

Monte Carlo Computation of the Influence of Carbon Contamination Layer on the Energy Distribution of Backscattered Electrons Emerging from Al and Au

A. M. D. Assa'd

Department of Basic Sciences Faculty of Arts and Sciences, Al-Ahliyya Amman University, Amman 19328, Jordan.

Received on: 2/7/2018;

Accepted on: 4/10/2018

Abstract: The influence of carbon contamination layer (5nm) on the energy distribution of backscattered electrons (BSEs) emerging from the top of Al- and Au-substrates at a wide range of normal primary electron energies ($E_p = 0.5\text{-}20\text{keV}$) has been theoretically examined. The study is based on using a CASINO Monte Carlo model. Generally, the results show a clear effect of the contamination on the backscattering coefficient and the energy distribution of backscattered electrons. This appeared as a reduction of the number of BSE emerging from the surface with energies close to the primary energy. For primary energy less than 5keV, the contamination effects are clearly seen in the reduction of the number of BSEs emerging with energy close to E_p and the increment of the number of BSEs with low energies. The backscattered electron spectrum starts with a wide peak at low energies and becomes sharper as the primary energy increases. For high primary electron energies (10-20keV), the influence of the carbon contamination layer is restricted on the energy distribution of the backscattered electrons with energies above 95% of the primary energy. The influence of the carbon contamination layer was observed more clearly for the Au-substrate than for the Al-substrate as a reduction of the number of backscattered electrons.

Keywords: Backscattered Electrons, Monte Carlo Model, CASINO, Backscattering Coefficient, Carbon Contamination, Energy Distribution.

Introduction

Backscattered electrons (BSEs) are defined as those incident primary electrons (PEs) that exit the target surface with energy greater than 50eV after they penetrated the target surface and traveled through it. The backscattering coefficient (η) is the ratio of the number of backscattered electrons (BSEs) to the number of primary electrons (PEs). η depends strongly on the primary electron energy (E_p) and the average atomic number (Z_{avr}) of the tested target. Therefore, it is useful in providing an atomic contrast mechanism in a Scanning Electron Microscope (SEM) [1]. However, η determination faces a lot of problems, both experimentally and theoretically. Experimentally, the first main problem is that of keeping the surface clean of contamination [2].

Another problem is having a stable incident beam current during the measurement [3]. El-Gomati *et al.* [2] measured η from 24 different elements at low primary electron beam energy (250-5000eV). η was measured for both clean and unclean surfaces under an ultra-high vacuum condition in order to protect the surface from any contamination that could happen during the experiment. The results showed an increment in η obtained from clean surface elements. Theoretically, the η calculation accuracy depends on having accurate elastic and stopping power formulae [4]. In the case of elastic scattering, there is a significant variation in the predication of the small angle elastic scattering between the provided formulae in the literature [5]. This variation reflects strongly on η calculation [6].

The importance of studying the behavior of backscattered electrons (BSEs) is due to their contribution to generating other signals, such as secondary electrons (SEs), Auger electrons (AEs) and X-ray, which are used in Scanning Electron Microscopy (SEM), Scanning Auger Microscopy (SAM) and X-ray microscopy, respectively. This can be exemplified in the case of SEs generation. The number of SE generated per BSE is greater by a factor of $\beta > 1$ than the number generated per PE [1]. This is due to the reduction in the mean energy of BSEs and to the fact that BSEs pass the surface layer with a shallow exit angle relative to the surface normal. Therefore, any changes in the BSE behavior could reflect on the intensity of the other signals used to image the samples in the mentioned microscopes. BSE energy distribution should be also studied in parallel with the backscattering coefficient (η). This will help to understand the behavior of incident primary electrons during their travel in the solid before being backscattered from the surface.

In this study, Monte Carlo simulation is used to examine theoretically the effect of a contamination layer (5-nm carbon layer) on η and on the energy distribution of backscattered electrons emerging from the Al- and Au-surface targeted at primary electron energy range (0.5-20 keV), where most of the modern SEMs are operated. The exact thickness of the C contamination is not known. So, in this work, a 5-nm C-layer thickness is chosen with the belief that qualitatively the same results would be found for a somewhat different thickness, higher or lower.

