Quantitative Modeling of Depth Profiling in Glow Discharge Spectrometry with Preferential Sputtering Effects

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(Background)

Thin films are critical in applications from semiconductors to coatings, where accurate depth profiling ensures performance and quality. Glow Discharge Spectroscopy (GDS) offers high depth resolution, modeled by the MRI (Mixing-Roughness-Information) framework. MRI-CRAS improves this by accounting for crater curvature during sputtering. However, preferential sputtering remains a major source of distortion in multicomponent systems.

Abstract

We present PCRAS, an extended model integrating preferential sputtering into MRI-CRAS for more accurate GDS depth profiling quantitative analysis . This paper presents PMRI-CRAS, an extended model integrating preferential sputtering into MRI-CRAS for more accurate quantitative GDS depth profiling. A modularized code is proposed to incorporate both preferential sputtering and the crater effect, enabling faster execution and extensibility to other sputter-based techniques

1 Model

MRI

- **M**ixing length w : (sputtering)

$$g_w = \frac{1}{w}\exp\left[-(z - z_0 + w)/w\right]$$

- **R**oughness σ : (specimen)

$$g_\sigma = \frac{1}{\sqrt{2\pi}\,\sigma}\exp\left[-(z - z_0)^2/2\sigma^2\right]$$

- **I**nformation depth λ : (analyzer)

$$g_\lambda = \frac{1}{\lambda}\exp\left[-(z_0 - z)/\lambda\right]$$

(CRAS) Crater Effects Simulation

$$I = k\int_0^1 r\cdot W(r)\cdot q(X,r)\cdot I^{MRI}(q\cdot t\cdot FR(r))\,dr$$

$$\begin{cases} W(r)=\dfrac{1}{r+1} & \text{Transfer function (detects signal weights)} \\ q(z) & \text{Sputtering rate (sputtering yield)} \\ FR(r)=\dfrac{b+2}{b+2p}\left[1+(p-1)r^b\right] & \text{Relative flux function (crater morphology)} \\ K=1/\int_0^1 r\cdot\omega(r)\cdot q(r)_{X=1}\,dr & \text{Normalisation factor} \end{cases}$$

