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Computation of Refractive Index Values of Inert Gases at Near-Infrared and XUV Region Based on Mathematica Software

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Abstract

In this study, refractive indices in the visible, near-infrared, and extreme ultraviolet (XUV) regions are calculated based on Mathematica software. Atomic scattering factors are simulated for a high photon energy range (20-60 eV). By using the atomic scattering factors, the real and imaginary part of the index of refraction values are plotted as a function of photon energy. This work aims to present a computational program, which calculates the index of refraction of the inert gases at different wavelength regions. The refractive indices of gases, namely helium (He), neon (Ne), argon (Ar), and xenon (Xe) in the near-infrared and XUV region are computed by using Mathematica software. The applications of the index of refraction are discussed in the paper. The Mathematica program calculating the refractive indices is presented in the Appendix.

Keywords: Refractive index; Inert gas; Infrared region; Extreme ultraviolet.

Mathematica Yazılımı Kullanılarak Yakın Kızılötesi ve XUV Bölgesinde Asal Gazların Kırılma İndisi Değerlerinin Hesaplanması

Öz

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Bu çalışmada, görünür, kızılötesi ve aşırı ultraviyole (XUV) bölgesindeki kırılma indisleri Mathematica yazılımı kullanılarak hesaplanmıştır. Atomik saçılma faktörleri yüksek foton enerji aralığı (20-60 eV) için simülasyonu gerçekleştirilmiştir. Atomik saçılma faktörleri kullanılarak kırılma indisi değerlerinin gerçek ve sanal kısmı, foton enerjisinin bir fonksiyonu olarak hesaplandı. Bu çalışmanın amacı, farklı dalga boyu bölgelerinde asal gazların kırılma indisini hesaplayan bir simülasyon programı sunmaktır. Yakın kızılötesi ve XUV bölgesindeki helyum (He), neon (Ne), argon (Ar) ve xenon (Xe) kırılma indisleri Mathematica yazılımı kullanılarak hesaplandı. Kırılma indisinin uygulama alanları bahsedilmiştir. Kırılma indislerini hesaplayan Mathematica programı Ek'te sunulmaktadır.

Anahtar Kelimeler: Kırılma indisi; Asal gaz; Kızılötesi bölge; Aşırı ultraviole.

1. Introduction

The laser-matter interaction paves the path for a new avenue to many research areas. Laser light is modified while propagating in the nonlinear medium, i.e. gas species that affect the propagation of light in a medium. The refractive index of the medium gives information about the modification of the laser light. Thus, the variation of the refractive index at different wavelength regions must be determined in the near-infrared region (at around 800 nm) and extreme ultraviolet (XUV) region (10 nm – 60 nm) to predict how the laser beam propagates and is shaped through the medium. Spectroscopic measurements are usually taken in a gas medium. For accurate measurements, the corresponding wavelength needs to be known, $\lambda_{medium}=\lambda_{vac}/n_{medium}$, here n_{medium}, λ_{medium}, and λ_{vac} are the index of refraction of the medium, the wavelength of light in the medium and wavelength of light in the vacuum, respectively. For this reason, the refractive index value of the used medium is to be known to accurately determine the behavior of the corresponding wavelength.

Technological devices require detailed studies. For example, optoelectronic devices find a wide range of applications in electronic and optical devices such as laser diodes, photodetectors, and nanotechnology [1-8]. The optical and electronic properties of a device are determined by fundamental science, e.g. properties of refractive index, which is a measurement of how light behaves in the medium. Moreover, the electronic properties such as atomic polarizability and dielectric constant depend on the refractive index of the materials as well.

In this paper, the refractive index of the inert gases in the infrared and XUV region is determined by using Mathematica software. The calculations of refractive indices of helium (He), neon (Ne), argon (Ar), and xenon (Xe) are performed using the various models in the visible and near-infrared region presented in the literature [9-15]. In addition, the refractive indices of these species in the XUV region are calculated using the atomic scattering factors [16-18]. The atomic scattering factors help calculate the real and imaginary part of the refractive indices in the XUV region. Wolfram Mathematica 10.0 program [19] has been used for calculation by using a personal computer. The complete Mathematica program is given in the Appendix.

