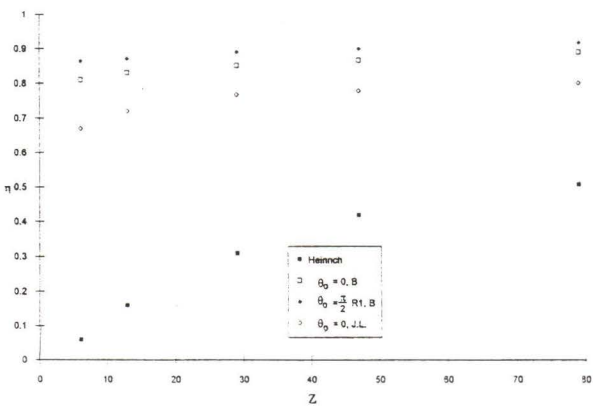

Figure 9. η as a function of Z from Heinrich (1966). Also, η as a function of Z computed at 30 keV assuming complete random walk with θ_0 computed with equation (22a) and (22b) respectively with Bethe law (B) of energy loss (Livingston and Bethe, 1937) and computed with equation (22a) with Joy and Luo (1989) (J.L.) law of energy loss.

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program has been modified to simulate electron trajectories which are described by a pure random walk process. This has been done by computing the polar angle in this way :

$$\theta_i = \pi R_1 \ (i > 0) \qquad (20)$$

and θ_0 by two different ways :

$$\theta_0 = 0, \qquad (21a)$$

or

$$\theta_0 = \frac{\pi R_1}{2} \qquad (21b)$$

Figure 9 shows η as a function of Z computed at 30 keV with equations (20) and (21a) or (21b) respectively for C, Al, Cu, Ag and Au. Also, the values measured by Heinrich (1966) are shown for comparison. From these results, it is clear that when electrons scatter into solids with a complete random walk process that the backscattering coefficient is significantly greater than those measured experimentally or simulated with θ_i computed with equation (1) since Murata et al. (1973) have obtained η values which are in excellent agreement with those measured by Heinrich (1966). Therefore, the fact that measured η values are significantly smaller than those simulated with complete randomness is the proof that the persistent part of the diffusion of electrons

in solids plays a major role in the behaviour of electron scattering in solids. When Z decrease, measured η values decreases meaning that the persistent part of electron trajectories in solids increases, as predicted by equation (18). Thus, the general meaning of equation (19) and of Figure 8 seems to be logical. Also, since η varies significantly less with Z in a complete random walk process than in reality, this proves that the outstanding chemical contrast of backscattering images in the scanning electron microscopes is the result of the strong variation of the fraction of electron trajectories which are described by a persistent process as a function of Z. Also, this is confirmed when we compare η computed with equation (20) and equations (21a) or (21b), respectively. Equation (21a) is the case when the first trajectory of electrons in solids is persistent and all the others random, and equation (21b) is the case of complete randomness. When equation (21a) is used, for all Z, η are smaller than those computed with equation (21b). The difference is about 6% for C and decreases as Z increases and equals about 3% for gold. Therefore, only one step of electron trajectories which is persistent (the initial speed only) is sufficient to give a variation of about 5% on η.

Concerning the maximum value of η in the case of complete randomness, it is clear that this value, for a given Z, is smaller than 1 but greater than 1/2 and that these values depend on the energy loss, since values computed with the energy loss of Joy and Luo (1989) are smaller than those computed with dE/dS given by equation (5). Therefore, the way that electron loss energy certainly affects the values of the real backscattering coefficients. If there was no energy loss, a complete random walk, for all Z values, should give $\eta = 1$ as the number of collisions goes to infinity. It is because of the energy loss, that the η values computed with complete randomness, are smaller than one.

Multifractal

The Hausdorff-Besicovitch dimension obtained from the plot of log (N(δ)) versus log (δ) has a serious limitation. If the number of times that the electron trajectory cut a given box of size δ is greater than 1, this information is not included because, each time that the electron trajectory cuts a box, only one count is counted. Thus, to overcome this difficulty, for each box which cut by the electron trajectory, a probability μ_i is measured. μ_i is equal to the number of times that the electron cuts the box i divided by the total number of counts. Because of the way in which we are computing the number of times that an electroncuts a box i, our computed values μ_i are the respective fraction of the total length of the electron trajectory in the box i. With the probabilities μ_i, the function N(δ, q) is defined in this way :

$$N(\delta,q) = \sum_{i=1}^{N} \mu_i^q \qquad (22)$$

where N is the number of boxes covering the electron trajectory and q is the moment order of the measure. N(δ, q) is related to the size of the boxes δ by :

$$N(\delta, q) = k\, \delta^{-\tau(q)} \qquad (23)$$

where k is a constant and $\tau(q)$ is the mass exponent that controls how the moments of the probabilities $\{\mu_i\}$ scale with δ. For q = 0, N(δ, 0) is equal to N and $\tau(0)$ is equal to the Hausdorff-Besicovitch dimension D.

