Study of zinc coating thickness gauge by Monte Carlo simulation

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Abstract. This paper introduces how to utilize the Monte Carlo N-Particle Transport Code (MCNP) in calculating the thickness of zinc coating which distributed homogeneously in an analyzed specimen. Experiments were performed on the specimens that made of 2 mm thickness steel substrates which covered by intermediate thickness (40-175 gm⁻²) zinc layer, with the purpose of analyzing the x-ray fluorescence spectra and comparing the changes of zinc fluorescence detection efficiency under different energy monochrome photons or different detector distance. The results show that when the energy of monochrome photons is equal to 10 keV as well as the distance of detector is equal to 4 cm, the fluorescence of zinc Kα has a very good linear relationship with the thickness of zinc coating. It indicates that the MCNP code can be applied for simulating the galvanizing thickness gauge. In addition, under the same other conditions, the experimental results were not affected by different incident spot sizes (0.01-1cm).

1. Introduction
In recent years, studies on the control of zinc coating thickness have been primarily focused on two areas: process control, and modeling and prediction. Studies on process control have investigated many aspects, including improvements to the air knife system[1], optimization of air knife control parameters[2], composition of the zinc bath[3], dipping duration[4], and withdrawal speed[5], while studies on modeling and prediction have investigated methods for the prediction and control of zinc coating thickness through mathematical models developed based on production line parameters[6][7]. However, from the perspective of automatic control of zinc coating thickness, the measurement of zinc coating thickness is a prerequisite and key factor in process control. Automatic thickness control can only be realized with the acquisition of real-time zinc coating thickness data through zinc coating thickness gauges and joint involvement in feedback control with the air knife system.

X-ray fluorescence (XRF) is a method of measurement in online zinc coating thickness gauges used in large-scale integrated steel corporations in China[8]. In thickness gauges that operate based on this method, the x-ray source, ionization chamber, high-pressure system, and cooling system are contained within a measuring head[9]. However, as x-rays have high penetrating power, when the conventional XRF measurement method is used, a simultaneous entry of fluorescence emitted by the galvanized steel sheet and scattered x-rays with a much higher energy than the emitted fluorescence into the measuring head[10][11]. This results in an elevated baseline in the measurement system and reduced measurement precision and accuracy[12]. Therefore, the development of novel x-ray fluorescence analytical techniques is necessary to meet the testing requirements for galvanized steel sheets.

2. Experimental
The Monte Carlo Neutron and Photon Transport (MCNP) Code\[^1\] is a large-scale multipurpose Monte Carlo code developed by Los Alamos National Laboratory in the United States for the resolution of particle transport problems. By using the MCNP code, measurement model for the application of XRF in measurements of zinc coating thickness can be established.

Figure 1 is a schematic diagram of the measurement model. The base material was a stainless steel cylinder with a height of 0.2 cm and a radius of 15 cm, and its upper surface was located on the XZ plane. The zinc layer was homogeneously distributed over the base material, which consists of pure zinc. An annular ionization chamber filled with xenon gas was arranged above the galvanized steel plate h cm as a detector. The inside and outside diameters of ionization chamber were 2 cm and 40 cm respectively, and the height was 14 cm. The bottom of the ionization chamber near the galvanized steel plate end was 0.01 cm thick beryllium window. The x-ray source was monochromatic energy photons, and irradiates the galvanized layer with a conical shape. The radius of the beam spot was L/2.

![Figure 1. Schematic drawing of zinc thickness gauge.](image)

The annular ionization chamber can effectively increase the window area of the detector, improve the detection efficiency as well as reduce the statistical error. It measures the zinc coating by collecting the fluorescence stimulated by x-ray beam from the source. After these x-rays are absorbed by the zinc coating atom, photons with certain energy are released from the atom. Due to the different thickness of zinc coating, the number of photons reflected back varies.

The simulation space was filled with air, which is composed of the elements C, N, O and Ar. The substrate is composed of the elements Si, Cr, Mn, Fe, Ni and Mo. To achieve a good approximation of actual conditions in the simulation, the concepts of ZAIDs (obtained by combining the atomic number and atomic weight) and atomic fractions (respective proportions of elements, with minus sign prefixes as required by the program) is introduced in the model construction process to indicate the actual material composition and proportions of the respective elements\[^1\]. Table 1 shows the ZAIDs, atomic fractions and characteristic K\textsubscript{α} x-ray energy of main elements. The Zn is the main target element of zinc coating measurement.

| Material       | Element | ZAID   | Atom fraction | Characteristic K\textsubscript{α} x-ray energy (keV) |
|----------------|---------|--------|---------------|-----------------------------------------------------|
| Steel substrate| Si      | 14028  | -0.01         | 1.740                                               |
|                | Cr      | 24052  | -0.17         | 5.411                                               |
|                | Mn      | 25055  | -0.02         | 5.894                                               |
|                | Fe      | 26056  | -0.655        | 6.399                                               |
|                | Ni      | 28059  | -0.12         | 7.471                                               |
|                | Mo      | 42096  | -0.025        | 17.443                                              |
| Coating layer  | Zn      | 30066  | -1.0          | 8.630                                               |
| Air            | C       | 6012   | -0.000124     | 0.282                                               |
|                | N       | 7014   | -0.755268     | 0.392                                               |
3. Results and discussion

3.1 Incident beam energy

Firstly, 30 keV monochrome photons were selected as the incident beam, and the half taper angle was 30°. The thickness of zinc coating was 10 μm. The tally type F1:P[15] was divided into 145 intervals according to the interval of 0.2 keV in the range of 1-30 keV. The calculated value represents the photons number of x-ray in each interval. The calculated results of MCNP are normalized to each source particle. The number of photons is counted by energy binning, which is similar to multichannel energy spectrum statistics.