2. Materials and Methods

The list of refractive index coefficients and atomic scattering factors has been obtained from Ref. [9, 10] and the official website of the physical measurement laboratory of the National Institute of Standards and Technology, https://www.nist.gov/. The refractive index constant in the IR region is obtained, and the atomic scattering factors calculate the index of refraction values in the XUV region.

3. Calculation of Index of Refraction in the Infrared Region

Refractive indices of inert gases have been calculated using the model at room temperature and pressure presented in Ref. [9]. The refractive index model for the inert gas is formulated by Eqn. (1) [9]

$$n = \sqrt{1 + a(1 + \frac{b}{\lambda^2} + \frac{c}{\lambda^4} + \frac{d}{\lambda^6} + \frac{e}{\lambda^8} + \frac{f}{\lambda^{10}})} \quad (1)$$

where λ is the wavelength in angstroms, and a, b, c, d, e, and f are coefficients for each gas species. The coefficients are given in Table 1 [9, 10].

Table 1: Refractive index coefficients used to calculate refractive indices of different gases in the infrared region

Gas species	*a*	*b*	*c*	*d*	*e*	*f*
Helium	6.927×10^{-5}	2.24×10^{5}	5.94×10^{10}	1.72×10^{16}	0	0
Neon	1.335×10^{-4}	2.24×10^{5}	8.09×10^{10}	3.56×10^{16}	0	0
Argon	5.547×10^{-4}	5.15×10^{5}	4.19×10^{11}	4.09×10^{17}	4.32×10^{23}	0
Xenon	1.366×10^{-3}	9.02×10^{5}	1.81×10^{12}	4.89×10^{18}	1.45×10^{25}	4.34×10^{31}

Figure 1 shows the refractive indices (n-1) of inert gases in the infrared region (from 600 nm to 800 nm) at room temperature and pressure. The variation of refractive index (n-1) values in the visible and near-infrared region is small, Fig. 1. The refractive indices (n-1) are small and positive for all gas species, and they give refractivity of the gas species in the optical path.

