

P(ND)<sup>2</sup>-2 SECOND INTERNATIONAL WORKSHOP  
ON PERSPECTIVES ON NUCLEAR DATA FOR THE  
NEXT DECADE

14–17 October 2014 — Bruyères-le-Châtel, France

**Modelling odd-even staggering in fission  
fragment yields in the Brownian shape-motion  
approach: Current results and prospects**

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Collaborators on this and other projects:

W. D. Myers, J. Randrup(LBL), H. Sagawa (Aizu), S. Yoshida (Hosei), T. Ichikawa(YITP), A. J. Sierk(LANL), A. Iwamoto (JAEA), S. Aberg (Lund), R. Bengtsson (Lund), S. Gupta (IIT, Ropar), and many experimental groups (e. g. K.-L. Kratz (Mainz), H. Schatz (MSU), A. Andreyev (York), K. Nishio (JAEA) ...).

More details about fission (PRC 79 064304, PRC 84 034613, PRC 88 064606), other projects (beta-decay, masses), associated ASCII data files, interactive access to data (type in Z, A and get specific data, contour maps) and figures are at

<http://t2.lanl.gov/nis/molleretal/>

## Potential Energy of Deformation

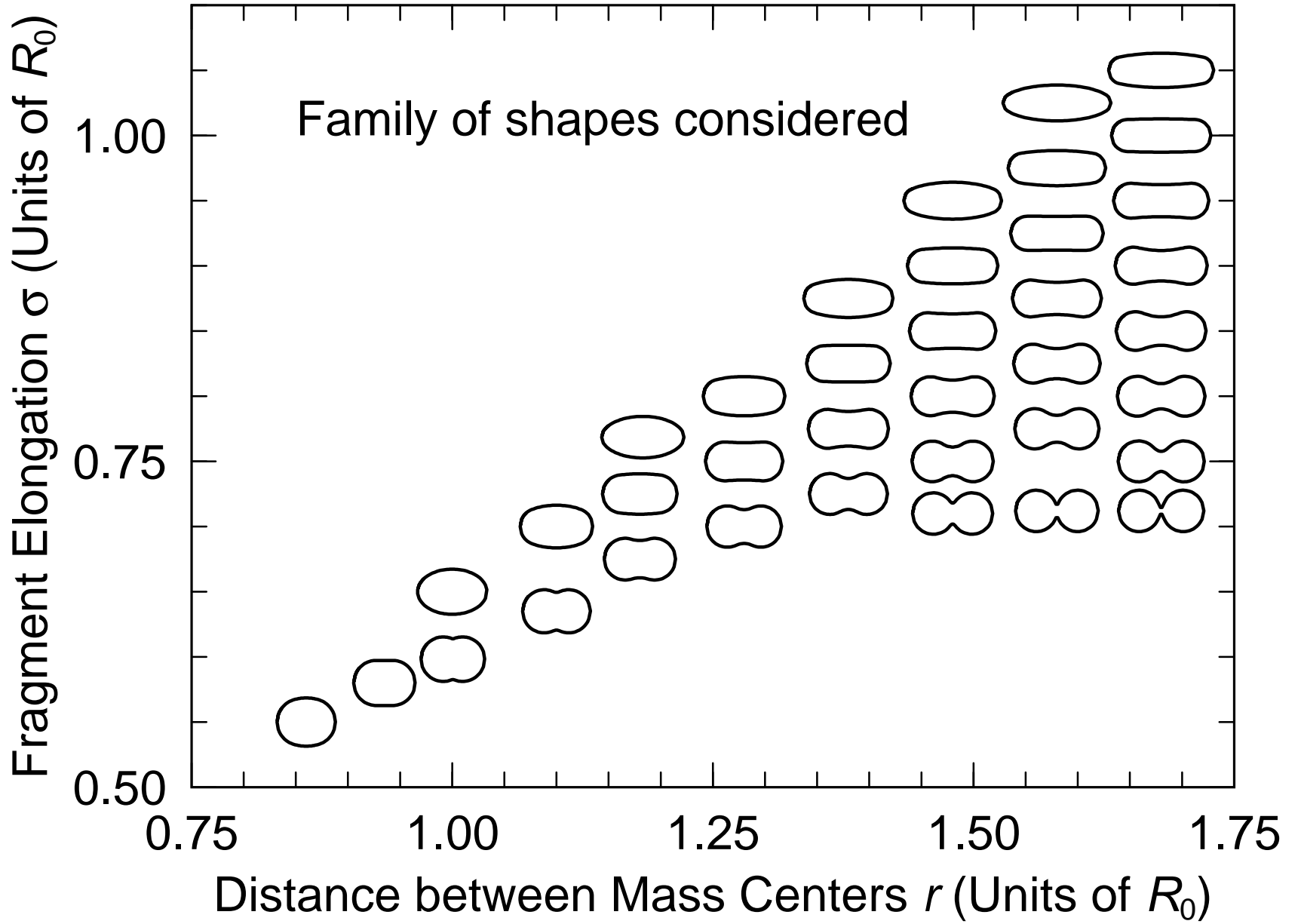
We use the macroscopic-microscopic method introduced by Swiatecki and Strutinsky:

$$E_{\text{pot}}(\text{shape}) = E_{\text{macr}}(\text{shape}) + E_{\text{micr}}(\text{shape}) \quad (1)$$

