



e-ISSN: 2319-8753 | p-ISSN: 2347-6710

# IJRSET

International Journal of Innovative Research in  
**SCIENCE | ENGINEERING | TECHNOLOGY**

# INTERNATIONAL JOURNAL OF INNOVATIVE RESEARCH

IN SCIENCE | ENGINEERING | TECHNOLOGY

Volume 13, Issue 5, May 2024

**ISSN** INTERNATIONAL  
STANDARD  
SERIAL  
NUMBER  
INDIA

Impact Factor: 8.423

9940 572 462

6381 907 438

[ijrset@gmail.com](mailto:ijrset@gmail.com)

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# Investigations on the Hard X-ray Reflectivity of Speculum and Other Metal Mirrors Using Computational Techniques

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**ABSTRACT:** Recent technological developments in mirror-based grazing incidence X-ray optics have stimulated the need for basic research in high-quality metallic mirror materials for novel applications. Among different metallic mirror materials, a binary alloy of copper and tin called speculum metal was used to make vital optical components in early studies of experimental astronomy and X-ray optics. It is highly reflective and suitable to make brilliant polishing surfaces with excellent resistance to tarnishing. In this context, we have studied for the first time the reflectivity of the speculum and other mirror materials in the hard X-ray region based on theoretical calculations. Furthermore, theoretical calculations are verified well with the X-ray database program of computer simulation. The results obtained reveal that the reflectivity of speculum metal in the hard X-ray region at grazing angles below 10 arc minutes is higher than that for commonly used high-density mirror materials. This hard X-ray reflectivity of speculum metal will open up promising possibilities for it to use as a vital optical component in various technological applications including X-ray astronomy, X-ray microscopy, X-ray imaging, synchrotron beamlines, X-ray lasers, X-ray reflection spectroscopy and other areas of high energy physics.

**KEYWORDS:** Compton Effect, X-ray reflectivity, Speculum metal, Metal mirror X-ray astronomy.

## I. INTRODUCTION

The total reflection of X-rays from solid samples with smooth surfaces first reported by A. H. Compton in 1923 can be assumed to mark the birth of grazing incidence X-ray optics [1- 4]. With this technique, the field of X-ray astronomy became a major scientific discipline in astrophysics and cosmology [5, 6]. It has made great progress in the past several years with technological advances in X-ray observations and instrumentations. The remarkable scientific observations in that field have enriched and guided new views of the universe. They have also shed light on dark matter and dark energy [7, 8]. However, future space missions in X-ray astronomy require the integration of highly reflective thin mirror segments into a light weight, high-resolution telescope housing without distortion [9]. Mirror materials like nickel, gold, platinum and Iridium are good reflectors and are commonly used for making X-ray mirrors in space missions[10]. However, recent advances in grazing incidence X-ray optics have stimulated the need for basic research in high-quality optically active mirror materials for novel applications. In this context, a detailed study of the reflectivity of speculum metal in the X-ray region, especially in the hard X-ray region will be highly useful and it forms the theme of the present paper.

Speculum metal is a typical binary alloy of copper and tin in the proportion of about 2:1. It is suitable to make brilliant polishing surfaces and it has a pleasing silvery white colour with excellent resistance to tarnishing. The antiquity of this particular alloy dates back to the Bronze Age [11-13]. It regained its prominence for a short period from the time of Isaac Newton in the 17th century to the early decades of the 20th century as mirrors, gratings, etc. for making large reflecting telescopes and other optical precision instruments [14, 15]. Speculum metal is not only a material of the past but also is relevant today because of its excellent applications in diverse fields of science and technology apart from its archaeometallurgical importance. In recent years, it finds several engineering applications in various fields such as slit material in transmission electron microscopy, an alternative to nickel undercoating for gold or chromium electroplating,

anode material for lithium-ion batteries, etc. [16- 18]. It can also be used in several scientific observations and discoveries covering different areas including experimental astronomy, optical and nuclear instrumentations, spectroscopic and other studies in modern physics [19-21].