Monte Carlo Model

For several decades, Monte Carlo simulation has been used as the main tool to investigate theoretically the electron solid interaction [7, 8, 9, 10]. An appropriate Monte Carlo model must operate for a wide range of primary electron energies and solid atomic numbers. In the present work, a free CASINO V2.51 (2017) Monte Carlo simulation model provided by the Université de Sherbrooke - Canada is used. The model can be downloaded from this link: <http://www.gel.usherbrooke.ca/casino/index.html> web page [11]. The model is based on the continuous slowing-down approximation (CSDA) method. A full description of the model can be found in reference [12]. For the elastic scattering cross-section, the model lists four

options that could be used. These are: the tabulated Mott cross-section provided by Mott and Massey [13], Gauvin and Drouin formula [14], Browning *et al.* equation [15] and the modified Rutherford cross-section equation proposed by Murata and Kyser [16]. The Gauvin and Drouin formula and the constants therein have been obtained from the values of the total elastic Mott cross-sections computed by Czyżewski *et al.* [17] using Thomas-Fermi-Dirac atomic potentials. The Browning *et al.* equation is an empirical form of cross-sections derived from trends in tabulated Mott scattering cross-sections. However, the model uses an equation proposed in Joy and Luo [18] in order to determine the primary electron energy loss due to inelastic scattering and the mean free path length between two scattering events. This equation is applicable for a wide range of primary electron energies, thus overcoming the weakness of the Bethe equation [19] at low energies.

In other studies, the use of the Browning *et al.* equation for the elastic scattering cross-section gave good agreement between the measured and the calculated η for Al and Au compared with the Mott tabulated cross-section [20, 21]. Therefore, Browning *et al.* equation is used in the present study.

Results and Discussion

Fig. 1 shows the trend of backscattering coefficient (η) for pure clean surfaces of C, Al, Au and for 5-nm C on top of Al- and Au-substrates (unclean target surface) as a function of normal incidence primary electron energy (E_p). The results show the effect of the presence of 5-nm C on top of Al- and Au-substrates. It can be classified into three categories: 1) at $E_p = 0.5$ keV, η is the same for both tested targets C/Al and C/Au. 2) For $E_p > 0.5$ keV, η values increase toward the values of clean Al and Au. 3) The difference between the values of η for clean and unclean surfaces vanished at $E_p \geq 5$ keV for Al, while for Au, it vanished at $E_p = 10$ keV. By using the Kanaya and Okayama formula [22], the electron range at $E_p = 0.5$ keV on a pure C target is 9 nm, while the BSE range is around 4.5 nm as calculated by Monte Carlo simulation, Table 1. This means that the BSEs did not reach the substrates and their behavior is controlled by the C top layer. As E_p increases, the BSE range (R_{BSE}) increases, Table 1, and an increasing effect of the substrate atomic number on η values

can be noticed in Fig. 1. For a 5-nm C-layer on top of an Al-substrate, the η value increases as E_p increases until it becomes constant at $E_p \geq 5$ keV and equal to those of clean Al target. However, for a 5-nm C-layer on top of an Au-substrate, the η value increases until it becomes constant at $E_p \geq 10$ keV. The data of Table 1 shows that as E_p increases, the BSE range increases until it becomes as high as that of the

clean Al and Au targets at $E_p \geq 5$ keV and 10 keV, respectively. For example, at $E_p = 5$ keV, the BSE range ($R_{BSE} = 195$ nm) for 5-nm C-layer on top of Al is close to that of the clean surface Al target $R_{BSE} = 190$ nm. Also, for higher E_p , R_{BSE} data of both targets is equal, Table 1. This means that the 5-nm C-layer has no more effect on η values. This is also applicable for Au substrate at $E_p \geq 10$ keV.