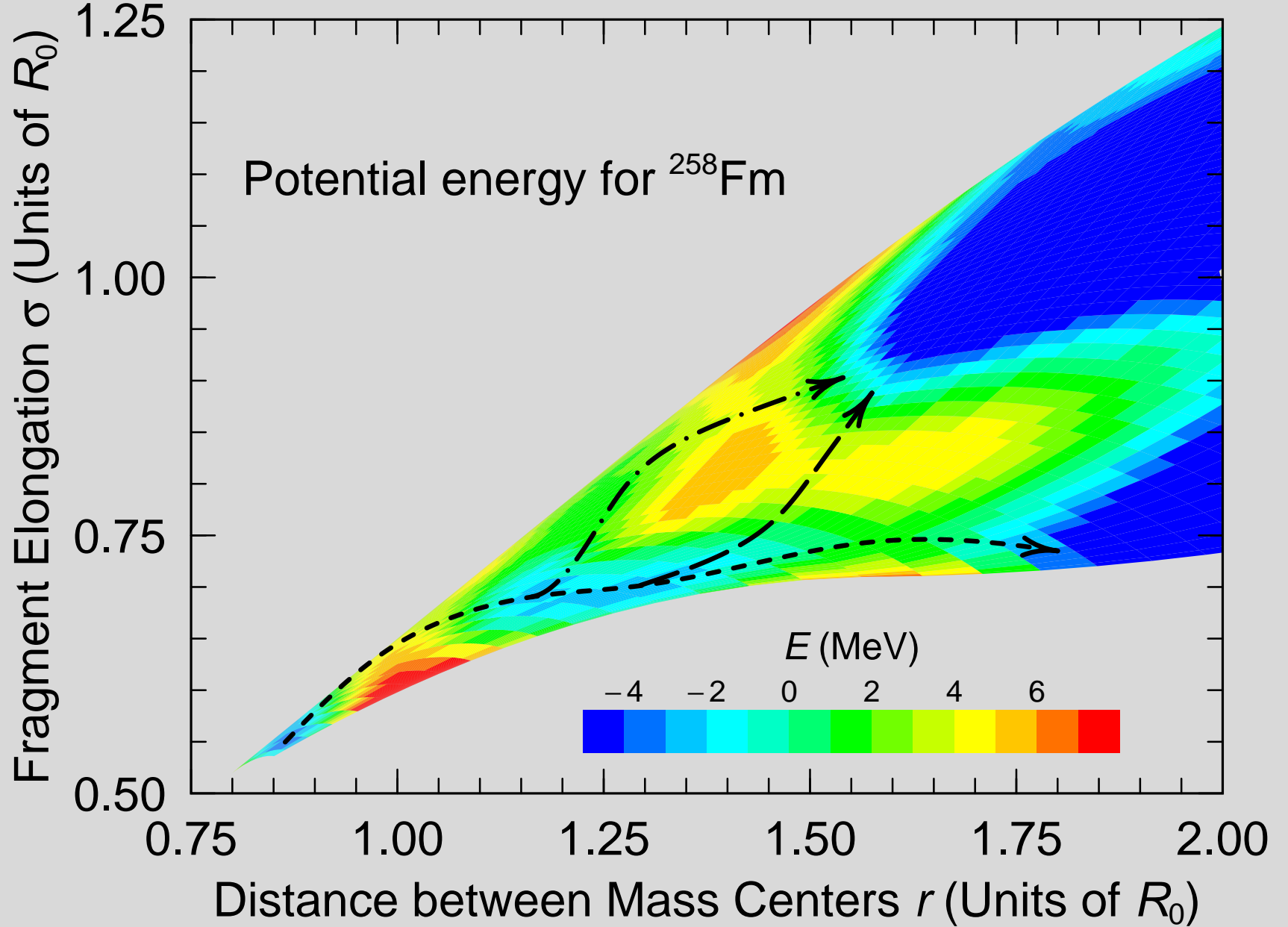
The macroscopic term is calculated in a liquid-drop type model (for a specific deformed shape).