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Preferential -Sputtering

$$dz\cdot N = dt\cdot J$$

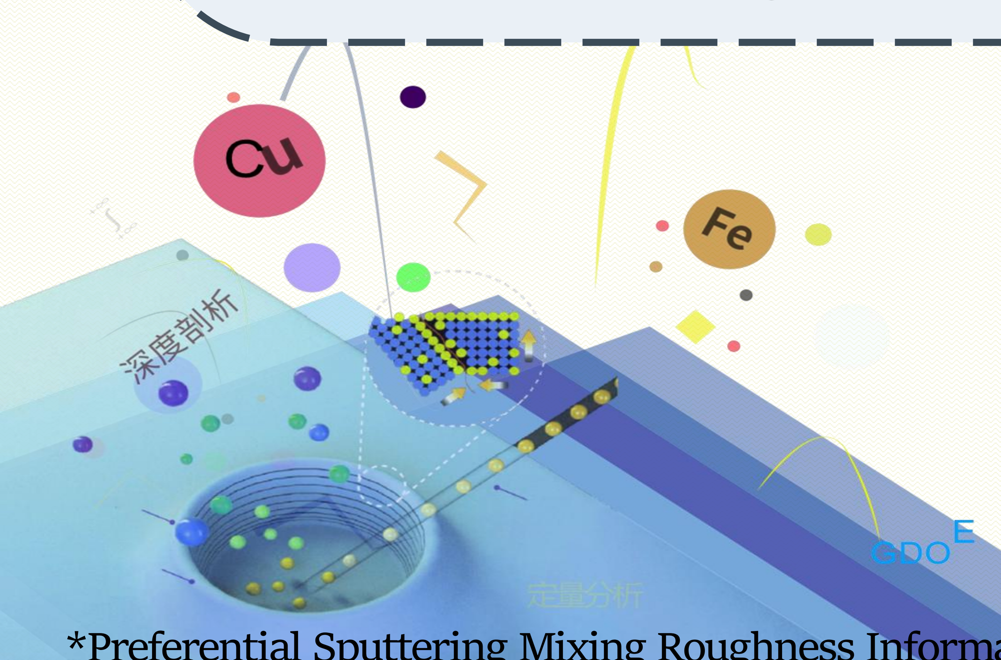
$$N=\sum_i^m N_i$$

$$J=\sum_i^m J_i$$

PCRAS*

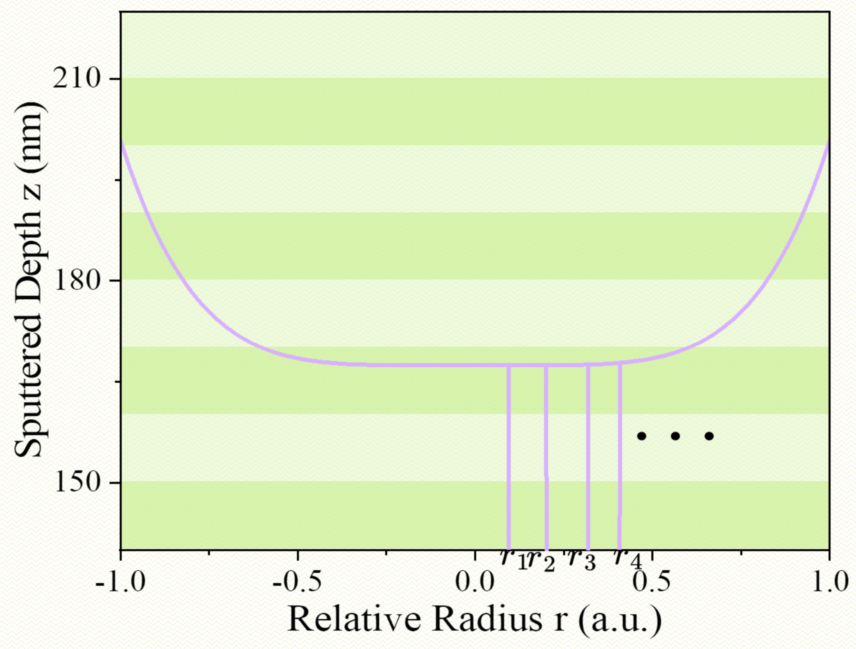
$$I = k\int_0^1 r\cdot W(r)\cdot q(X,r)\cdot I^{PMRI}(q\cdot t\cdot FR(r))\,dr$$

$$\begin{cases} W(r)=\dfrac{1}{r+1} \\ q(z)=\sum_i^N q_i X_i(z) \\ FR(r)=\dfrac{b+2}{b+2p}\left[1+(p-1)r^b\right] \\ K=1/\int_0^1 r\cdot\omega(r)\cdot q(r)_{X=1}\,dr \end{cases}$$



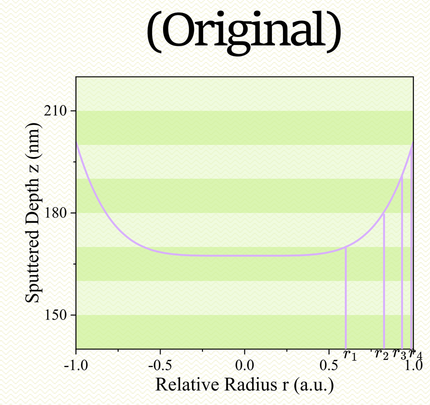
2 Experiment

Instrument: Glow Discharge Time-of-Flight Mass Spectrometry
Sample: 8xNi(30 nm)/Cr(30 nm)



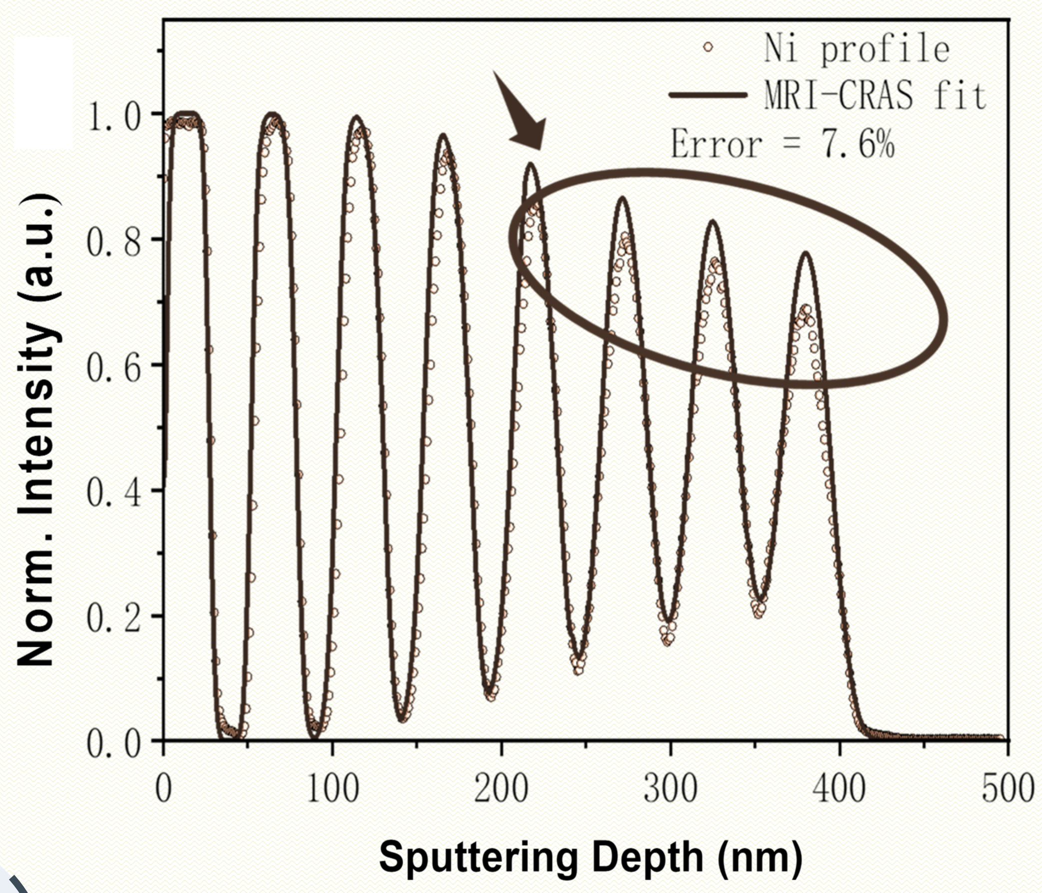
With modular segmentation, (figure left) the code runs 20 times slower