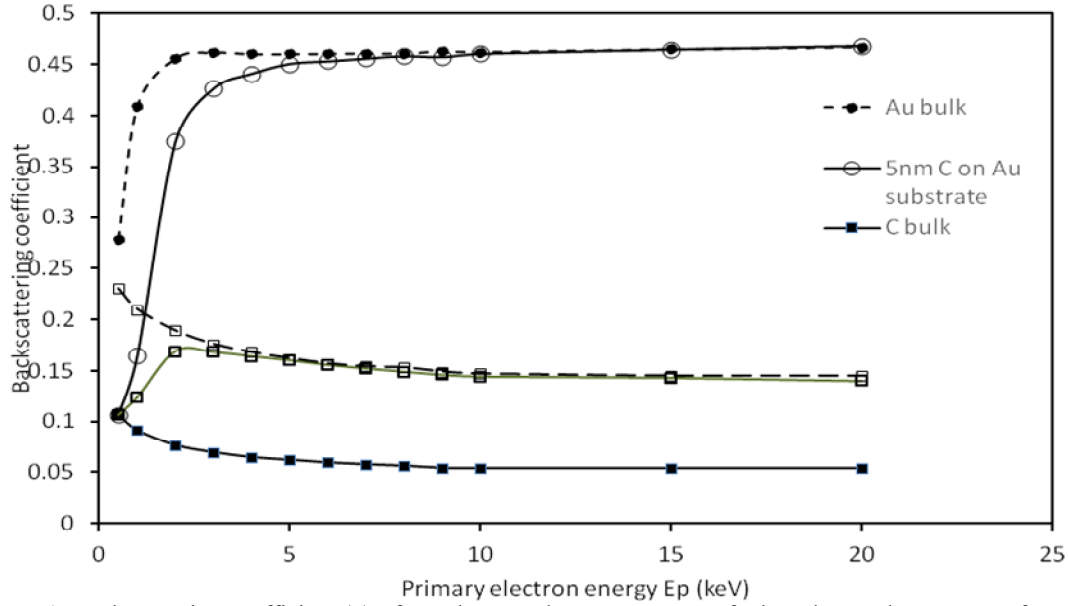


FIG. 1. Backscattering coefficient (η) of C, Al, Au and 5-nm C on top of Al- and Au-substrates as a function of primary electron energy (E_p).

TABLE 1. The maximum range of the primary (R_E) and backscattered (R_{BSE}) electrons as a function of primary energy (E_p). R_E is calculated by Kanaya and Okayama formula [22], while R_{BSE} is calculated by the present Monte Carlo model.

	Carbon		Aluminum		5-nm C on Al-substrate	Gold		5-nm C on Au-substrate
(E_p) keV	R_E (nm)	R_{BSE} (nm)	R_E (nm)	R_{BSE} (nm)	R_{BSE} (nm)	R_E (nm)	R_{BSE} (nm)	R_{BSE} (nm)
0.5	9.19	4.5	8.85	5	4.5	2.65	3	4.5
1	29.23	9	28.15	15	13	5.24	6	8.5
2	93.01	40	89.58	41	40	16.67	15	17
3	183.06	67	176.32	80	85	32.82	25	28
4	295.97	110	285.06	130	140	53.06	33	37
5	429.62	159	413.79	190	200	77.02	43	50
6	582.53	220	561.06	270	270	104.43	58	65
7	753.57	280	725.79	340	340	135.09	71	85
8	941.82	370	907.11	460	460	168.84	91	92
9	1146.55	480	1104.29	490	490	205.54	110	115
10	1367.12	510	1316.74	640	640	245.08	135	140
15	2690.79	1200	2591.62	1300	1300	482.38	260	265
20	4350.39	1750	4190.05	2100	2100	779.90	450	450

FIG. 2 shows the backscattered electron energy distribution for pure C, Al and Au as the targets are bombarded by a 20 keV normal incidence beam of primary electrons. It is clear

that the shape of the spectrum depends on the atomic number of the target material as shown by different experimental results [23, 24].