The microscopic correction is determined in the following steps

1. A shape is prescribed
2. A single-particle potential with this shape is generated. A spin-orbit term is included.
3. The Schrödinger equation is solved for this deformed potential and single-particle levels and wave-functions are obtained
4. The shell correction is calculated by use of Strutinsky's method.
5. The pairing correction is calculated in the BCS or Lipkin-Nogami method.

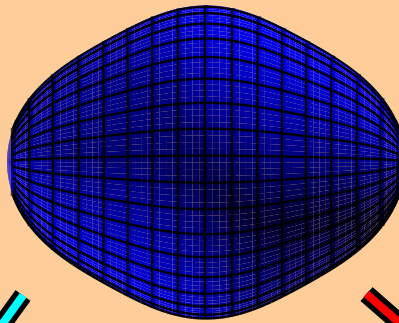


From: [Journ. Phys. G: Nucl. Part. Phys. 20 \(1994\) 1681](#)

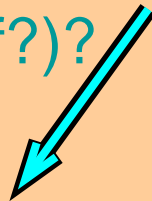


In fission, what are the shapes and related energies involved in the transition from a single ground-state shape to two separated fission fragments?

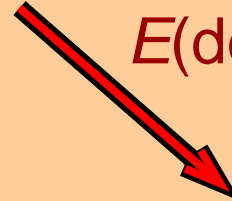
$^{234}\text{U}$



$E(\text{def?})?$



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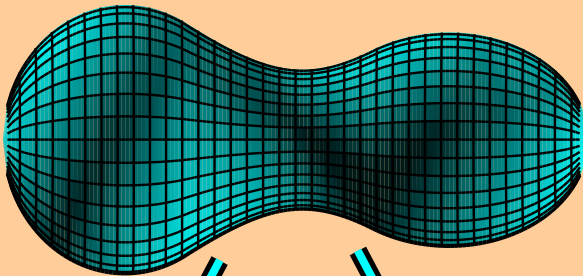


$^{234}\text{U}$  : Asymmetric valley at  $Q_2 = 76$

$\epsilon_{f1} = -0.1000$   $\epsilon_{f2} = 0.2500$   $M_H/M_L = 135.7/98.3$

$^{234}\text{U}$  : Symmetric valley at  $Q_2 = 76$

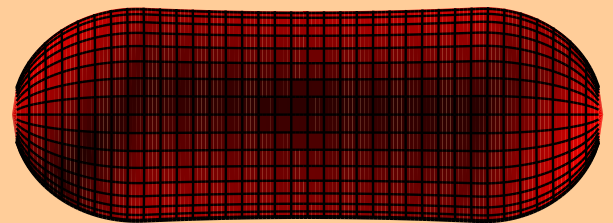
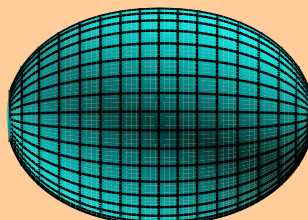
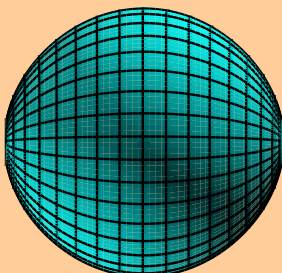
$\epsilon_{f1} = 0.1500$   $\epsilon_{f2} = 0.1000$   $M_H/M_L = 119.3/114.7$



$^{136}\text{I}$



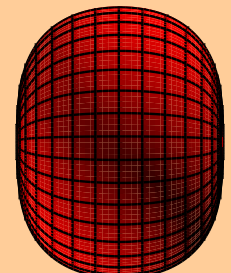
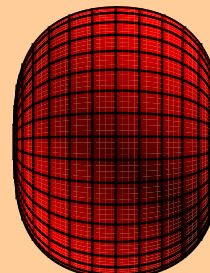
$^{98}\text{Y}$