## II. BASIC CONCEPTS OF X-RAY REFLECTION

The interaction of X-rays with matter can be described by an index of refraction less than unity, and is given by,

$$n = 1 - \delta - i\beta \quad (1)$$

With real part  $\delta$ , a decrement of the refractive index describing the reflection, given by

$$\delta = \frac{N_A}{2\pi} r_e \frac{Z}{A} \rho \lambda^2 = C_m \lambda^2 \quad (2)$$

and  $\beta$  determining the absorption properties of the material, given by  $\beta = \frac{\lambda\mu}{4\pi}$ , where  $N_A$  is the Avogadro number,  $r_e$  is the classical electron radius,  $Z$  is the atomic number,  $A$  is the atomic mass,  $\rho$  is the mass density,  $\lambda$  is the wavelength of X-ray photon,  $C_m$  is the material constant and  $\mu$  is the linear absorption coefficient. X-rays undergo total external reflection only for the grazing angle of incidence ( $\theta$ ) less than the critical angle,

$$\theta_c = (2\delta)^{1/2} = \frac{1.651}{E} \left(\frac{Z}{A} \rho\right)^{1/2} \quad (3)$$

Where  $E$  is the photon energy.

The reflection of X-rays is described by the Fresnel equations, which are derived by Compton and Allison. Reflectivity is calculated by three approximation relations, given by

$$\begin{aligned} \text{(i)} \quad R &= 1 - \sqrt{\frac{2}{\delta}} \cdot \frac{\beta}{\delta} \theta \quad \text{when } \theta = \theta_c \text{ (4. a)} \\ \text{(ii)} \quad R &= \frac{\delta + \beta - \sqrt{2\beta\delta}}{\delta + \beta + \sqrt{2\beta\delta}} \quad \text{when } \theta < \theta_c \text{ (4. b) and} \\ \text{(iii)} \quad R &= \frac{\delta^2}{4\theta^4} \quad \text{when } \theta > \theta_c \text{ (4. c)} \end{aligned}$$

Where  $\theta$  is the grazing angle of incidence [22- 25].

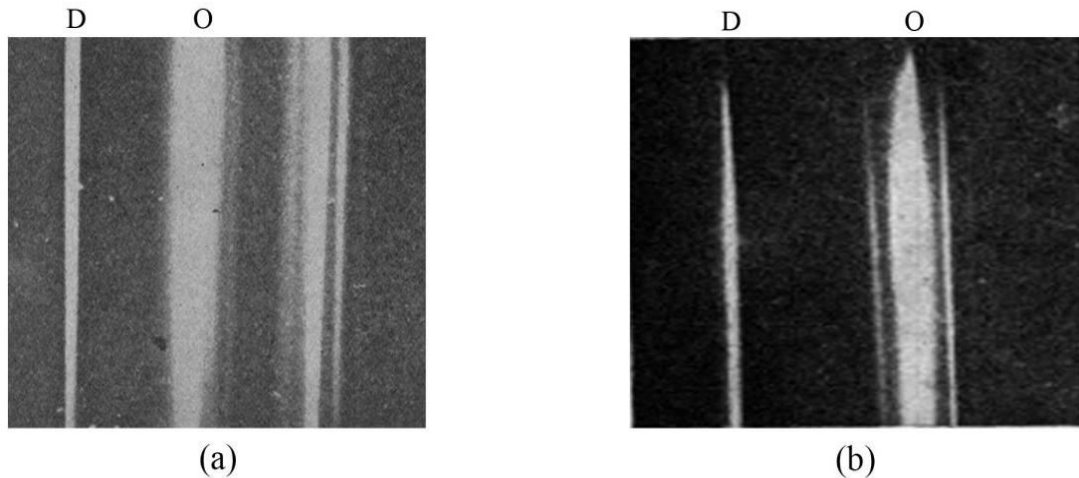
## III. MATERIALS AND METHODS

Experimental investigations are carried out by using a highly reflecting speculum metal mirror, cast and polished using traditional techniques from Aranmula, a village in Kerala, Southern India [26- 28]. The purchased mirror (Aditi Handicrafts Centre, Aranmula) with an aperture of 0.05m, separated from the brass base is cleaned and sectioned into several fragments of different dimensions using a diamond cutter, which is used for experimental characterization. X-ray reflection parameters are calculated theoretically by using the above basic equations and verifications of these calculations are carried out by using computer simulation programmes based on Henke- Gullikson-Davis database at Lawrence Berkeley Laboratory and Sergey's X-ray library database at Argonne National Laboratory [29,30].

