Lindhard Doc

Tong

Ref

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STOPPING POWER OF ELECTRON GAS AND EQUIPARTITION RULE

BY

JENS LINDHARD AND AAGE WINTHER

第四章 非弹性碰撞过程及电子阻止本领

程序中相关的参量根据中文的定义，像alpha1,alpha2 对应于Lindhard文献中的f1,f2

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```
class epsilon:
    'use gauss unit'
    def __init__(self):
        pass

    def alpha1(self,z,u):
        a=z-u; b=z+u
        p1=0.5
        if abs(a)==1.0:
            p2=0
        else:
            p2=1.0/8.0/z*(1.0-a*a)*math.log(abs((a+1.0)/(a-1.0)))

        if abs(b)==1.0:
            p3=0
        else:
            p3=1.0/8.0/z*(1-b*b)*math.log(abs((b+1.0)/(b-1.0)))

        return p1+p2+p3

    def alpha2(self,z,u):
        a=z-u; b=z+u
        if b<=1:
            return PI/2.0*u
        if b>1 and abs(a)<1:
            return PI/8.0/z*(1-a*a)
        if abs(a)>=1:
            return 0
```

$$\alpha_1(z,u)=\frac{1}{2}+\frac{1}{8z}(1-a^2)\ln\left|\frac{a+1}{a-1}\right|+\frac{1}{8z}(1-b^2)\ln\left|\frac{b+1}{b-1}\right| \qquad (4.2\text{-}29)$$

$$\alpha_2(k,u)=\begin{cases}\dfrac{\pi}{2}u & b<1\\ \dfrac{\pi}{8z}(1-a) & |a|<1<b\\ 0 & |a|>1\end{cases} \qquad (4.2\text{-}30)$$

其中 $a=z-u$ 和 $b=z+u$。

$$E_F=\frac{1}{2}mv_F^2=\frac{\hbar^2k_F^2}{2m}=\frac{\hbar^2}{2m}(3\pi^2n)^{2/3}.$$

The summation in (5) may now be performed and the result is conveniently written in the form

$$\varepsilon^1(u,z)=1+\frac{\chi^2}{z^2}\{f_1(u,z)+if_2(u,z)\}, \qquad (6)$$

where

$$f_1(u,z)=\frac{1}{2}+\frac{1}{8z}\{1-(z-u)^2\}\log\left|\frac{z-u+1}{z-u-1}\right|+\frac{1}{8z}\{1-(z+u)^2\}\log\left|\frac{z+u+1}{z+u-1}\right|,$$

and

$$f_2(u,z)=\begin{cases}\dfrac{\pi}{2}u, & \text{for } z+u<1,\\ \dfrac{\pi}{8z}\{1-(z-u)^2\}, & \text{for } |z-u|<1<z+u,\\ 0, & \text{for } |z-u|>1.\end{cases} \qquad (6')$$