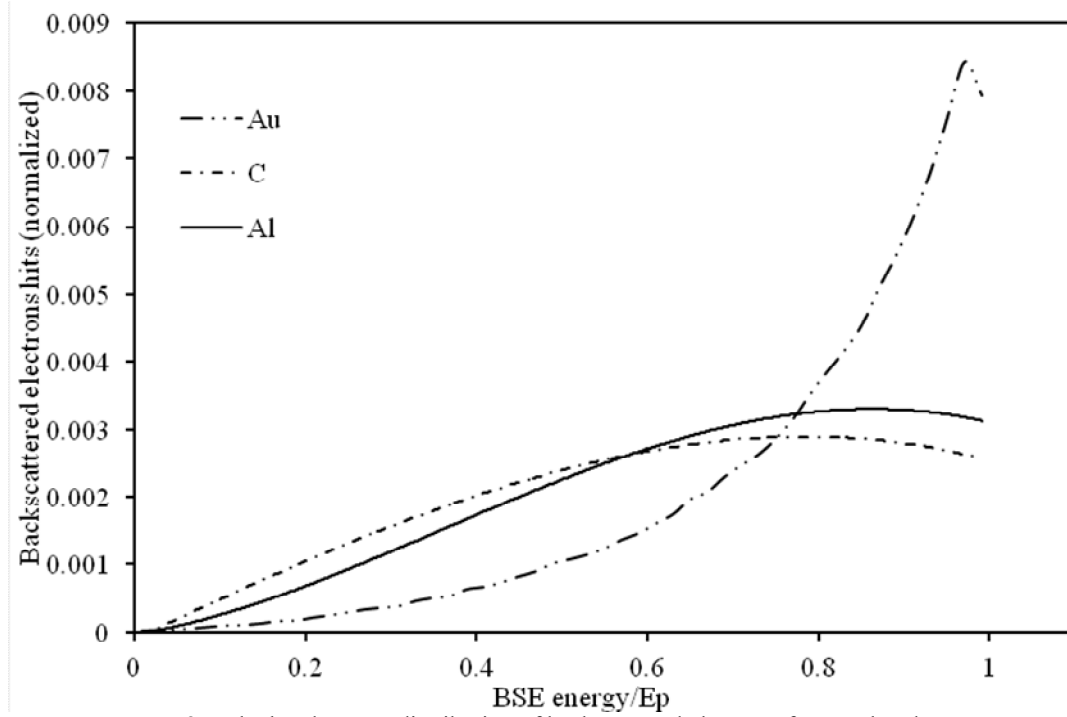


FIG. 2. Calculated energy distribution of backscattered electrons for C, Al and Au.

The dependence of the collected BSE spectrum on the primary electron energy (E_p) for the clean surface Al and Au targets is shown in Figs. 3 and 4, respectively. As E_p increases, the peak of the spectrum becomes sharper, higher and closer to E_p . Moreover, a reduction in the spectra at backscattered energies below $0.4 E_p$ for Al and $0.75 E_p$ for Au is demonstrated as E_p increases. The probability of having elastic scattering increases as E_p increases, which makes the primary electrons backscatter with minimum loss of their energy. Those BSEs collected with energies close to E_p escaped after they penetrated a depth of a few nanometers below the surface and suffered more elastic scattering than inelastic scattering even without losing much of

their energy. So, as E_p increases, more BSEs with high energy escape from the surface. However, the peak sharpness depends on the target average atomic number. This is rather more clear in the case of Al, where the probability of having inelastic scattering increases compared to the case of Au. Therefore, the primary electrons will travel deeper in the target and suffer more energy loss before escaping from the surface with low energies. This makes the BSE spectrum look wider and not as sharp as in the case of Au. So, the behavior of high energetic BSEs is surface-sensitive and can be used to investigate the surface topography, since these have a small exit depth.

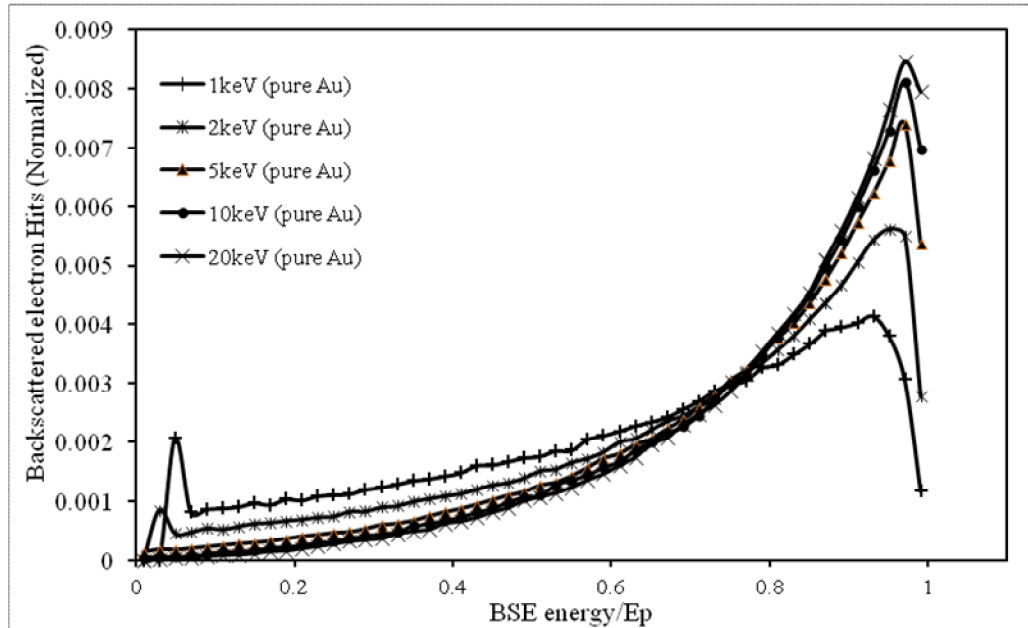


FIG. 3. Energy distribution of backscattered electrons for a pure Au target and primary electron energy range (1-20keV).