The probabilities $\{\mu_i\}$ are a function of the size of the boxes, δ. These probabilities can be related to the Lipschitz-Hölder exponent α according to:

$$\mu_i = \delta^{\alpha} . \qquad (24)$$

Each probability $\{\mu_i\}$ is then characterized by a specific exponent α for a given δ. The multifractal spectrum of the Lipschitz-Hölder exponents is given by the function f(α) which is obtained from the curve which relates $\tau(q)$ as a function of q by the use of the Legendre's transform (see Feder, 1988) :

$$\alpha(q) = -\frac{d}{dq}\tau(q) \qquad (25)$$

and

$$f(\alpha(q)) = q\,\alpha(q) + \tau(q) \qquad (26)$$

Let $N(\mu_\alpha)$ be the number of probabilities $\{\mu_i\}$ defined by the exponent α for a given δ value. Then, $N(\mu_\alpha)$ scales with δ according to :

$$N(\mu_\alpha) = K\, \delta^{-f(\alpha)} \qquad (27)$$

where K is another constant and f(α) is the fractal dimension of the subset of probabilities $\{\mu_\alpha\}$. As a

result, a curve described by a multifractal measure has a continuous spectrum of fractal dimensions.

Gauvin and Drouin (1992) have shown, from the trajectory of an electron simulated in Au with E_0 equal to 30 keV, that the distribution of the trajectory of incident electrons in solids that cut boxes of size δ, is described by a multifractal measure. Here, the energy distribution of backscattered electrons is studied using multifractal analysis for electron trajectories simulated in C, Cu and Au with E_0 equals 30 keV. The probabilities μ_i^δ are computed as follows :

$$\mu_i^\delta = \frac{N_i^\delta}{N_T} \qquad (28)$$

where N_i^δ is the number of backscattered electrons having an energy between $(i-1)\frac{E_o}{\delta}$ and $\frac{iE_o}{\delta}$ with $1 \leq i \leq \delta^{-1}$.

Figure 10 shows the energy distribution of backscattered electrons in C, Ag and Au with E_0 = 30 keV. These distributions are presented as $d\eta/dW$ as a function of W where $W = E/E_0$ and E is the energy of the backscattered electron. These distributions have been obtained from simulations of 100,000 electrons. For Au, Ag and C, the most probable energies are equal to 0.92, 0.88 and 0.56, respectively. As Z decreases, the mean energy decreases and the distribution becomes broader. This behaviour is well known.

Figure 11 shows the $f(\alpha)$ curves for these three energy distributions. In these curves, the largest α values correspond to the smallest μ_i^α, so they show the information concerning the tails of these distributions. Since silver has the greatest variation of α, this means that more information is included in the tails of $d\eta/dW$ versus W than in the other distributions. C has the least information in the tails and Au is in between. To characterize the nature of the distribution of $d\eta/dW$ versus W, the $f(\alpha)$ curves are a powerful tool and they will certainly be very useful to characterize all distributions generated by Monte Carlo simulations because the scattering of electrons in solids is a physical phenomenon which is generated by a set of independent physical process acting simultaneously. $f(\alpha)$ curves play a central role to describe such phenomena.