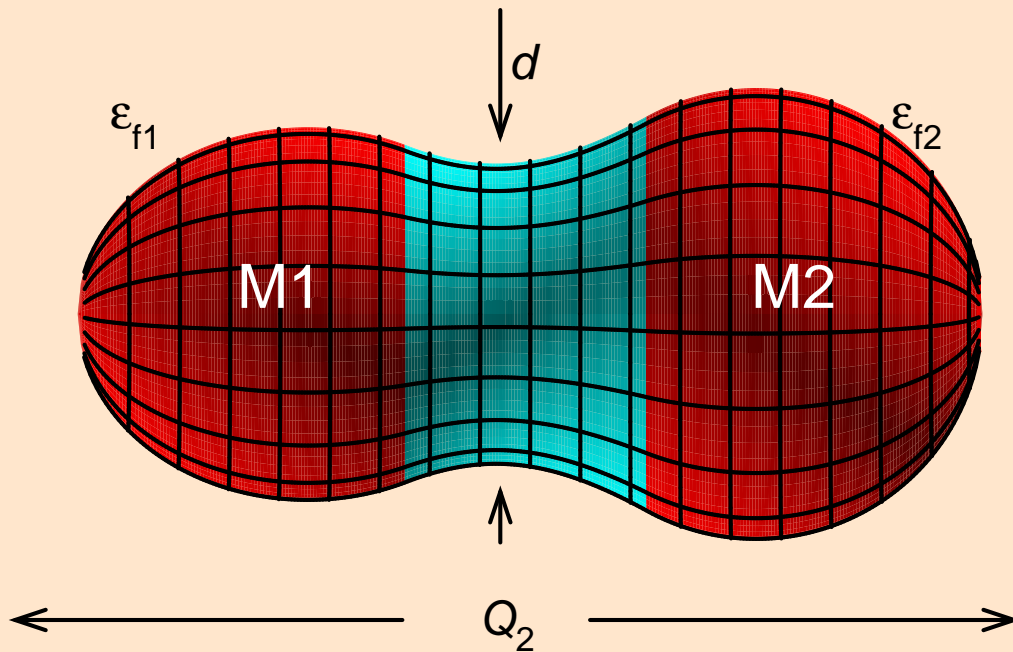
$^{117}\text{Pd}$



$^{117}\text{Pd}$



## Five Essential Fission Shape Coordinates

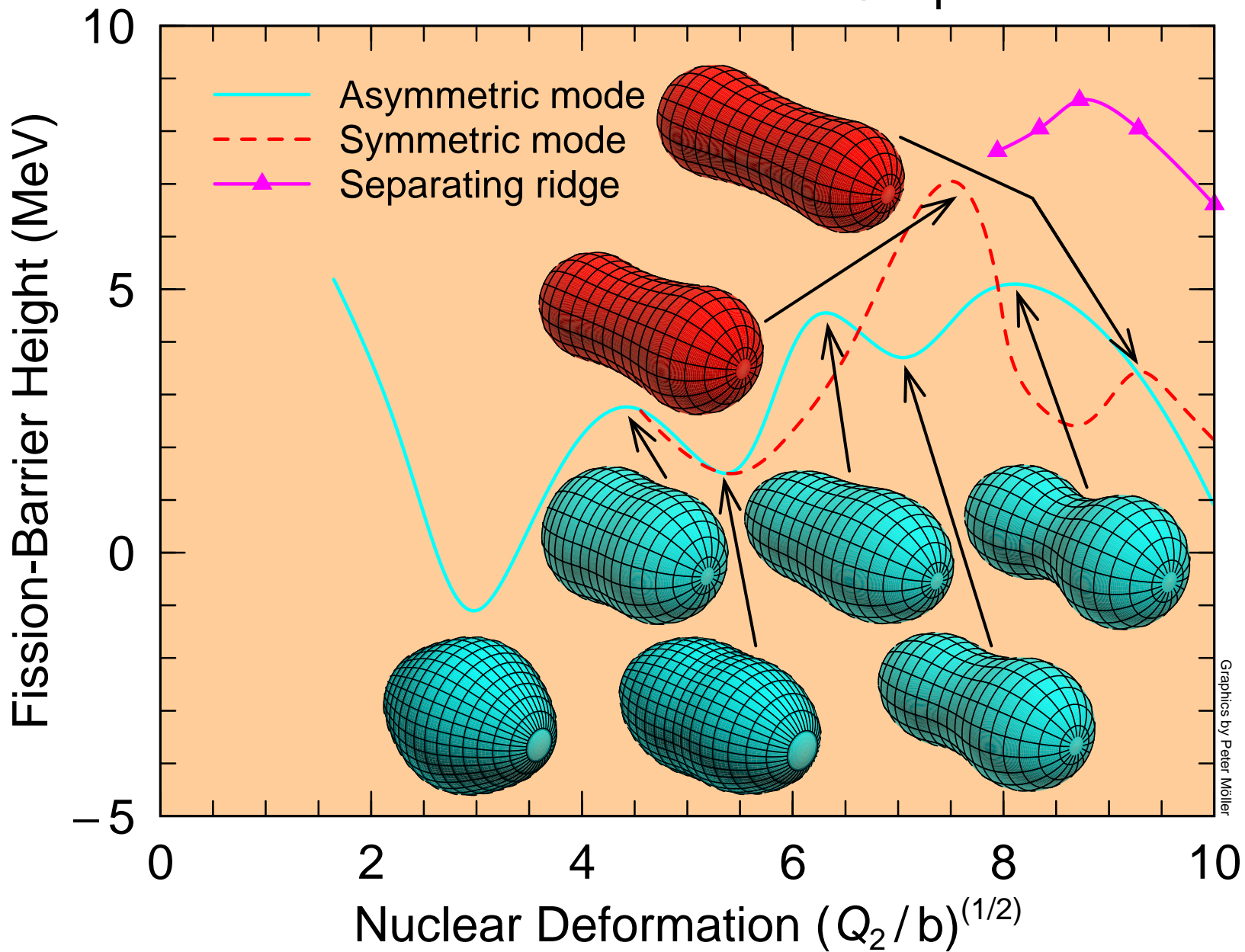


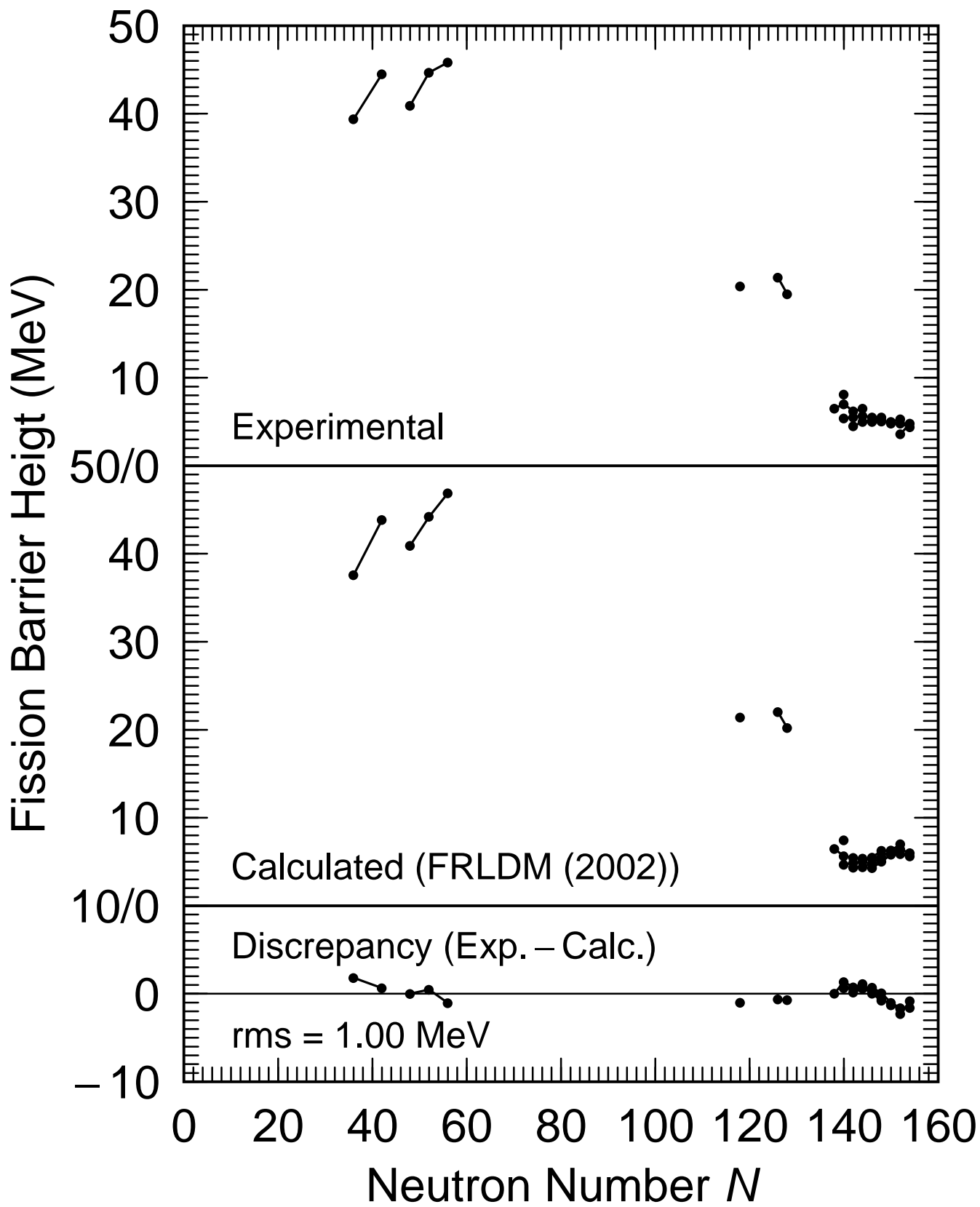
45	$Q_2$ ~ Elongation (fission direction)
⊗	
15	$d$ ~ Neck
⊗	
15	$\epsilon_{f1}$ ~ Left fragment deformation
⊗	
15	$\epsilon_{f2}$ ~ Right fragment deformation
⊗	
35	$\alpha_g$ ~ $(M1-M2)/(M1+M2)$ Mass asymmetry