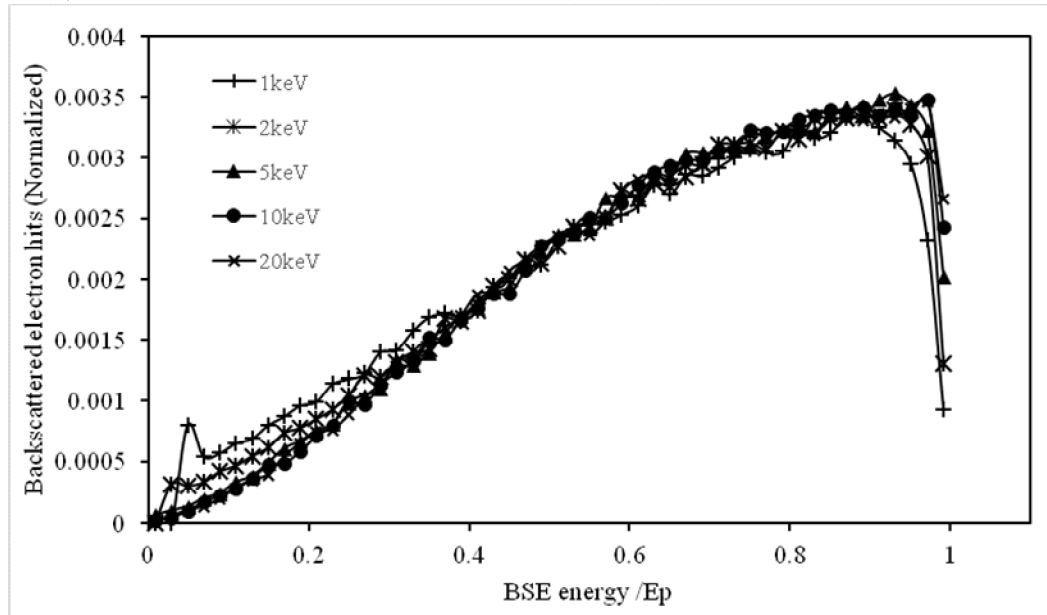


FIG. 4. Energy distribution of backscattered electrons for a pure Al target and primary electron energy range (1-20keV).

Figs. 5 and 6 show the energy distribution of the backscattered electrons as a function of E_p for a 5-nm C-layer deposited on Al- and Au-substrates, respectively. The BSE spectrum of primary electron energy $E_p = 0.5\text{keV}$ is not shown, because it is similar to that of the pure C target. Figs. 5a and 6a show a comparison between the BSE spectra of clean Al- and Au-surfaces and those from 5-nm C-layers on top of

Al- and Au-substrates (unclean surfaces). The effect of the C top layer on the shape of BSE spectrum is clearly shown at low E_p and for high-energy BSEs (E_{BSE}). The BSE spectrum shows a massive reduction of BSEs with energy close to E_p ($E_{BSE} \geq 0.6E_p$) and an increase of BSEs with low energies ($E_{BSE} < 0.6E_p$). This could make BSEs more effective in generating secondary and Auger electrons from C layer and X-ray from C-layer and from Al- and Au-

substrates at high E_p . More investigation could be done in the future to study the effect of BSEs on the other signals in the presence of contamination. The increase of the BSE spectrum at low E_{BSE} is due to the energy loss that BSEs suffered in the C top layer in their way back to surface. As E_p increases, the peak of BSE spectrum shifts toward E_p and η value increases toward the data of clean Al and Au targets, Figs. 5b and 6b. A greater number of BSEs escaped from the surface, particularly those with higher energies. The reason for this is the increase in the primary electron range (R_E), which means having a larger depth of electron-solid interaction volume, Table 1. Hence, the

primary electron will suffer more scattering events in the substrate before coming back to the C top layer in its way back to the surface. As E_p increases, the interaction volume increases and the importance of the C top layer thickness on the interaction volume decreases. So the effect of the C top layer on the BSE spectrum will be minimized. The only effect of the C top layer on the BSE spectrum will remain on BSEs with energy above $0.95E_p$, Fig. 7. These electrons are backscattered from a small exit depth less than the C top surface thickness which has low backscattering coefficient compared to the substrate materials.