Figure 2 shows the x-ray energy spectrum of zinc fluorescence which are excited by the incident beam of 30 keV and then collected by the beryllium window. The fluorescence energy of each element is consistent with the characteristic x-ray energy calculated in the table 1. Element Zn has the highest fluorescence intensity, and Zn Kα peak is about 7 times stronger than Zn Kβ peak. Iron and molybdenum in the substrate were also excited, indicating that the incident beam has penetrated the zinc coating. In addition to the photoelectric absorption effect, some photons generate Rayleigh and Compton scattering.

![Figure 2. 30 keV energy spectrogram.](image)

After confirming that the measurement model can effectively stimulate the fluorescence of zinc element and penetrate the coating, the most suitable source energy should be found. The characteristic x-ray energy of Zn Kα is 8.63 keV. Therefore, the energy of incident monochromatic photons must be greater than this value. For the convenience of calculation, the energy of the smallest monochrome photons is set to 10 keV. Figure 3 is a comparison of energy spectra of 10 keV, 20 keV, 30 keV and 40 keV. Figure 3 shows that the fluorescence intensity of Zn Kα produced by 10 keV monochrome photons is the highest.

With the increase of incident photons energy, the fluorescence of Zn Kα decreases gradually. This is due to more Rayleigh and Compton scattering of high energy incident photons. Therefore, the most suitable source energy in the measurement model should be 10 keV.
Figure 3. The comparison charts of Zn characteristic Kα fluorescence excited by 10-40 keV energy incident x-rays.

3.2 Detector distance
The distance (h) of detector is another important factor in the model construction process. Figure 4 is the contrast data of Zn Kα intensity collected by beryllium window at the distance of 1 cm to 10 cm respectively. The fluorescence intensity reaches the maximum when the detector distance is between 3 and 4 cm. When the detector is close to zinc coating, part of the fluorescence enter the blind area of the inner diameter of the detector and therefore is not collected. When the detector distance increases gradually, part of the fluorescence escape from the outside of the detector. Considering the actual production, the larger detector distance can effectively reduce the errors caused by the vibration of steel plate and the risk of instrument damage. Therefore, the most suitable detector distance in the measurement model should be 4 cm.

Figure 4. Comparison of fluorescence intensity at different detector distances (h).

3.3 Measurement curve
After the source energy and detector distance were determined, the zinc coating with intermediate thickness of 40-175 gm^{-2} was measured. Figure 5 (a) is the correlation between the thickness of zinc coating and the photon counting of Zn Kα. The linear correlation coefficient is 0.9997. The results show that under the above conditions, the thickness of zinc coating has a good linear relationship with the photon counting of Zn Kα. Figure 5 (b) is the comparative data of 20 keV monochrome photons. This is because the fluorescence of Zn Kα produced by high energy x-rays is less, and after passing through the thicker zinc coating, the fluorescence of Zn Kα is further reduced, so that the weak change trend could not be shown.
Figure 5. Corresponding relationship between thickness of galvanized layers and photon counting of zinc Kα at h=4.

3.4 Incident beam spot size
Finally, in order to verify the influence of conical shape x-ray beam spot size on the results, the half taper angle was set to 26.6 ° and 88.855 ° (respectively corresponding spot radius L/2 is 0.01 cm and 1 cm) and carried out two groups of repetitive simulation experiments. The results are shown in table 2. As can be seen from table 2, when the spot size was between 0.01cm and 1cm, there was a good linear correlation between the thickness of zinc coating and Zn Kα fluorescence.

Table 2. Comparisons of linear correlation coefficients for different half taper angle. The zinc coating weight (d) was 40 gm-2, 80 gm-2, 120 gm-2 and 160 gm-2, respectively.

| Half taper angle (degree) | Number of zinc fluorescence photons | Linear correlation coefficient |
|--------------------------|------------------------------------|------------------------------|
|                          | d=40 | d=80 | d=120 | d=160 |                             |
| 26.6                     | 0.0895045 | 0.0895292 | 0.0895513 | 0.0895761 | 0.9995                              |
| 88.855                   | 0.0001531 | 0.0001533 | 0.0001535 | 0.0001537 | 1                            |

4. Conclusions
1) The MCNP model constructed in the present study passed 10 tally convergence checks, and all calculation errors were within the confidence interval. This shows that the tally process and results were true and effective.

2) Proposed physical model effectively simulates the XRF-based measurement process. It provides a new method for the design and simulation of zinc coating thickness gauge.

3) Under the condition that the source energy is 10 keV monochrome photons and the detector distance h=4, the measuring curves of zinc coatings on conventional steel sheets in the range of 40-175 gm-2 are obtained.

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