⇒ 5 315 625 grid points – 306 300 unphysical points

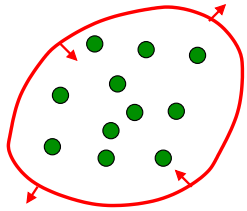
⇒ **5 009 325 physical grid points**

# Fission Barrier and Associated Shapes for $^{232}\text{Th}$









## Brownian shape motion

Nuclear deformation energy:  $E_{\text{def}}(i,j,k,l,m)$

Bias potential:  $V_{\text{bias}}(i) = V_0 (Q_0/Q_2)^2$

Level density parameter:  $a_A = A/(8 \text{ MeV})$

Temperature  $T$ :  $E^* - E_{\text{def}} = a_A T^2$

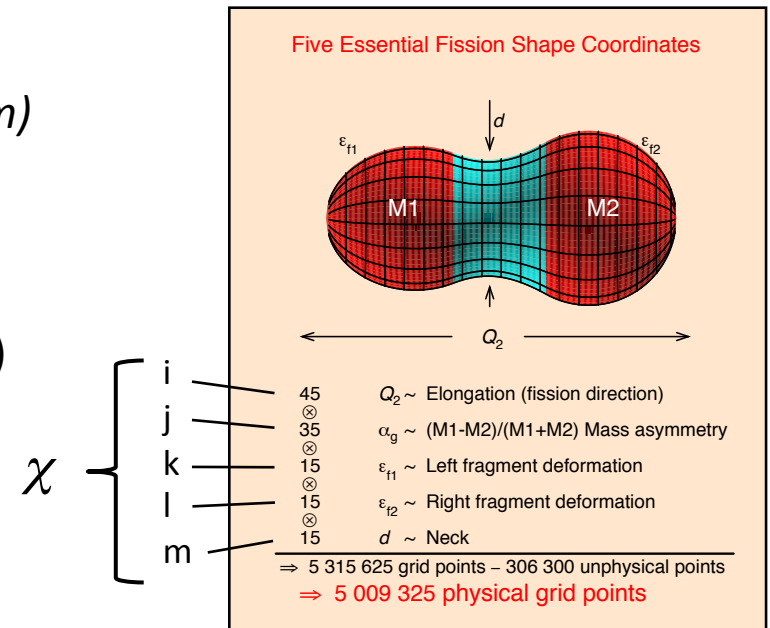
$$\Rightarrow V(\chi) = E_{\text{def}} + V_{\text{bias}}$$

Metropolis walk:

Change shape:  $\chi \rightarrow \chi'$  ?

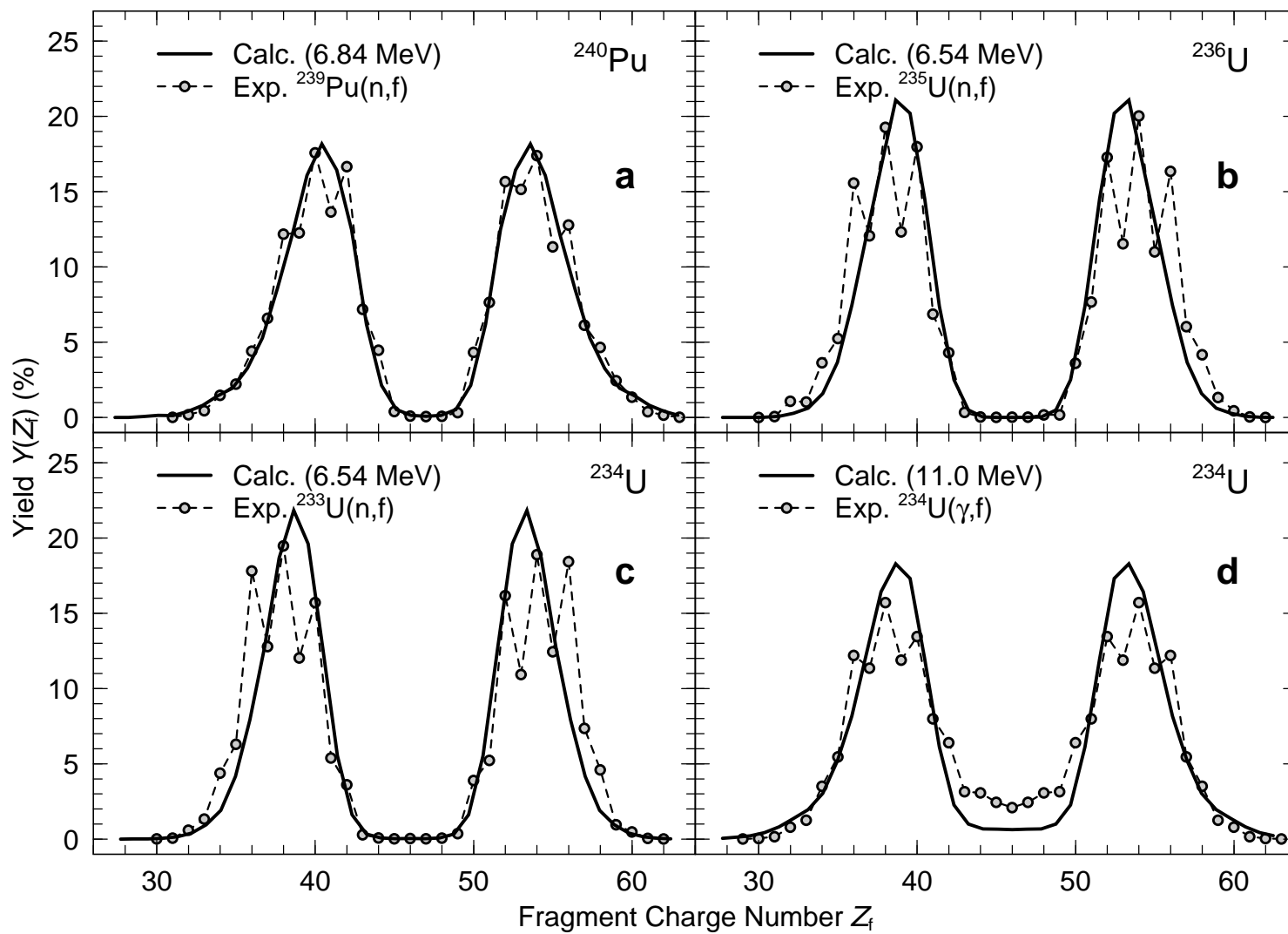
$$\begin{cases} V(\chi') < V(\chi): \text{ move with } P = 1 \\ V(\chi') > V(\chi): \text{ move with } P = \exp(-\Delta V/T) \end{cases}$$