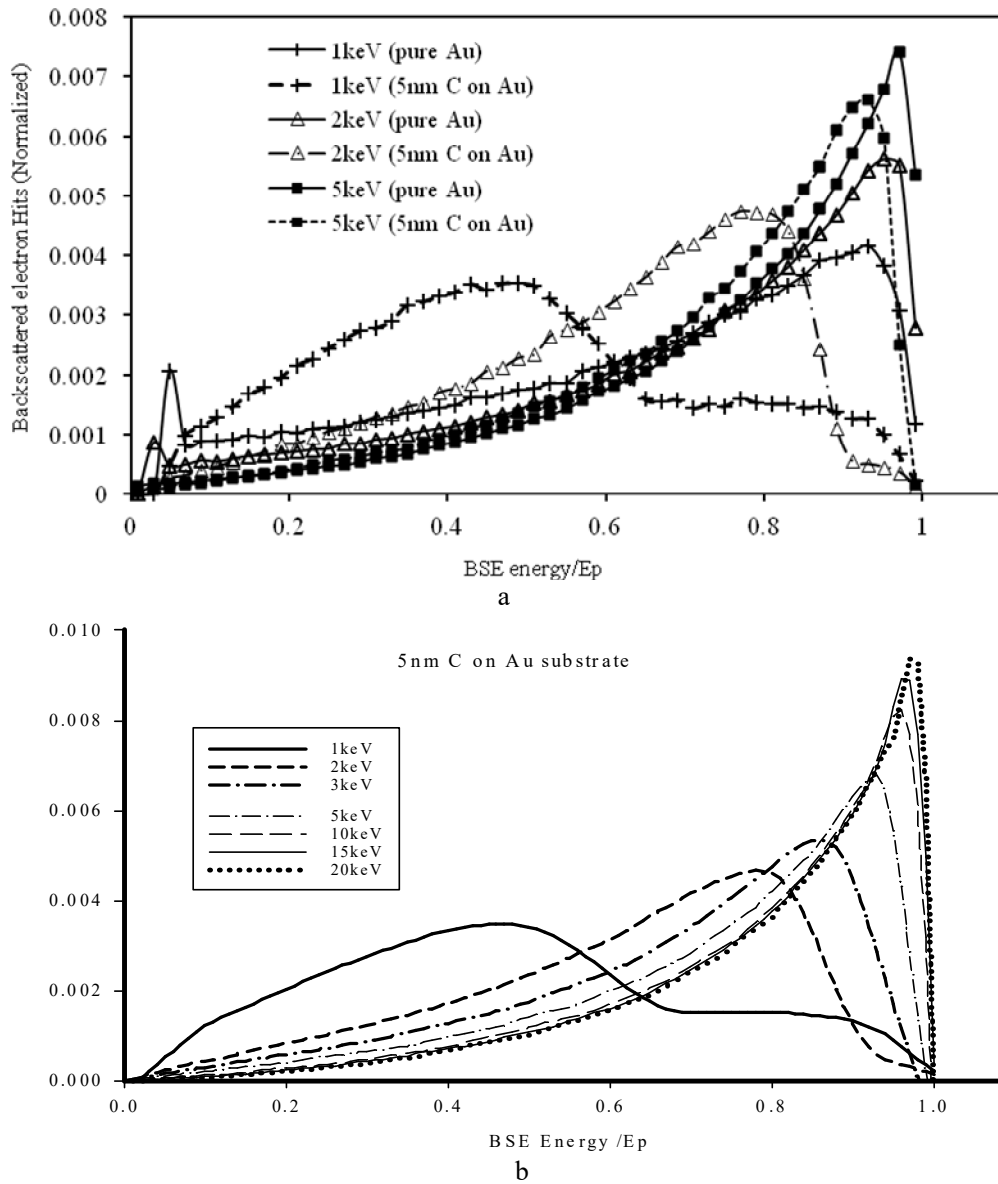
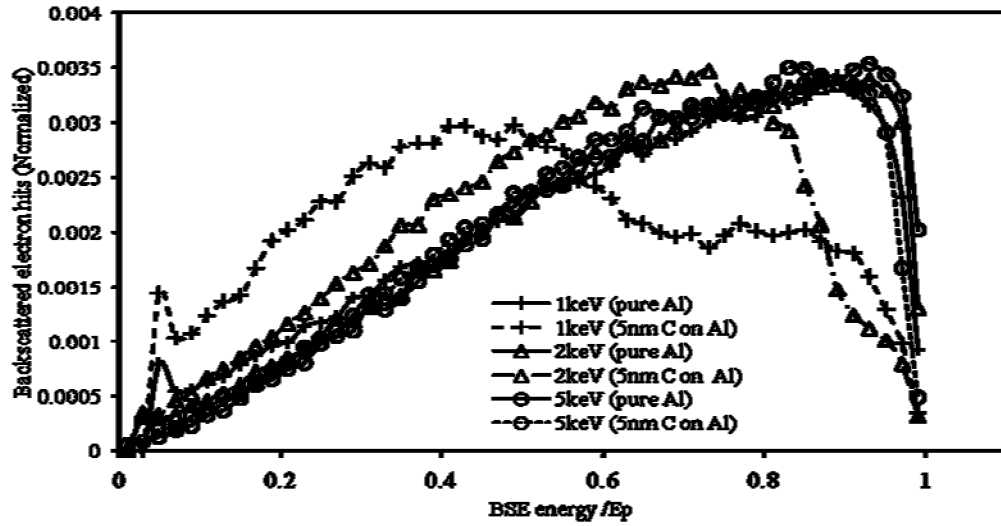
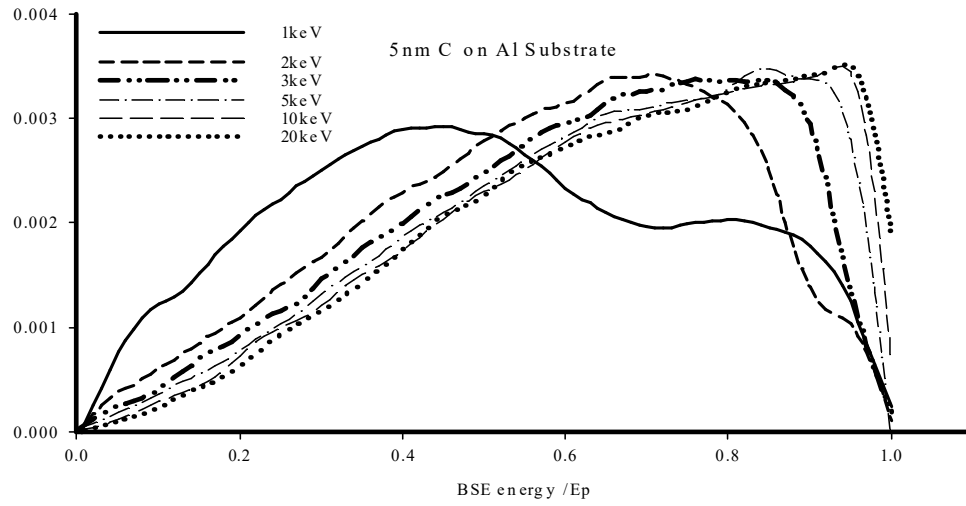