## IV. EXPERIMENTAL EVIDENCE FOR HIGH X-RAY REFLECTIVITY OF SPECULUM METAL

A unique X-ray reflection property of speculum metal is observed from early experiments related to X-ray optics carried out by A. H. Compton and R. L. Doan. Compton pointed out in his literary article that considerable X-ray reflection does occur from a speculum surface when it strikes the surface at small glancing angles, within the critical angle for total reflection. Later, Doan confirmed this fascinating experimental investigation results in collaboration with Compton and they obtained the spectra of ordinary X-rays by reflection at very small glancing angles from a grating ruled on speculum metal [31, 32]. Some of these spectra are used to measure X-ray wavelengths with considerable precision. Spectra of K-series radiations both from copper and molybdenum obtained by reflection at a small glancing angle from a grating ruled on speculum metal are shown in Fig. 1 (a) and (b). In connection with these experimental results, the X-ray reflectivity of

speculum metal in comparison with a variety of other mirror materials as functions of different photon energies at different grazing angles of incidence have been studied.



**Fig. 1. (a) Reflection on speculum using Cu K $\alpha$  X-rays (b) Reflection on speculum using Mo K $\alpha$  X-rays**

**D - Image of a direct beam, O - Directly reflected beam [38, 39]**

## V. RESULTS AND DISCUSSION

Based on the fundamental theory of X-ray reflection, we have calculated the total external reflection critical angle for speculum metal with other mirror materials for photon energies from 8.05 keV to 300 keV, which is shown graphically in Fig. 2. It is observed from our study that the critical angle reduces as the x-ray photon energy increases from 8.05 keV to 300 keV and is high for iridium and low for aluminium. These observations led us to the conclusion that the critical angle for total external reflection reduces inversely as the photon energy increases and also high-density materials with higher atomic numbers have a larger critical angle at any photon energy. Theoretically, the estimated total external reflection critical angle of Cu K $\alpha$  and Mo K $\alpha$  X-rays for different substances like Al, Ni, Cu, Pt and Au is similar to that reported by N. V. Alov and Klockenkämper in their literary work [23, 33].

In the next step, a theoretical study of the critical angle reflectivity of the speculum and other materials for different photon energies from 8.05 keV to 300 keV is made and is graphically represented in Fig. 3. Critical angle reflectivity of the speculum is found to be gradually increased from 54.2 to 88.3% for photon energies from 8 keV to 300 KeV, compared with other materials. It is also found that the critical angle reflectivity of the speculum is higher than that of high-density common X-ray mirror materials such as iridium, platinum, and gold and comparable with that of lighter elements such as silver, nickel and copper.

Theoretical reflectivity of speculum metal with other mirror materials for various grazing angles of 1- 10 arc minutes using Cu K $\alpha$  and Mo K $\alpha$  X-rays with energies 8.05 keV and 17.5 keV are given in Tables 1 and 2. In the X-ray region of Cu K $\alpha$ , the speculum shows higher reflectivity, which is comparable with that of commonly used high-density X-ray mirror materials, but slightly less than that of lighter elements. The reflectivity in the region of Mo K $\alpha$  X-ray is found to be higher than that of commonly used high-density X-ray mirror materials and comparable with that of light elements. But aluminium shows poor reflection in this hard X-ray region, which is about 1-2% only. Henke-Gullikson-based computer simulated reflectivity of speculum with various mirror materials at different grazing angles for Cu K $\alpha$  and Mo K $\alpha$  X-rays are given in Tables 3 and 4, which are broadly in good agreement with theoretical calculations. The simulated spectral reflecting power of perfectly smooth speculum metal surface for Mo K $\alpha$  compared with other mirror materials are shown in Fig. 4 and 5. Reflectivities of more than 80 % are observed for X-ray energies up to 17.5 keV at all grazing angles, but a reduction in reflectivity is observed in all cases at higher X-ray energies.