(Original)

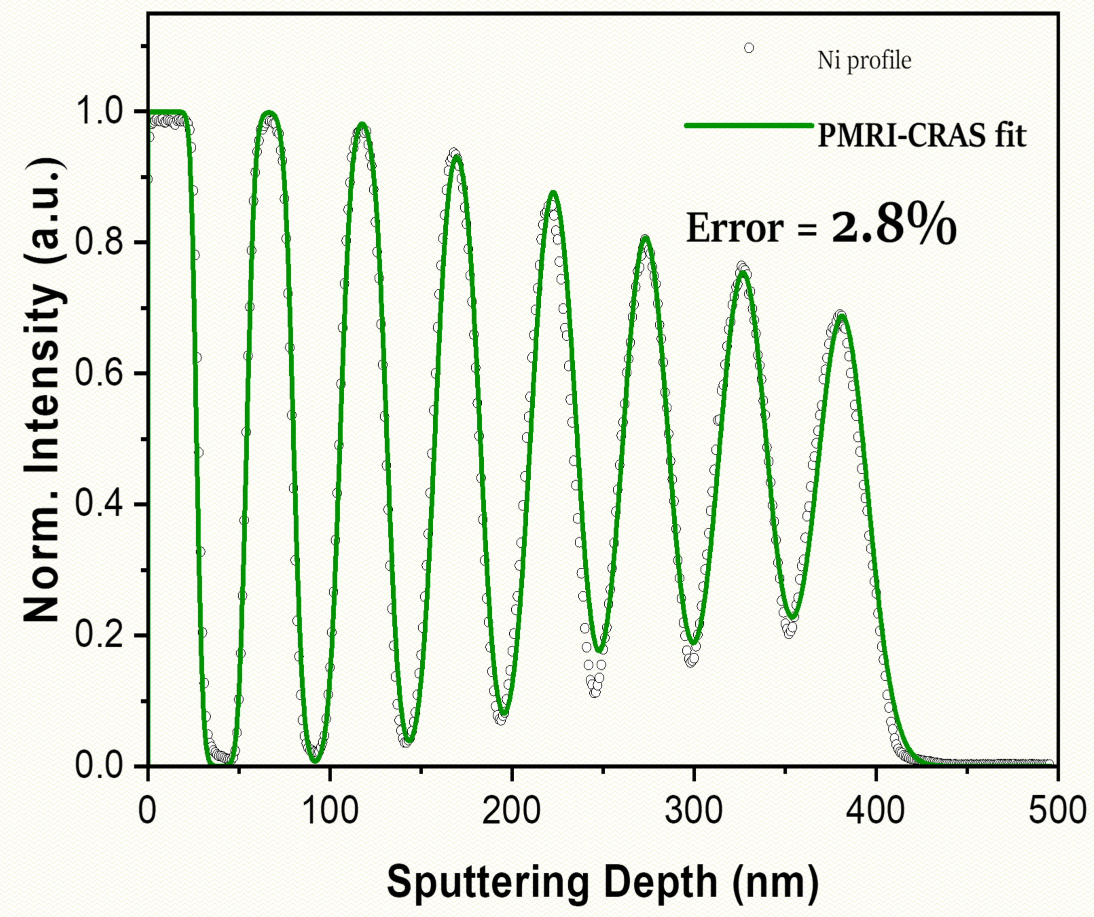


Time: 20h→1h
Error: 0.076 →0.028

MRI-CRAS fitting result



PMRI-CRAS fitting result



3 Conclusion

- Developed PCRAS model, integrating crater effect and preferential sputtering into MRI.
- Improved accuracy and depth resolution in quantitative profiling
- Program~20× faster than previous version
  - Modular design allows adaptation to different instruments and physical conditions
  - Suitable for efficient multi-parameter fitting and complex thin-film analysis

*Preferential Sputtering Mixing Roughness Information depth Crater Simulation Model