FIG. 5. Energy distribution of backscattered electrons comparison between those for a pure Au target and those calculated in the presence of a 5-nm C-layer on top of the Au surface.



a



b

FIG. 6. Energy distribution of backscattered electrons comparison between those for a pure Al target and those calculated in the presence of a 5-nm C-layer on top of the Al surface.

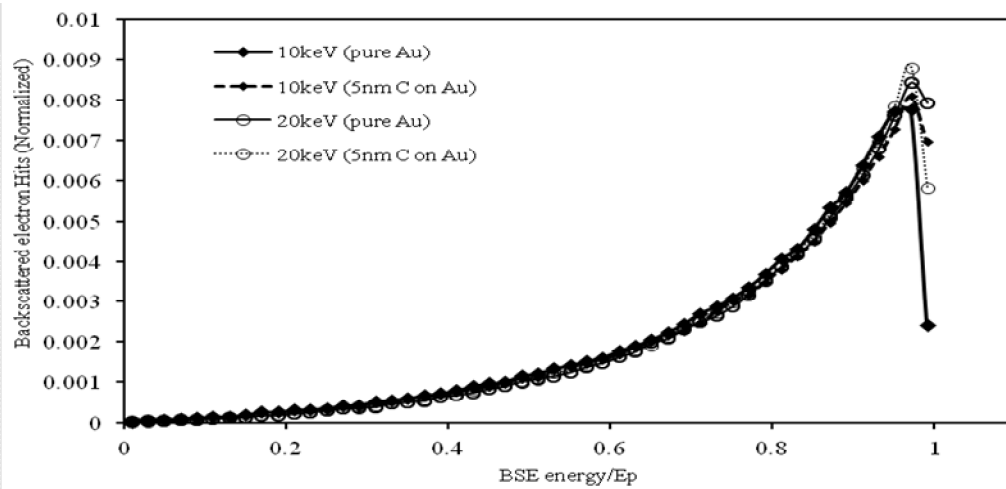


FIG. 7. Energy distribution of backscattered electrons comparison between those for a pure Au target and those calculated in the presence of a 5-nm C-layer on top of the Au surface.