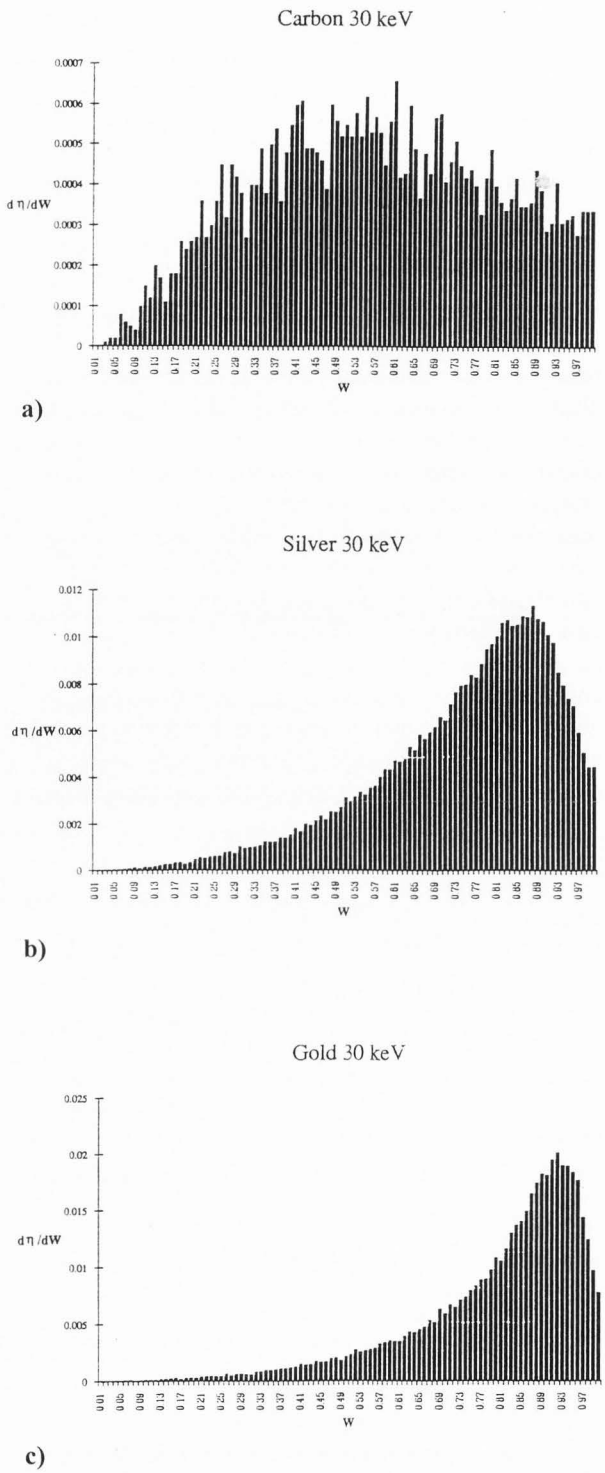

Figure 10. $d\eta/dW$ as a function of W for E_0 = 30 keV. a) C, b) Ag, c) Au.

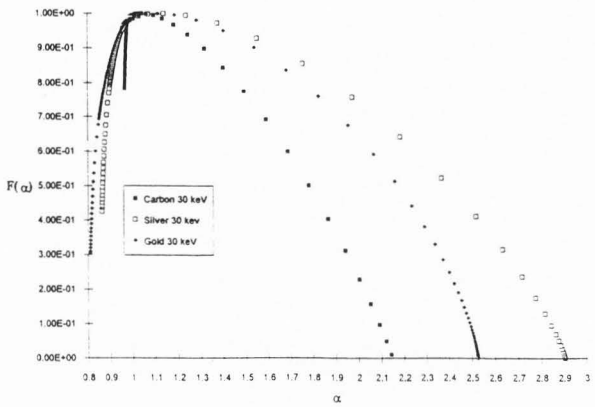

Figure 11. f(α) versus α obtained from the energy distribution of bascattered electrons simulated in C, Ag and Au at 30 keV.

Conclusions

Fractal analysis is a powerful tool to describe electron scattering in solids from a fundamental point of view and this will certainly help to validate the numerous Monte Carlo codes used to simulate the trajectories of electrons in solids. The electron trajectory in $\Re^3$ simulated by the Monte Carlo's method is fractal for a given range of δ where δ is in the order of the electron trajectory and $1 \leq D \leq 2$. The first part of the scattering of an incident electron in solids is described by a persistent process where the last part is described by a random walk process. The cumulative effect of the azimuthal angle of collision gives this transition. When Z decreases, the fraction of persistence increases when electron scatters into the solid.

A simple model to compute D has been proposed and a relation has been found between D and η. This model, which depends on Z only, is expected to be valid when $E_0 \geq 10$ keV. When $E_0 \leq 10$ keV, a more elaborate model will give D as a function of Z and E_0. The variation of the fraction of an electron trajectory in a solid which is described by a persistent process with the atomic number explains the outstanding chemical contrast of backscattered images. The energy distribution of backscattered electrons is described by a multifractal measure and the shape of the corresponding f(α) curves is function of the atomic number of the target.