Moreover, the simulated reflectivity plot of speculum metal for Cu  $K\alpha$  and Mo  $K\alpha$  X-rays as functions of different photon energies up to 30 keV at various grazing angles of incidence using a computer simulation program based on Henke-Gullikson database and Sergey's X-ray library database are graphically shown in Fig. 6 and 7. The reflectivity is decreased at all grazing angles of incidence but more reduction in reflectivity is observed at grazing angles of 10 and 7 arc minutes. Early literary work proposed by Henke et al. also reported the reflectivity of Al, Ni, Cu and Pt at various grazing angles for different energies, which has a close resemblance to our estimation [35]. It also suggested that the reflectivity of gold, copper and nickel in the soft X-ray region (using Copper  $K\alpha$ , particularly for energy 8 keV at a grazing angle of 5 mrad) are above 88 to 96%, but aluminium shows a reflectivity of 7.6%. However in the hard X-ray region using Molybdenum  $K\alpha$  with energy 17.479 keV at a grazing angle of 5 mrad, all these materials show poor reflectivity. Theoretical reflectivity at the perfectly smooth surface of speculum metal for Mo  $K\alpha$  X-ray is plotted as functions of different photon energies and various grazing angles of incidence and is shown in Fig. 8. The reflectivity plot shows that speculum reflects with high efficiency at energies 8.05 keV and 17.5 keV and it decreases very rapidly at higher photon energies at a grazing angle of 10 arc minute. However, it reflects with high efficiency and gives a finite value up to 300 keV at a grazing angle of one arc minute. This implies that the efficiency of reflection is high as the grazing angle within the critical angle regime reduces to its lower value. In brief, theoretical studies of the X-ray reflectivity of speculum metal in comparison with a variety of other mirror materials and its verification based on the Henke- Gullikson- Davis database and Sergey's X-ray library database confirm the results of Compton and Deon experiments (1923) on the X-ray reflectivity of speculum metal using Cu  $K\alpha$  and Mo  $K\alpha$  X-rays, that is about above 80%. Thus the reflectivity of speculum metal in the X-ray region, particularly in the hard X-ray region is highly interesting and it will find excellent applications for this typical alloy as mirrors, gratings, filters, light pipes, etc. in various fields of astrophysics, especially in X-ray astronomy, X-ray optics, X-ray microscopy, X-ray reflection spectroscopy and other areas of high energy physics.

## VI. CONCLUSIONS

X-ray reflectivity of various mirror materials including speculum metal is studied in detail for different photon energies ranging from 8.05 keV to 300 keV at various grazing angles of incidence. Speculum metal shows a gradual increase in critical angle reflectivity with the increase of photon energy. Low-density materials generally show high reflectivity at small grazing angles compared to high-density materials. The reflectivity of speculum metal in the hard X-ray region at various grazing incidence angles of 1–10 arc minutes is found to be high in comparison with commonly used high-density mirror materials such as gold, platinum and iridium. This also confirms the results of Compton and Deon experiments (1923) on the X-ray reflectivity of speculum metal using Cu  $K\alpha$  and Mo  $K\alpha$  X-rays that is about above 80%. The high reflectivity may be due to the presence of a thin transparent layer of a well-polished smooth surface containing nanoscale crystalline particles. The high reflectivity of speculum metal in the hard X-ray region may open up promising possibilities for this alloy to be used as mirrors, gratings, filters, light pipes, etc. in various fields of astrophysics, especially in X-ray astronomy, X-ray microscopy, X-ray imaging including medicine and industry, X-ray lithography, X-ray reflection spectroscopy and other areas of high energy physics.

## ACKNOWLEDGEMENTS

Authors are extremely grateful to Dr. S. NarayanaKalkura, Dr. K. MuraleedharaVarier, Mr.Midhun, Dr.Gopchandran, Dr. Abdul Kalam, for their constructive comments, valuable suggestions, continuing support and contributions during the entire work, the director of NCESS, the staffs of SICC, University of Kerala, for providing useful reference materials and laboratory facilities to conduct experimental analyses.

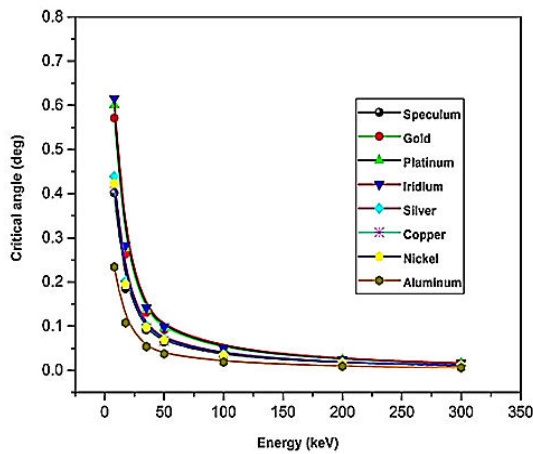


Fig. 2 Critical angle for various materials calculated for different photon energies.

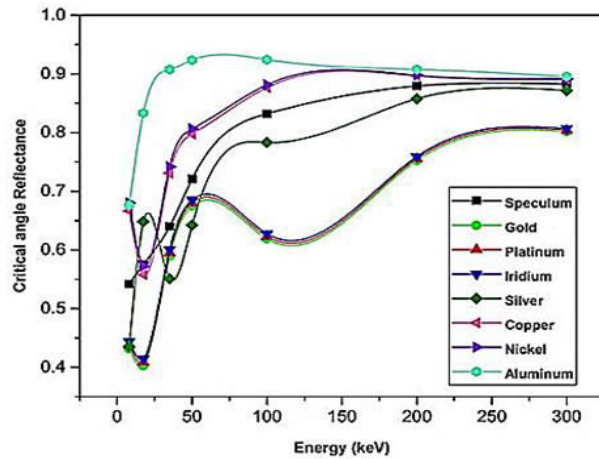


Fig. 3 Critical angle reflectivity of various materials as a function of different photon energies.