The variables k and ω are here replaced by dimensionless variables z and u, where

$$z=\frac{k}{2k_F} \text{ and } u=\frac{\omega}{kv_F}.$$

Moreover, the parameter χ^2 in (6), defined by

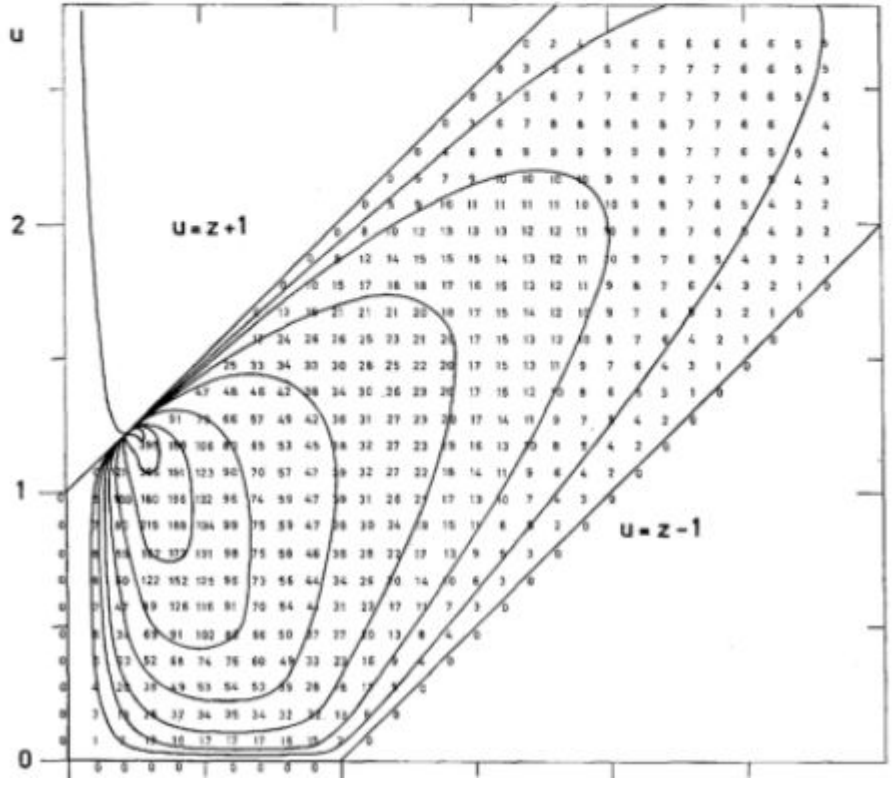
$$\chi^2=\frac{e^2}{\pi\hbar v_F}, \qquad (7)$$

积分分段，普通的面积分和一段线积分。线积分并没有直接积分。而是采用了后面（20）的简化的算法。这就导致在临近点附近，有点差异。共振线的minimum点，用二分查找，求得零点。

$$L = \frac{-6}{\pi\chi^2}\int_0^{v/v_F} u\,du \int_0^{\infty} z\,dz\ \mathrm{Im}\left(\frac{1}{\varepsilon}-1\right)$$

$$= -\frac{6}{\pi}\int_0^{v/v_F} u\,du \int_0^{\infty} dz\ \frac{z^3 f_2(u,z)}{\{z^2+\chi^2 f_1(u,z)\}^2+\{\chi^2 f_2(u,z)\}^2}. \qquad (8)$$

It is seen from (6) that the integral (8) receives contributions from the domain $|u-z|<1$ where $f_2(u,z) \neq 0$, and also from a curve in the region $u>z+1$, for which $\varepsilon^I = 0$, i.e. $z^2+\chi^2 f_1(u,z) = 0$. In the latter case the double integral degenerates to a line integral. The former contribution



and neglecting terms of higher order in χ^2 we obtain

$$L(v_1) - L(v_2) = \left\{u^3 \log\frac{u+1}{u-1} + \log(u^2-1) - 2u^2 + o\left(\frac{\chi^2}{u^4}\right)\right\}\Bigg|_{v_2/v_F}^{v_1/v_F}. \qquad (19')$$

Combining (19') with (17), and taking only the first terms in a series expansion in v_F^2/v^2, the result is

$$L = \log\frac{2mv^2}{\hbar\omega_0} - \frac{3v_F^2}{5v^2} - \frac{3v_F^4}{14v^4} - \cdots + o\left(\frac{\chi^2 v_F^4}{v^4}\right) - \qquad (20)$$

$$= \log y - \frac{3^{3/2}}{5\chi}\frac{1}{y} - \frac{9}{14\chi^2 y^2} - \cdots .$$

The formula (20) is applicable when v/v_F is above the minimum of the resonance curve. According to the equipartition rule, every term in (20) is contributed equally from the resonance curve and from close collisions,

```
def ucFun(self,chi2, u):
    return (u-1)**2 + chi2/2.0*(1 - u*math.log(u/(u-1)))