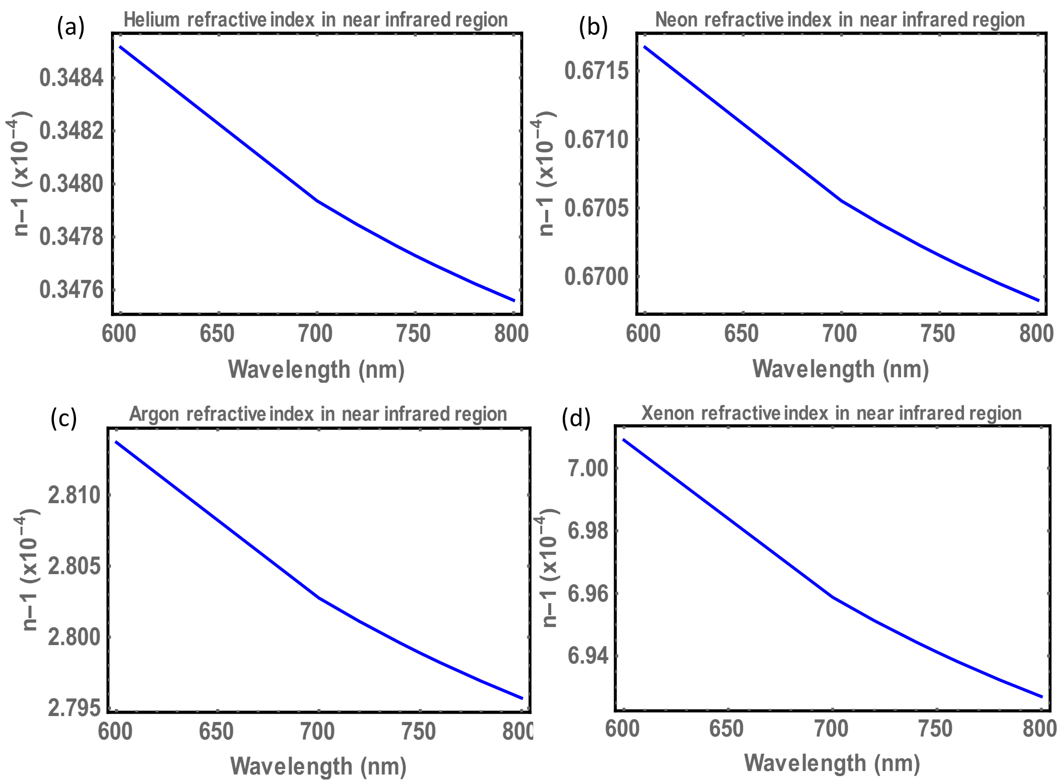

Figure 1: Simulation of refractive index (n-1) of inert gas species in the infrared region. (a) Helium, (b) Neon (c) Argon (d) Xenon

The index of refraction values is calculated at room temperature and pressure. If the refractivity of the gas species is required at a specific temperature and pressure, the conversion formula is given by Eqn. (2) [10, 20]

$$\begin{aligned} n &= 1 + (n_0 - 1)\frac{T_0}{T} \\ n &= 1 + (n_0 - 1)\frac{P_0}{P} \end{aligned} \tag{2}$$

here n_0, T_0, P_0 are the reference refractive index, temperature, and pressure, respectively.

4. Calculation of Refractive Index in the Extreme Ultraviolet Region

The refractive indices in the XUV region are not known very well compared to those in the infrared region. The estimation of the refractive index in the XUV region is obtained from the atomic scattering factors, f_1 and f_2 [16, 21]. The atomic scattering factors measure the scattering power of individual atoms. Each species has a different scattering factor, which shows how X-ray radiation response to each species. Each component of atomic scattering factors gives information about the dispersive and absorptive components, f_1 and f_2, respectively.

The atomic scattering factors are defined as $f=f_1+if_2$ [10, 21]. The atomic scattering is described by the complex refractive index, n. The refractive index value is proportional to the atomic scattering factor, and it is given by [16, 21].

$$n = 1 - \frac{r_0}{2\pi}\lambda^2 \rho f \tag{3}$$

where ρ, f, and r_0 are the density of atoms, the atomic scattering factor, and the classical electron radius, respectively.

Figure 2 presents the scattering factors for the used gas species. The values are taken from the references [16-18] and are used as the input parameters in the simulation program, Appendix. f_1 and f_2 describe the refraction and absorption of the species. The refractive indices of the gases at the XUV region are determined from the scattering factors, Eqn. (3). The solid blue line shows scattering properties of the species, while the red dotted line gives information about the absorptive components of the species, Fig. 2.