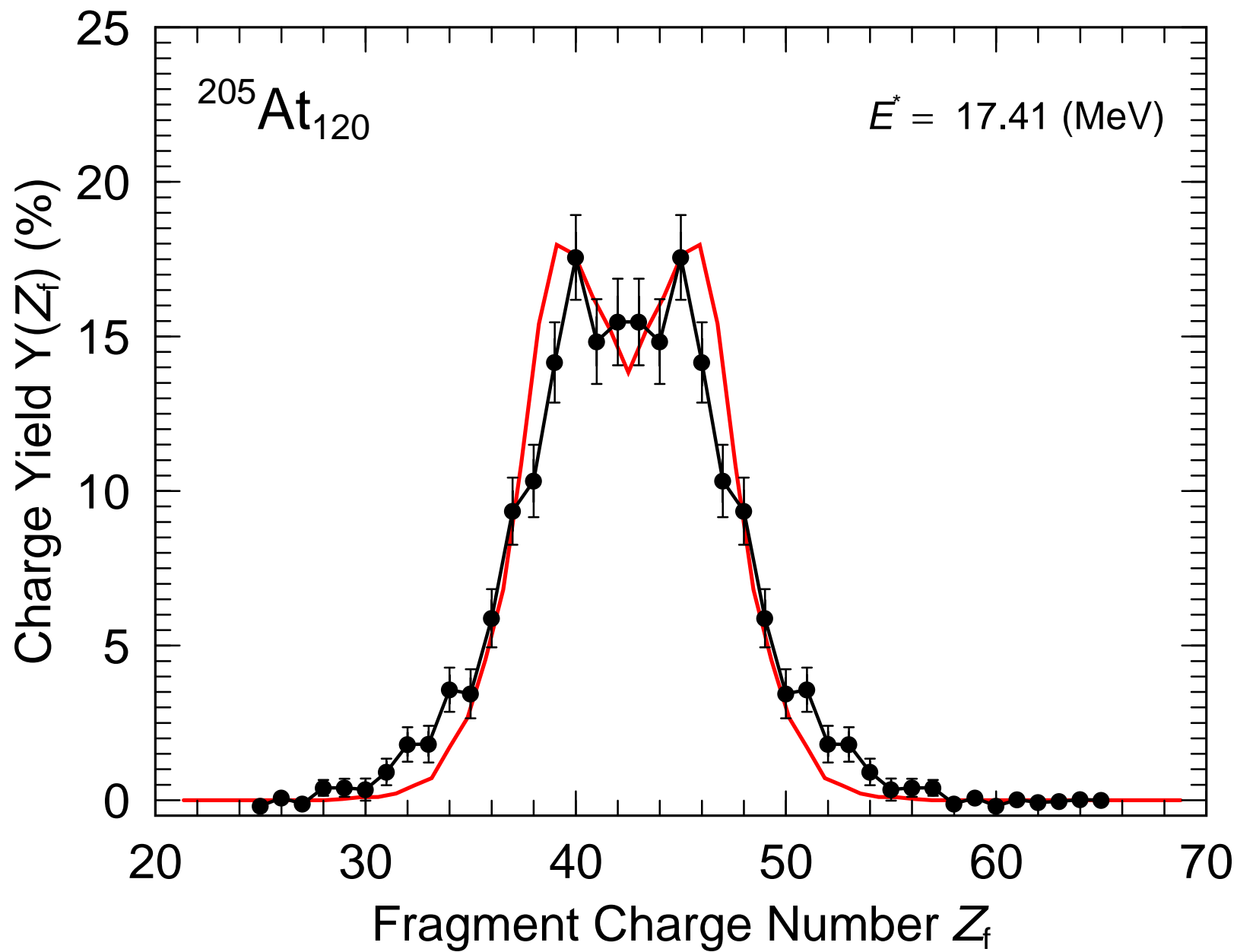
Scission: Critical neck radius  $c_0 \approx 2.5 \text{ fm}$