def calZeroPoint(self,fun,u0,u1,pre):
    f0=fun(u0); f1=fun(u1)
    du=u1-u0
    while du>pre and f0*f1<0:
        f0=fun(u0); f1=fun(u1)
        u=(u0+u1)/2.0
        f=fun(u)
        if f*f0<=0:
            u1=u
        if f*f1<=0:
            u0=u
        du=u1-u0
    return (u0+u1)/2.0
```

LFun 测试

TABLE 2

The factor L in the specific energy loss computed numerically as a function of the particle velocity for six values of the density parameter in (7), $\chi^2 = 1$, $10^{-1/3}$, 10^{-1}, $10^{-4/3}$, $10^{-5/3}$ and 10^{-2}. L is given as a function of the parameter y, defined in (11).

y	$\log y$	$\chi^2 = 0.01$		$\chi^2 = 0.02154$		$\chi^2 = 0.046416$	
		v/v_F	$L(y)$	v/v_F	$L(y)$	v/v_F	$L(y)$
0.10000	–	0.07598	0.0007995	0.09206	0.001145	0.1115	0.001540
0.31623	–	0.13512	0.004491	0.1637	0.006398	0.1983	0.008642
1.0000	0	0.2403	0.02522	0.2909	0.03575	0.3527	0.04839
1.7783	0.5757	0.3204	0.05963	0.3882	0.08459	0.4703	0.1141
3.1623	1.1513	0.4273	0.1407	0.5177	0.1990	0.6272	0.2675
5.6235	1.7269	0.5698	0.3306	0.6903	0.4647	0.8363	0.6220
10.000	2.3026	0.7598	0.7772	0.9206	1.067	1.115	1.420
14.678	2.6864	0.9205	1.341	1.115	1.833	1.351	2.247
21.544	3.0701	1.115	2.280	1.351	2.641	1.637	2.804
31.623	3.4539	1.351	3.029	1.637	3.191	1.983	3.285
56.235	4.0295	1.802	3.820	2.183	3.893	2.645	3.939
100.00	4.6052	2.403	4.496	2.909	4.530	3.527	4.555
316.23	5.7565	4.273	5.724	5.177	5.734	6.272	5.741
1000.0	6.9078	7.598	6.898	9.206	6.901	11.15	6.903

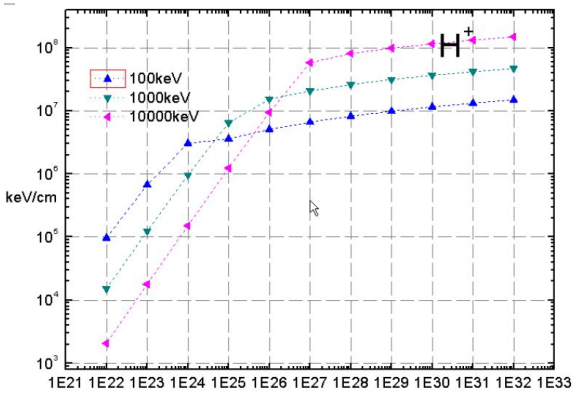
```
---- 0.01 ----
y= 0.1 L= 0.000801067888643
y= 0.31623 L= 0.0045016875364
y= 1.0 L= 0.0253333087232
y= 1.7783 L= 0.0599160374225
y= 3.1623 L= 0.14138029626
y= 5.6235 L= 0.332095325948
y= 10.0 L= 0.770035739198
y= 14.678 L= 1.33838519719
y= 21.544 L= 2.449217694
y= 31.623 L= 3.06096868504
y= 56.235 L= 3.82440967172
y= 100.0 L= 4.49481856611
y= 316.23 L= 5.72296382759
y= 1000.0 L= 6.89729868842
```

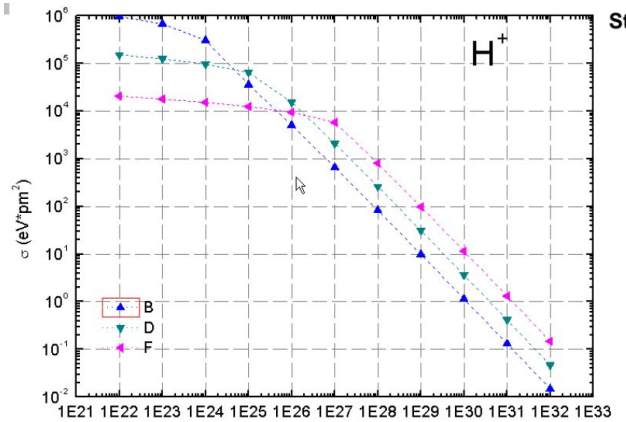
```
---- 0.02154 ----
y= 0.1 L= 0.00114283465472
y= 0.31623 L= 0.00640091107446
y= 1.0 L= 0.0359773845608
y= 1.7783 L= 0.0849608431497
y= 3.1623 L= 0.199882079577
y= 5.6235 L= 0.466687860515
y= 10.0 L= 1.07120122515
y= 14.678 L= 1.8370607298
y= 21.544 L= 2.67712461219
y= 31.623 L= 3.2001238892
y= 56.235 L= 3.89418546461
y= 100.0 L= 4.53137661282
y= 316.23 L= 5.73377971014
y= 1000.0 L= 6.90064452493
```