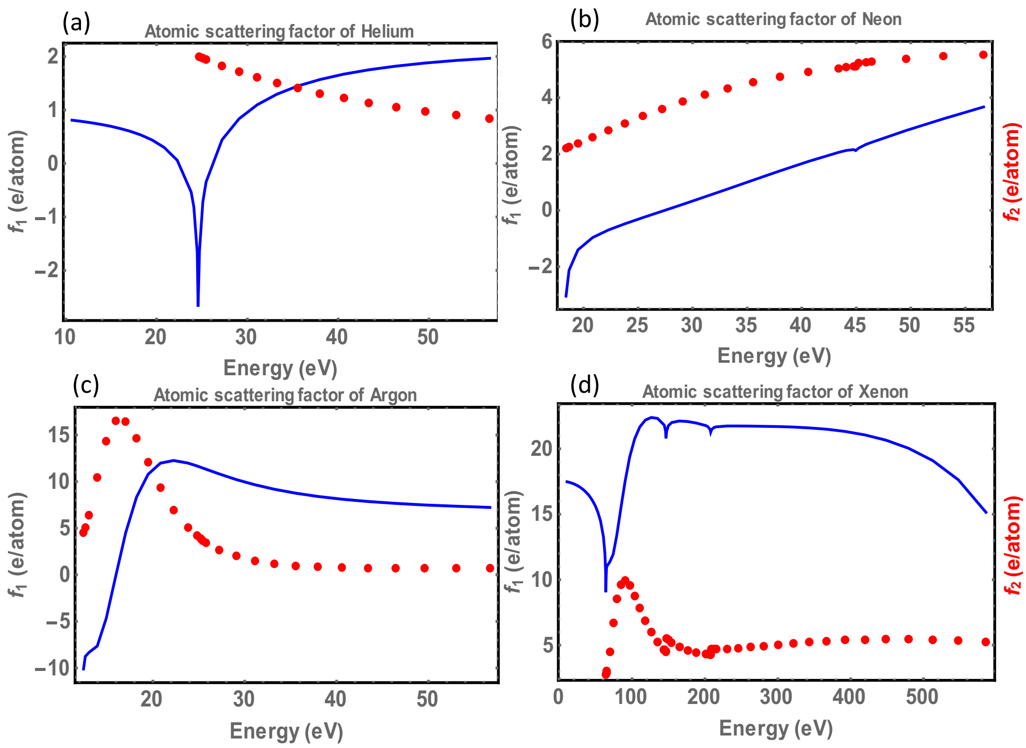

Figure 2: Atomic scattering factors of inert gases in the XUV region. (a) Helium, (b) Neon (c) Argon (d) Xenon. The solid blue line is for f_1, and the red dotted line is for f_2

The refractive indices in the XUV region are calculated using Eqn. (3) even though the refractive indices in the XUV region are not completely accurate in the energy range of interest. The simulation for refraction index values helps determine how a medium responds to a specific wavelength. The real and imaginary parts of the refractive indices are studied using Eqn. (3). Figure 3 presents the real part of the refractive indices for He, Ne, Ar, and Xe gas while Fig. 4 shows the imaginary part of the index of refraction values for these gas species. f_2 of xenon is plotted from 60 eV to 500 eV since f_2 is available for xenon gas at this range, Fig. 2 and 3.