Conclusion

The presence of contamination on the top of the examined targets affects the backscattering coefficient (η) as well as the backscattered electron energy distribution. The influence of contamination on the collected BSE spectrum depends on the thickness of the contamination layer and the incident primary electron energy. At low energies, $E_p \leq 5\text{keV}$, an increase in BSEs with energies below $0.70E_p$ and a massive reduction in BSEs with energies above $0.70E_p$

are observed. Even though the contamination layer has no effect on η values at high E_p , it has an effect on the BSE energy distribution. As E_p increases, the shape of the BSE spectrum goes toward the BSE shape of the clean target except for energies above $0.95E_p$. These high-energetic backscattered BSEs have a small exit depth, which is filled by the contamination layer (5-nm C top layer). The high energy BSEs are surface-sensitive and can be used to investigate the surface topography.

References

- [1] Reimer, L., "Scanning Electron Microscopy, Physics of Image Formation and Microanalysis". (Springer, Berlin, Germany, 1985).
- [2] El-Gomati, M.M., Walker, C.G.H., Assa'd, A.M.D. and Zadrazil, M., *Scanning*, 30 (2008) 2.
- [3] Assa'd A.M.D. and El-Gomati M.M., *Scanning Microscopy*, 12 (1998) 185.
- [4] Joy, D.C., *J. of Microsc.*, 147 (1987) 51.
- [5] Jablonski, A., Salva, F. and Powell, C.J., *J. Phys. Chem. Ref. Data*, 33 (2) (2004) 2004
- [6] Walker, C.G.H., Matthew, J.A.D. and El-Gomati, M.M., *Scanning*, 36 (2014) 241
- [7] Yan, H., El-Gomati, M.M., Prutton, M., Wilkinson, D.K. and Chu, D.P., *Scanning*, 20 (1998) 465.
- [8] Star'y, V., *J. Phys. D: Appl. Phys.*, 32 (1999) 1811.
- [9] Dapor, M., Bazzanella, N., Toniutti, L., Miotello, A., Crivellari, M. and Gialanella, S., *Surf. Interface Anal.*, 45 (2013) 677.
- [10] Walker, C.G.H., Luděk, F. and Müllerová, I., *Scanning*, 36 (2016) 802.
- [11] Drouin, D., <http://www.gel.usherbrooke.ca/casino/index.html>, web page.
- [12] Drouin, D., Couture, A.R., Joly, D., Tastet, X., Vincent, A. and Gauvin, R.M., *Scanning*, 29 (2007) 92.
- [13] Mott, N.F. and Massey, H.S.W., "Theory of Atomic Collisions". (Oxford University Press, London, 1965).
- [14] Gauvin, R. and Drouin, D., *Scanning*, 15 (1993) 140.
- [15] Browning, T.Z., Li, J.M., Chui, B., Ye, J., Pease, R.F.W., Czyzewski, Z. and Joy, D.C., *J. Appl. Phys.*, 76 (1994) 2016.
- [16] Murata, K. and Kyser, D.F., *Advances in Electronics and Electron Physics*, 69 (1987) 175.
- [17] Czyzewski, Z., O'Neill MacCallum, D., Romig, A. and Joy D.C., *J. Appl. Phys.*, 68 (1990) 3066.
- [18] Joy, D.C. and Luo, S., *Scanning*, 11 (1989) 180.
- [19] Bethe, H., *Ann. Phys.*, 5 (1930) 325.
- [20] Demers, H., Poirier-Demers, N., Couture, A.R., Joly, D., Guilmain, M., Jonge, N. and Drouin, D., *Scanning*, 33 (2011) 135.
- [21] Assa'd, A.M.D., *Appl. Phys. A*, 124 (2018) 699.
- [22] Kanaya, K. and Okayama, S., *J. Phys. D: Appl. Phys.*, 5 (1972) 43.
- [23] Napchan, E., "Backscattered Electrons in SEM", *Microscopy and Analysis*, (2001) January, 9-11.
- [24] Gineste, T., Belhaj, M., Teyssedre, G. and Puech, J., *App. Surf. Sci.*, 359 (2015) 398.