```
---- 0.046416 ----
y= 0.1 L= 0.00154158559386
y= 0.31623 L= 0.0086583590916
y= 1.0 L= 0.0486105601343
y= 1.7783 L= 0.114268660423
y= 3.1623 L= 0.26795916066
y= 5.6235 L= 0.623504915133
y= 10.0 L= 1.41752843526
y= 14.678 L= 2.29343130342
y= 21.544 L= 2.81635892449
y= 31.623 L= 3.28749808232
y= 56.235 L= 3.93938265704
y= 100.0 L= 4.55554844749
y= 316.23 L= 5.74107760852
y= 1000.0 L= 6.90291775427
```

v/vf > uc 时候，会有点差距，主要是由于采用了简化的算法

electron gas 测试





APPLIED PHYSICS REVIEWS

Stopping of energetic light ions in elemental matter

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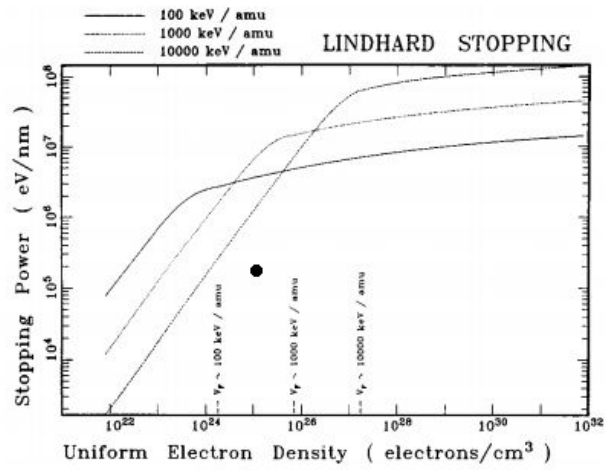

FIG. 24. Energy loss per unit distance in a free electron gas. The stopping power or energy loss per unit path length of a particle in a free electron gas is the product of the interaction strength shown in Fig. 23 times the electron density. These two factors compete since as the electron density increases, the