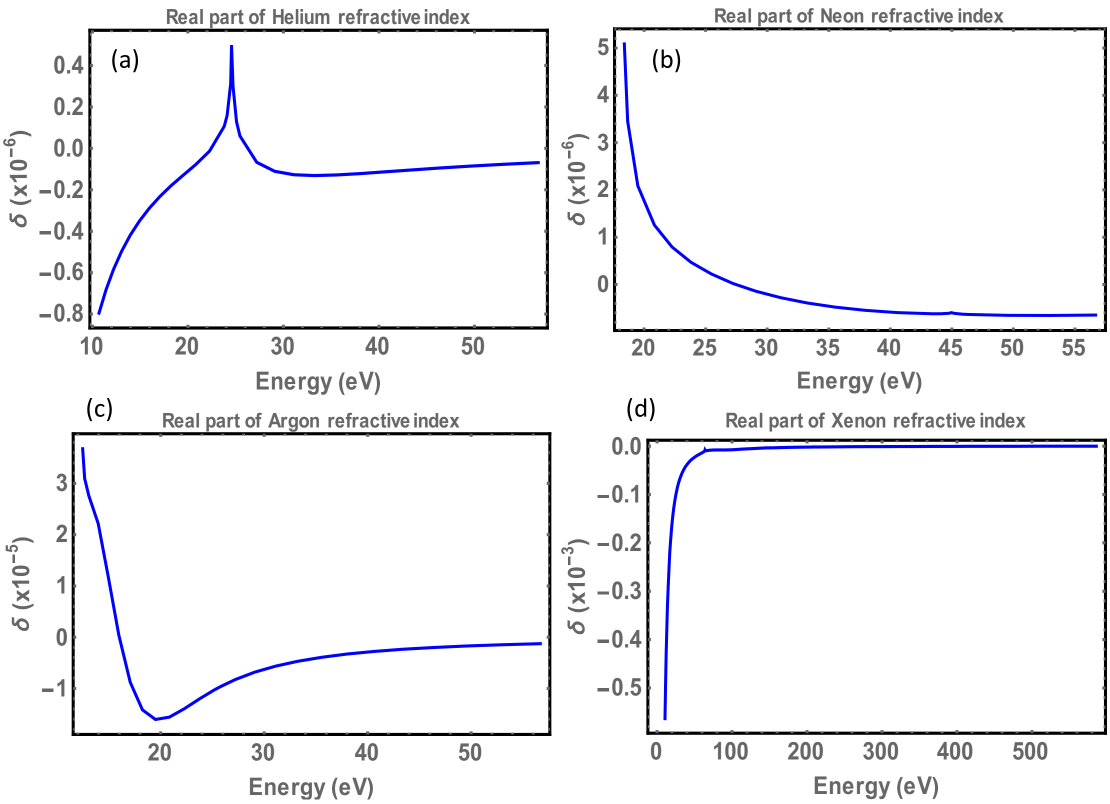

Figure 3: Simulation of the real part of the refractive index ($\delta = R(n) - 1$) in the XUV region for inert gases (a) Helium, (b) Neon, (c) Argon, (d) Xenon

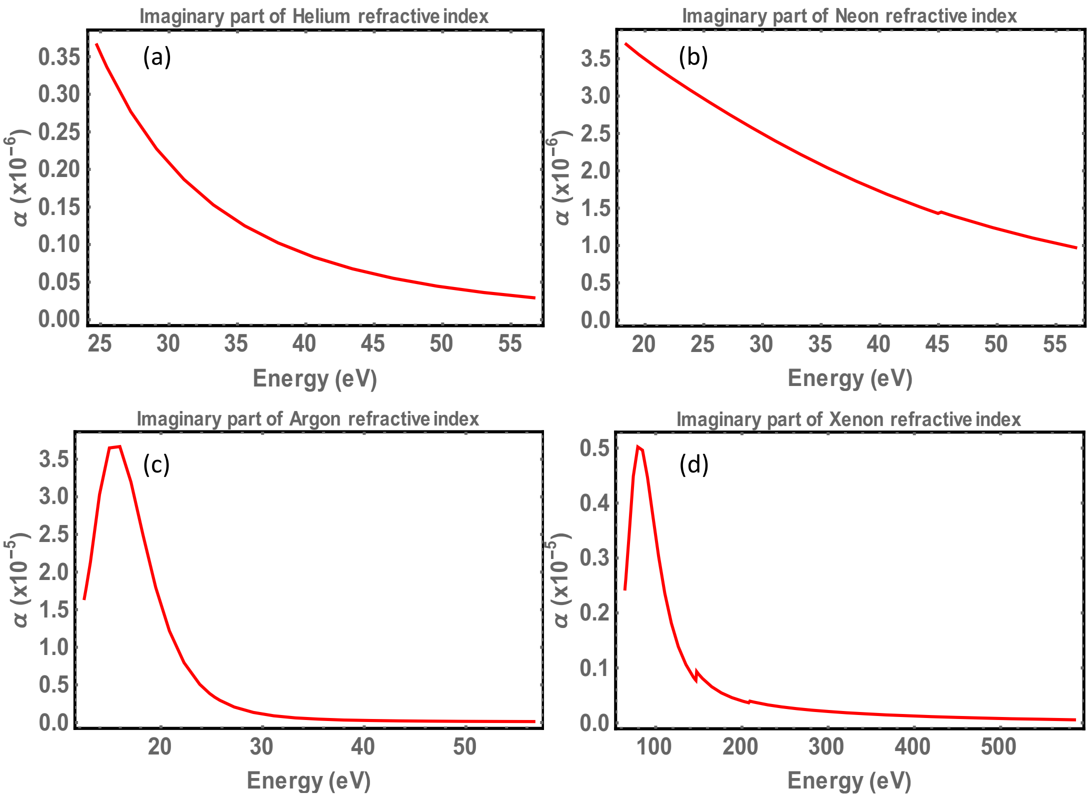

Figure 4: Simulation of imaginary part of the refractive index ($\alpha = Im(n)$) in the XUV region for inert gases (a) Helium, (b) Neon, (c) Argon, (d) Xenon

