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A General X-ray Fluorescence Correction for Electron Microanalysis by Monte Carlo Simulations

H. Demers[1] and R. Gauvin[1]

[1] Department of Mining, Metals and Materials Engineering, McGill University,
3610 University Street, Montreal, Quebec, Canada H3A 2B2

The x-ray fluorescence effect occurs when a x-ray of higher energy is absorbed by an atom of another element and increases the total x-ray intensity measured for this element. To understand in which conditions this effect is important, a Monte Carlo program is used to simulate the electron and photon interaction with a sample [1]. The fluorescence effect calculation is based on the general equation given by Armstrong and Buseck [2].

The Ni–Fe alloys is often used to illustrate the x-ray fluorescence effect. Figure 1 shows a variation of Fe K_α x-ray intensity with a variation of the Fe weight fraction. An increase of Fe weight fraction, f_w^{Fe}, naturally increases the intensity created by the primary electron, Fe K_α^p, which is directly related to the Fe concentration. Only a small increase of the x-ray intensity, Fe K_α^f, created by secondary fluorescence from the Ni K_α x-ray is observed for the same variation of Fe concentration. The ratio of the fluorescence intensity over the intensity from the primary electron (Fe K_α^f/K_α^p), presented in Figure 2, indicates a stronger effect of the x-ray fluorescence for low Fe concentration. A closer look at the results shows that the intensity of Fe K_α^p is doubled for a change in concentration from 0.1 to 0.2 of f_w^{Fe}, $1.1 \cdot 10^{-5}$ $(e-)^{-1}\mathrm{sr}^{-1}$ and $2.3 \cdot 10^{-5}$ $(e-)^{-1}\mathrm{sr}^{-1}$, respectively. In the other hand, a small decrease, 0.9, in the Ni K_α x-ray generated is observed ($8.3 \cdot 10^{-5}$ $(e-)^{-1}\mathrm{sr}^{-1}$ at 0.1 f_w^{Fe} and $7.5 \cdot 10^{-5}$ $(e-)^{-1}\mathrm{sr}^{-1}$ at 0.2 f_w^{Fe}). The decrease of Ni generation and the increase of Fe concentration result in a small increase, 1.3, of the Fe K subshell ionization probability by Ni x-ray fluorescence ($0.16 \cdot 10^{-3}(e-)^{-1}$ at 0.1 f_w^{Fe} and $0.21 \cdot 10^{-3}(e-)^{-1}$ at 0.2 f_w^{Fe}). Finally an increase of 1.4 is observed in the x-ray intensity of Fe K_α^f by fluorescence ($2.6 \cdot 10^{-5}$ $(e-)^{-1}\mathrm{sr}^{-1}$ at 0.1 f_w^{Fe} and $3.7 \cdot 10^{-5}$ $(e-)^{-1}\mathrm{sr}^{-1}$ at 0.2 f_w^{Fe}). The difference between the ratio value from ionization (1.3) and x-ray emission (1.4) is attributed to the difference in the mass absorption coefficient, for this x-ray energy, between Fe and Ni.

This example illustrates how the Monte Carlo simulation can be used to understand the x-ray fluorescence effect. The simulation provides a detailed description of the electron and photon interaction with the sample. Which allow us to explain the variation of the x-ray intensity with a change of the Fe concentration.