number of electrons per unit volume increases but the interaction strength decreases. The result is a linear increase of stopping power with electron density for dilute gases, and then a leveling off for more dense gases. The inflection point for a particle is where its velocity equals the Fermi velocity of a free electron gas as indicated by the arrows above.

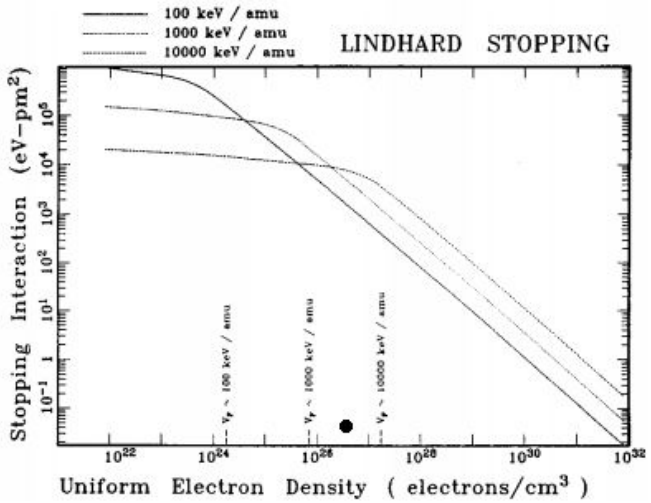

FIG. 23. Stopping interaction of a particle with a free electron gas. The stopping interaction derived by Lindhard is shown as [Eq. (A2)]. It has been calculated for ten orders of magnitude of electron density, and for three different particle velocities. Each curve is flat for the section where the particle is much faster than the electrons in low density electron gases. At about the point where the particle velocity equals the Fermi velocity of an electron gas (see arrows above) the interaction curve inflects. For greater density