5. Conclusions

In this paper, refractive index values in the IR and XUV region are calculated using the Mathematica program. This paper is the comparison of refractive indices of different inert gases in different wavelength regions. An explanation of the index of refraction at the IR and XUV region is described for room temperature and pressure values. This paper provides a calculation of the real and imaginary part of refractive indices of inert gases and covers a wide range of wavelengths from IR to XUV region. The study of the refraction index values in the near-infrared and the extreme ultraviolet region has been carried out. The atomic scattering factors for gas species help calculate the real and imaginary part of the refractive index values in the XUV region. The gas species of helium, neon, argon, and xenon are used. The atomic scattering factors of these gas species are used as input parameters in the simulation program, and so the real and imaginary parts of the refractive indices in the XUV region are determined. As simulation software, the Wolfram Mathematica program is used for the calculation of refractive indices.

The estimation of the index of refraction values in the infrared and XUV region can be used for the phase matching calculation for the generation of coherent XUV pulses, absorption, or transmission of a material for a specific wavelength region.

Appendix: Mathematica Program

```
a=1.366*10^-3; b=9.02*10^5; c=1.81*10^12; d=4.89*10^18; ee=1.45*10^25; f=4.34*10^31; (*Xe gas variables values*)
λ={6000,7000,7200,7400,7500,7600,7800,8000}; (*Wavelength angstrom*)
n=SetPrecision[Table[(1+a*(1+b/λ[[i]]^2+c/λ[[i]]^4+d/λ[[i]]^6+ee/λ[[i]]^8+f/λ[[i]]^10))^(1/2),{i,1,8}],10];
Print["Refractive index of Xe at 800 nm = ",n," at 1 bar for Xe gas"]
n=n-1;
ListLinePlot[Table[{λ[[i]]/10,n[[i]]*10^4},{i,1,8}],Frame->True,Axes->False,PlotRange->All,FrameLabel->{"Wavelength (nm)","n-1 (x10-4)"},FrameStyle->Thick,LabelStyle->{Bold,15},PlotStyle->{Thick,Blue},PlotLabel->"Xenon refractive index in near infrared region"]
MA=131.29; (*Xenon atomic weight gr/mol*) R=83.14; (*cm^3bar/Kmol*) T=22.8+273.15;
P=1; (*bar optimum presure for Xenon gas*) ρ=MA*P/R/T;Print["ρ=",ρ,"gr/cm^3"]
Nav=6.02*10^23; (*avagadro number*) natom=Nav*ρ/MA; (*number of atoms per cm^3*)
Print["natom= ",natom," atoms/cm^3"]

EEf1={10.69,11.4276,12.2161,13.059,13.9601,14.9234,15.9531,17.0538,18.2305,19.4884,20.8331,22.2706,23.8073,25.45,27.2061,29.0833,31.09,33.2352,35.5285,37.9799,40.6005,43.402,46.3967,49.5981,53.0204,56.6788,60.5896,62.72,63.68,63.936,64.32,64.7703,65.28,69.2394,74.017,79.1241,84.5837,90.42,96.6589,103.328,110.458,118.08,126.227,134.937,143.766,144.248,145.967,146.553,147.433,149.634,154.201,164.84,176.214,188.373,201.371,203.938,207.06,207.892,209.141,212.262,215.266,230.119,245.997,262.971,281.116,300.513,321.248,343.414,367.11,392.441,419.519,448.466,479.41,512.489,547.851,585.653}; (*eV for f1*)