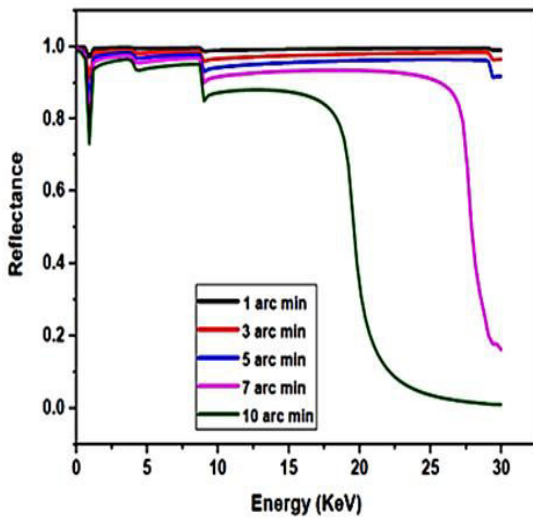


Fig. 4 Henke- Gullikson data based simulated reflectivity of perfectly smooth speculum metal for different photon energies up to 30 keV at various grazing angles of incidence.

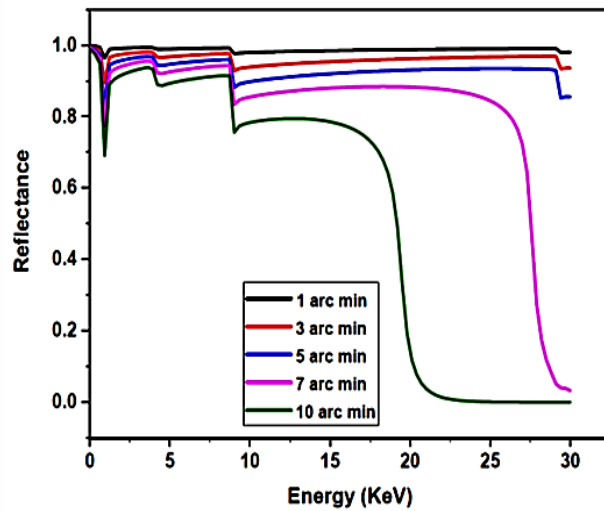


Fig.5 Henke-Gullikson data-based simulated reflectivity of speculum metal with a surface roughness of 3.3 nm as functions of photon energies up to 30 keV at various grazing angles of incidence.

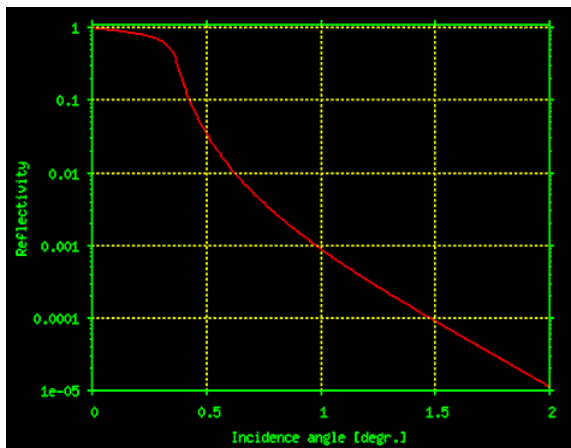


Fig. 6 Sergey’s X-ray library data-based simulated reflectivity of speculum metal for different photon energies up to 30 keV at various grazing angle.

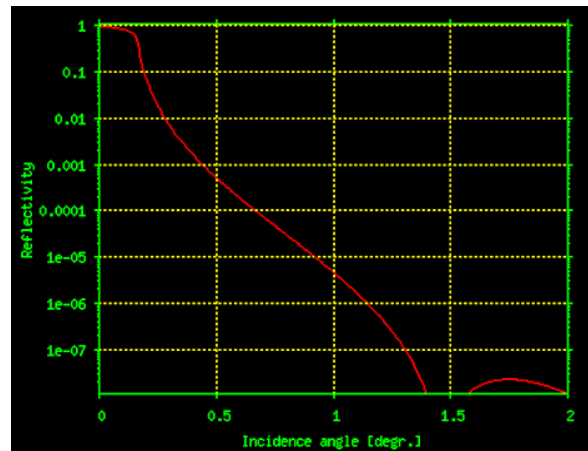


Fig. 7 Sergey’s X-ray library data-based simulated reflectivity of perfectly smooth speculum metal for different photon energies up to 30 keV at various grazing angle.