electron gases the interaction becomes less since some of the electrons are moving faster than the particle and these collisions become more adiabatic.

Al 测试

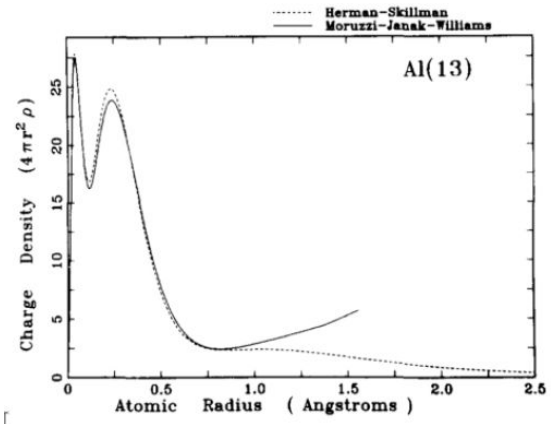

FIG. 2. Comparison of HFS radial charge density calculated by F. Herman and S. Skillman (Ref. 14) and solid-state spherically averaged radial charge densities by Moruzzi, Janak, and Williams (Ref. 16).

用density程序，把casp生成的所有dat文件，合并成总的密度分布函数。但这是孤立原子的密度分布，后面文章中用的是固体中的密度分布计算，发现两者差异很大。因此，后面计算中采用的密度分布，是根据文章中的图，取的几个点（对应al.orb_fit），计算的。

Application of Lindhard's dielectric theory to the stopping of ions in solids

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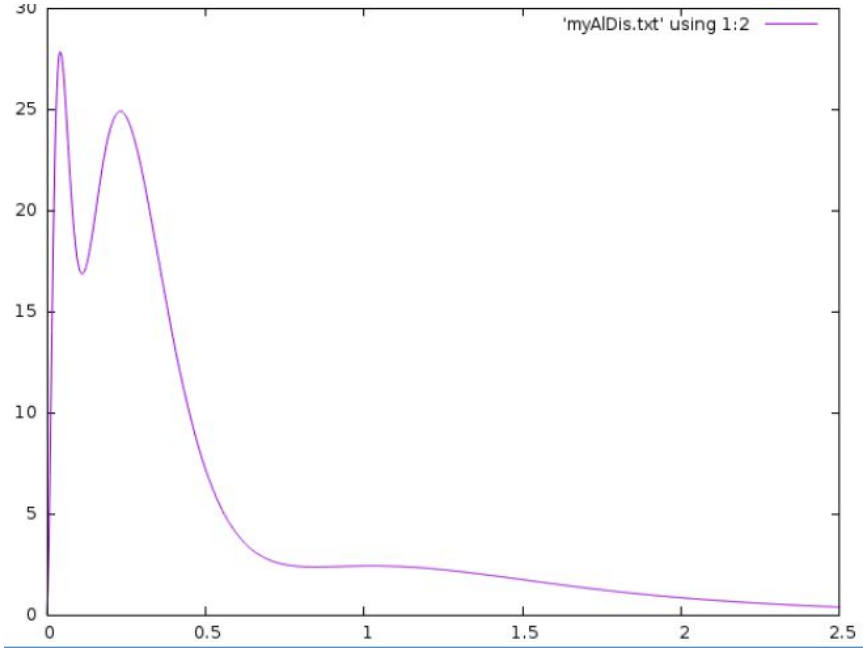

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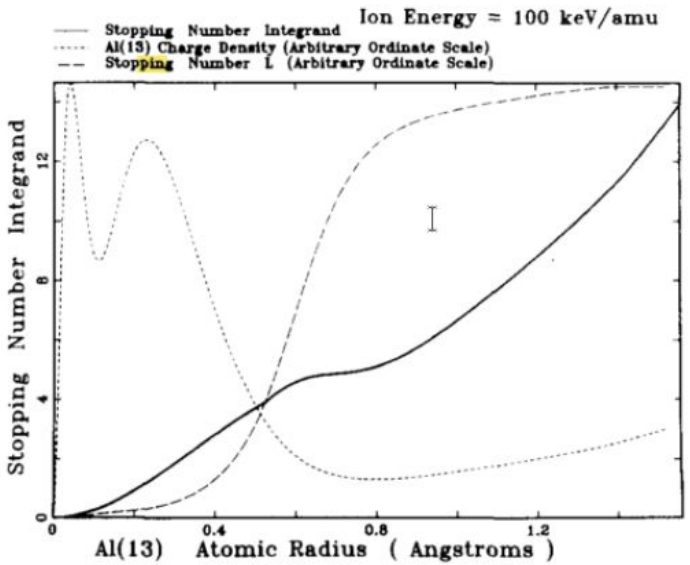
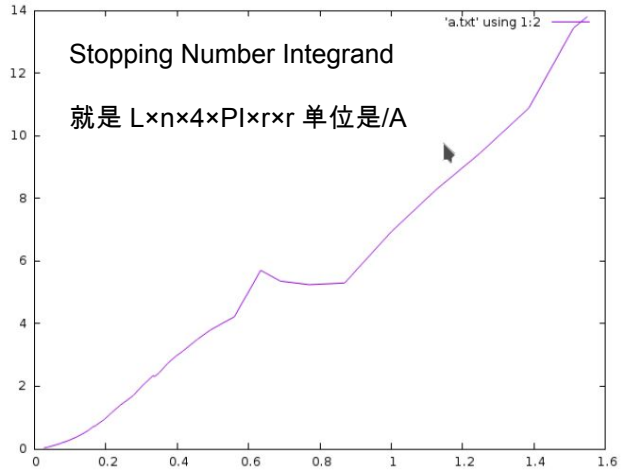
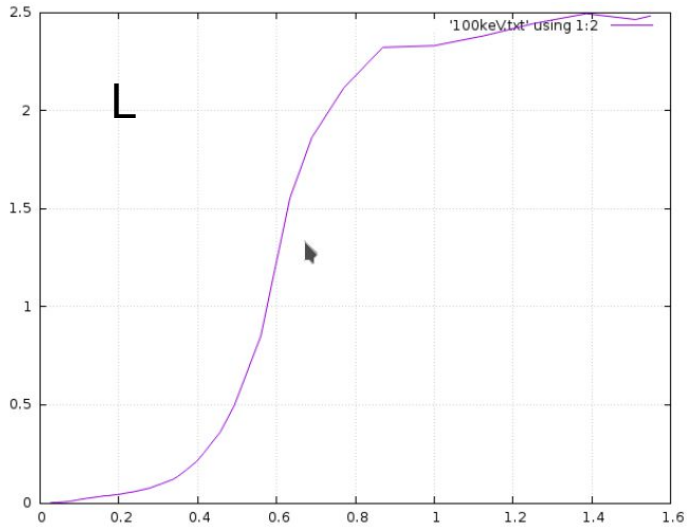