f1={17.4817,17.4729,17.4627,17.451,17.4376,17.4222,17.4044,17.3839,17.3603,17.333,17.3014,17.2647,17.2221,17.1724,17.1143,17.046,16.9653,16.8696,16.7551,16.6169,16.4483,16.2392,15.9749,15.631,15.1635,14.4787,13.2889,11.9994,10.5181,9.04168,10.1989,10.7681,11.0295,11.3451,11.9353,13.4352,15.4567,17.5482,19.3672,20.7487,21.6728,22.1972,22.3982,22.3204,21.8272,21.7629,21.3416,20.7968,21.3224,21.7567,22.0064,22.129,22.0852,21.9645,21.7702,21.6898,21.4862,21.2694,21.4691,21.6278,21.6791,21.7426,21.7454,21.7359,21.7211,21.6987,21.6617,21.5992,21.4951,21.3273,21.0644,20.6582,20.0448,19.1067,17.6322,15.1523}; (*Real atomic scattering factor*)
```

```
EEf2={64.32,64.7703,65.28,69.2394,74.017,79.1241,84.5837,90.42,96.6589,103.328,110.458,1
18.08,126.227,134.937,143.766,144.248,145.967,146.553,147.433,149.634,154.201,164.84,176
.214,188.373,201.371,203.938,207.06,207.892,209.141,212.262,215.266,230.119,245.997,262.
971,281.116,300.513,321.248,343.414,367.11,392.441,419.519,448.466,479.41,512.489,547.85
1,585.653}; (*eV for f2*)

f2={2.7373,2.8683,3.0230,4.4855,6.6806,8.5363,9.6404,9.9217,9.5457,8.7673,7.8187,6.8627,5.
9916,5.2451,4.6587,4.6310,4.5353,4.5038,5.5082,5.4034,5.2082,4.8526,4.5958,4.4226,4.3179,
4.3047,4.2913,4.2883,4.6957,4.6923,4.6913,4.7129,4.7685,4.8475,4.9411,5.0418,5.1427,5.237
5,5.3204,5.3862,5.4308,5.4507,5.4436,5.4084,5.3453,5.2553}; (*Imaginary atomic scattering
factor*)

r0=2.82*10^-6;(*classical electron radius*);
λ=1240/EEf1 (*nm*);
nr=SetPrecision[1-((r0)/(2*π))*λ^2*(ρ*f1),40];
λ=1240/EEf2 (*nm*);
ni=SetPrecision[((r0)/(2*π))*λ^2*(ρ*f2),40];
b1=ListLinePlot[Table[{EEf1[[i]],(nr[[i]]-1)*10^3},{i,1,76}],Frame->True,Axes-
>False,PlotRange->All,FrameLabel->{"Energy (eV)","δ (x10-3)"},FrameStyle-
>Thick,LabelStyle->{Bold,15},PlotStyle->{Thick,Blue},PlotLabel->"Real part of Xenon
refractive index"]

b2=ListLinePlot[Table[{EEf2[[i]],(ni[[i]]*10^5)},{i,1,46}],Frame->True,Axes-
>False,PlotRange->All,FrameLabel->{"Energy (eV)","α (x10-5)"},FrameStyle-
>Thick,LabelStyle->{Bold,15},PlotStyle->{Thick,Red},PlotLabel->"Imaginary part of Xenon
refractive index"]
Show[b1,b2,PlotRange->All]

a1=ListLinePlot[Table[{EEf1[[i]],(f1[[i]])},{i,1,76}],Frame->True,Axes->False,PlotRange-
>All,FrameLabel->{"Energy (eV)","f1 (e/atom)"},FrameStyle->Thick,LabelStyle-
>{Bold,15},PlotStyle->{Thick,Blue},PlotLabel->"Atomic scattering factor of Xenon"]

a2=ListPlot[Table[{EEf2[[i]],(f2[[i]])},{i,1,46}],Frame->True,Axes->False,PlotRange-
>All,FrameLabel->{"Energy (eV)","f2 (e/atom)"},FrameStyle->Thick,LabelStyle-
>{Bold,15},PlotStyle->{Thick,Red},PlotLabel->"Atomic scattering factor of Xenon"]
```

```
Show[a1,a2,PlotRange->All]
```

The gas variables are taken from Table 1, Ref [9, 10].

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