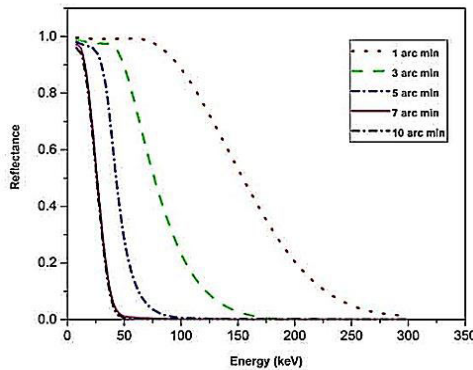


Fig. 8 Theoretical reflectivity of perfectly smooth surface of speculum metal for Mo  $K_{\alpha}$  X-rays as functions of different photon energies and various grazing angle of incidence

**Table 1. Theoretical reflectivity of various mirror materials for Mo  $K_{\alpha}$  X-rays**

Material	Reflectivity of various materials calculated for Cu $K_{\alpha}$ X-rays at different grazing angles				
	1 arc min	3 arc min	5 arc min	7 arc min	10 arc min
Speculum	99.60	98.79	98.0	97.19	95.98
Gold	99.43	98.34	97.25	96.13	94.48
Platinum	99.45	98.48	97.45	96.47	94.95
Iridium	99.53	98.58	97.63	96.68	95.26
Silver	99.30	97.90	96.50	95.12	93.10
Copper	99.83	99.45	99.16	98.82	98.32
Nickel	99.85	99.55	99.26	98.96	98.52
Aluminum	99.72	99.17	98.62	98.10	97.24



**Table 2. Theoretical reflectivity of various mirror materials for Mo K $\alpha$  X-rays**

Material	Reflectivity of various materials calculated for Mo K $\alpha$ X-rays at different grazing angles				
	1 arc min	3 arc min	5 arc min	7 arc min	10 arc min
Speculum	99.29	97.89	96.48	95.04	92.92
Gold	98.58	95.74	92.90	90.02	85.77
Platinum	98.70	96.10	93.49	90.85	86.95
Iridium	98.77	96.32	93.86	91.37	87.68
Silver	99.61	98.82	98.04	97.24	96.06
Copper	99.24	97.71	96.18	94.64	92.35
Nickel	99.31	97.95	96.59	95.20	93.15
Aluminum	99.87	99.61	99.36	4.50	1.09

**Table 3. Reflectivity of various mirror materials for Cu K $\alpha$  X-rays using Computer simulation based on the Henke-Gullikson-Davis database**

Material	Reflectivity of various materials for Cu K $\alpha$ X-rays at different grazing angles				
	1 arc min	3 arc min	5 arc min	7 arc min	10 arc min
Speculum	99.56	98.70	97.82	96.88	95.33
Gold	99.39	98.17	96.95	95.71	93.78
Platinum	99.44	98.33	97.22	96.09	94.34
Iridium	99.48	98.44	97.40	96.35	94.72
Silver	99.31	97.96	96.59	95.17	92.89
Copper	99.81	99.43	99.05	98.64	97.96
Nickel	99.82	99.47	99.11	98.73	98.09
Aluminu	99.74	99.21	98.62	97.94	96.40

**Table 4. Reflectivity of various mirror materials for Mo K $\alpha$  X-rays using Computer simulation based on Henke-Gullikson- Davis database**

Material	Reflectivity of various materials calculated for Mo K $\alpha$ X-rays at different grazing angles				
	1 arc min	3 arc min	5 arc min	7 arc min	10 arc min
Speculum	99.29	97.82	96.12	93.84	85.20
Gold	98.55	95.64	92.59	89.21	82.75
Platinum	98.65	95.95	93.14	90.06	84.36
Iridium	98.77	96.29	93.72	90.91	85.76
Silver	99.60	98.78	97.84	96.64	93.09
Copper	99.24	97.67	95.87	93.52	85.88
Nickel	99.32	97.93	96.35	94.30	88.00
Aluminu m	99.87	99.58	99.02	20.30	1.82



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