FIG. 3. Comparison of spatial variation in the stopping number integrand of Eq. (12), the stopping number of Eq. (12), and the solid-state radial charge density for aluminum (Ref. 16) with ion energy of 100 keV/amu.





Al 测试

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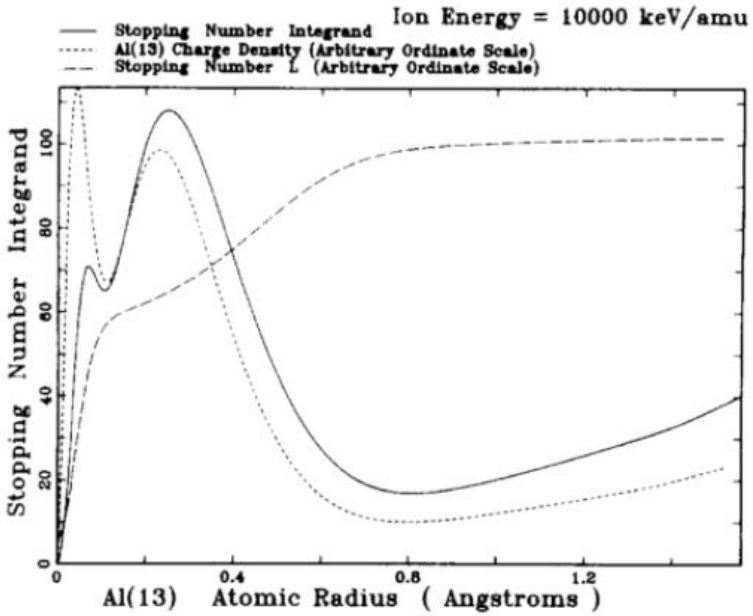
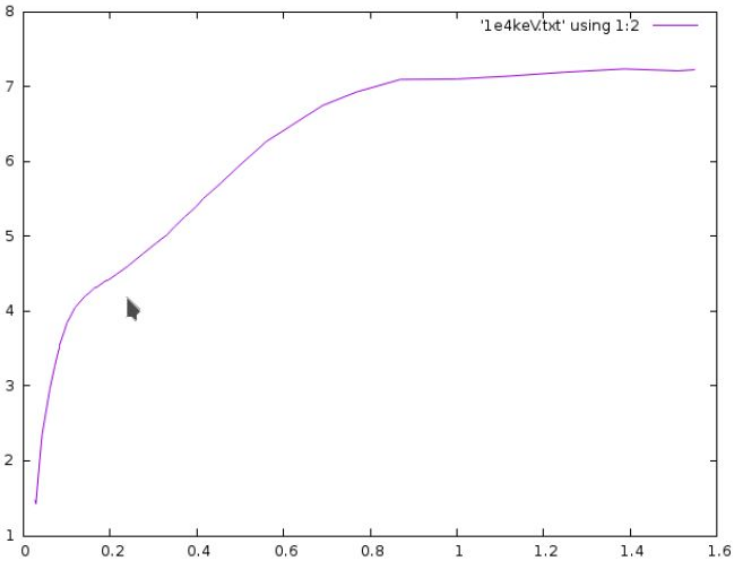


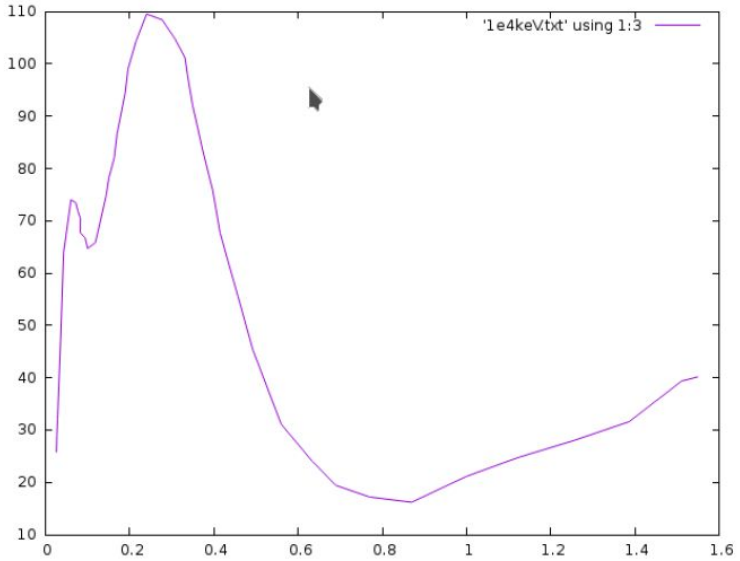
FIG. 4. Comparison of spatial variation in the stopping number integrand of Eq. (12), the stopping number of Eq. (12), and the solid-state radial charge density for aluminum (Ref. 16) with ion energy of 10 000 keV/amu.

L



Stopping Number Integrand

就是 L×n×4×PI×r×r 单位是/A



原子density 文件生成

在density文件夹下， 有d.py文件。
例子：

```
[zxt@fedora Al]$ ls
Al1s1.dat  Al2p1.dat  Al2p3.dat  Al2p5.dat  Al2s1.dat  Al3p1.dat  Al3s2.dat  a.txt  HFS1s.dat  HFS2s.dat  HFS3s.dat
Al1s2.dat  Al2p2.dat  Al2p4.dat  Al2p6.dat  Al2s2.dat  Al3s1.dat  al.orb     b.txt  HFS2p.dat  HFS3p.dat
[zxt@fedora Al]$ ../d.py Al*.dat
```