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References

Cosslett VE (1964) The diffusion depth for electrons in solid targets. Brit. J. Appl. Phys. **15**: 107-109.

Darlington EH, Cosslett VE (1972) Backscattering of 0.5-10 keV electrons from solid targets. J. Phys. D Appl. Phys. **5**: 1969-1981.

Feder J (1988) Fractals. Plenum Press, New York.

Gauvin R, Drouin D (1992) Fractal description of electron scattering in solids. Scanning **14**: 313-323.

Heinrich KFJ (1966) Electron probe microanalysis specimen current measurement. In: X-Ray Optics and Microanalysis. Castaing R, Deschamps P, Philibert J, eds. Hermann, Paris, pp 159-167.

Joy DC, Luo S (1989) An empirical stopping power relationship for low-energy electrons. Scanning **11**: 176-180.

Livingston MS, Bethe HA (1937) Nuclear physics. Rev. Mod. Physics **9**: 245-390.

Mandelbrot BB (1967) How long is the coast of Britain? Statistical self-similarity and fractal dimension. Science **155**: 636-638.

Mandelbrot BB (1975) Stochastic models for earth's relief, the shape and the fractal dimension of the coastlines, and the number-area rule for islands. Proc. Nat. Acad. Sci. USA **72**: 3825-3828.

Mandelbrot BB (1982) The Fractal Geometry of Nature. W. H. Freeman, New York.

Mandelbrot BB (1989) A class of multimonial multifractal measures with negative (latent) values for the "dimension" f(α). In: Fractals' Physical Origin and Properties. Pietronero L, ed. Plenum Press, New York, pp 3-29.

Mandelbrot BB (1991) Fractals and Multifractals, Selecta Vol. 1, Springer, New York.

Mandelbrot BB, Passoja DE, Paullay AJ (1984) Fractal character of fracture surfaces of metals. Nature **308**: 721-722.

Murata K, Matsukawa T, Shimizu R (1973) Monte Carlo calculations on electron scattering in a solid target. Jap. J. Appl. Physics **10**: 678-686.

Newbury DE, Joy DC, Echlin P, Fiori CE, Goldstein JI (1986) Advanced Scanning Electron Microscopy and X-Ray Microanalysis, Plenum Press, New York, pp 3-43.

Nigam BP, Sundaresan MK, Wu TY (1959) Theory of multiple scattering, second Born approximation and corrections to Moliere's work. Phys. Rev. **115**: 491-502.

Normant F, Tricot C (1991) Method for evaluating the fractal dimension of curves using convex hulls. Phys. Rev. **A 43**: 6518-6525.

Press WH, Flannery BP, Teckolsky SA, Vetterling WT (1986) Numerical Recipes. Cambridge University Press, Cambridge, pp. 191-225.

Rossi F, Parkin DM, Nastasi M (1989) Fractal geometry of collision cascades. J. Mater. Res. **4**: 137-143.

Uwaha M, Saito Y (1990) Fractal aggregation and dendritic crystal growth. J. Crystal Growth **99**: 175-178.

Voss RF (1985) Random fractals: characterization and measurement. In: Scaling Phenomena in Disordered Systems. Pynn R, Skieltorp A, eds. Plenum Press, New York, pp 1-11.

Discussion with Reviewers

Z. Czyzewski : The Mott scattering cross-section is a better approximation for elastic scattering than the Rutherford one. Could you show any comparison of the D dimension for electron trajectories calculated using Mott cross-section and Rutherford formula? Please, comment any differences between these two data sets.

Authors : Before commenting on any differences between different sets of data, we believe that we must assess the accuracy of the method used to measure D. We are currently valiating several methods using trajectories of complete random walk where D is known to be equal to 2.

Z. Czyzewski : Could you show an example of the D dimension when a mean value of $\overline{N(\delta)}$ is used for all electron trajectories as a function of the number of trajectories used in calculations. You suggest in the paper that it is much better approach than that which measures $\overline{N(\delta)}$ for all trajectories together.

Authors : Table 2 shows an example where the mean value of D is computed from 5 independent values of D obtained from 5 electron trajectories simulated in Au with E_0 = keV. Again, we believe that before comparing different results, we must validate the precision of the methods used to measure D.