References

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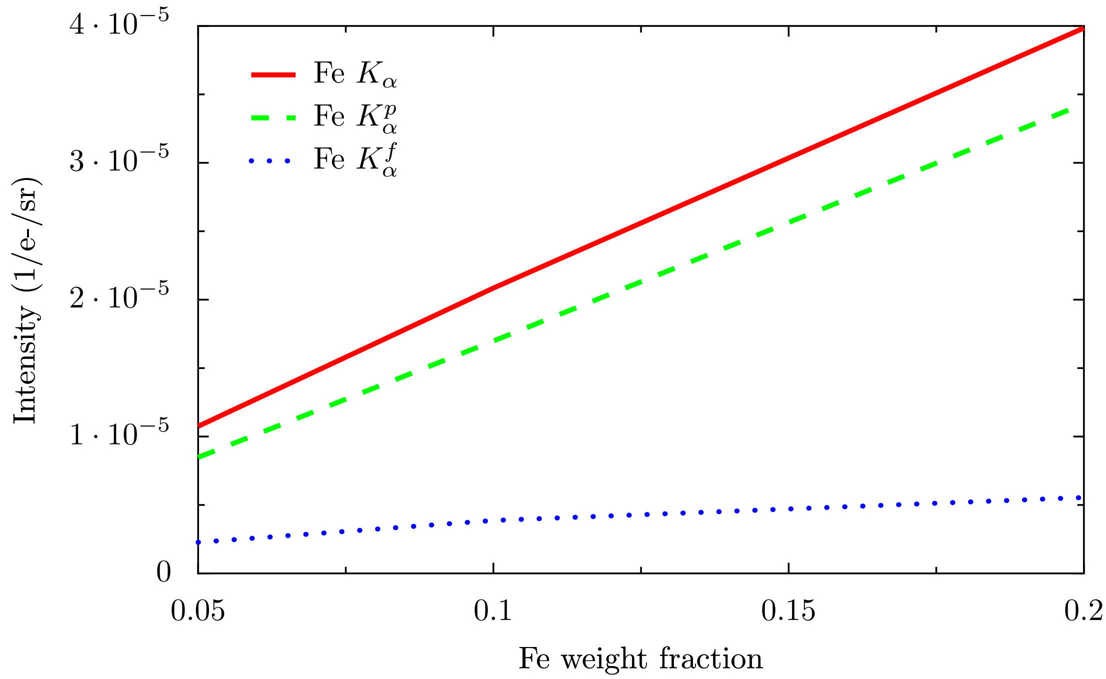

Figure 1: Emitted x-ray intensity for Fe in a Ni–Fe alloys (E_0 = 25 keV, ϕ = 40°): from primary electron (Fe K_α^p), from x-ray fluorescence emission (Fe K_α^f) by the Ni x-ray, and the total intensity (Fe $K_\alpha = K_\alpha^p + K_\alpha^f$).

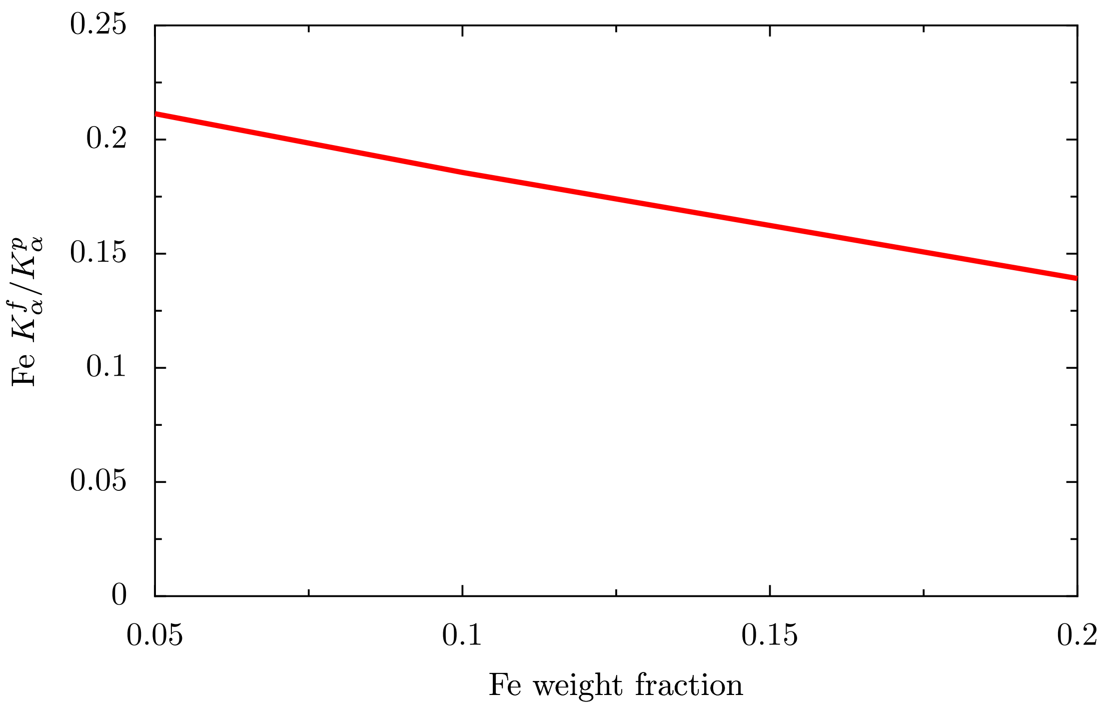

Figure 2: Ratio of Fe K_α x-ray intensity generated by x-ray fluorescence (Fe K_α^f) on the intensity created by primary electron (Fe K_α^p), for Fe in a Ni–Fe alloys (E_0 = 25 keV, ϕ = 40°).