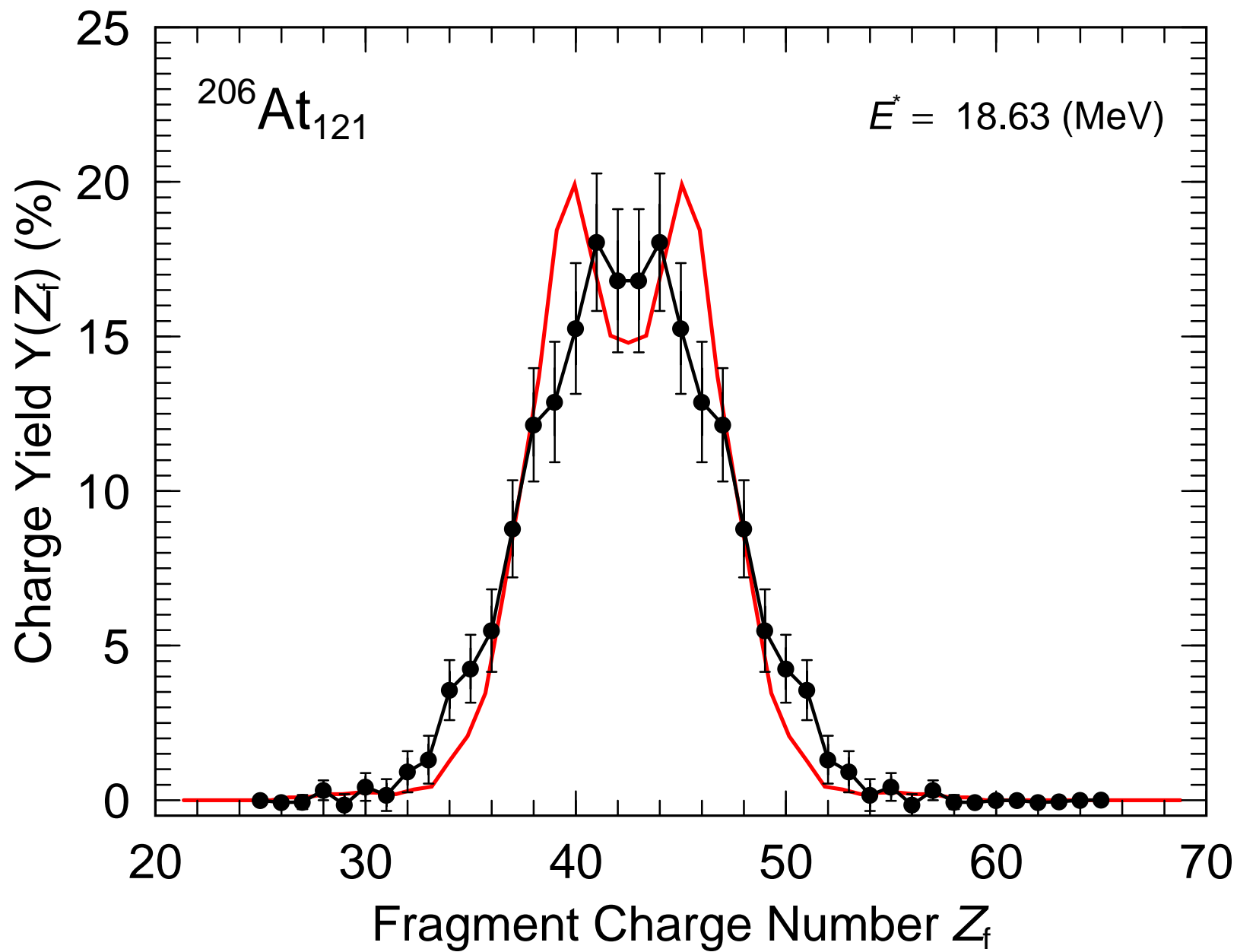


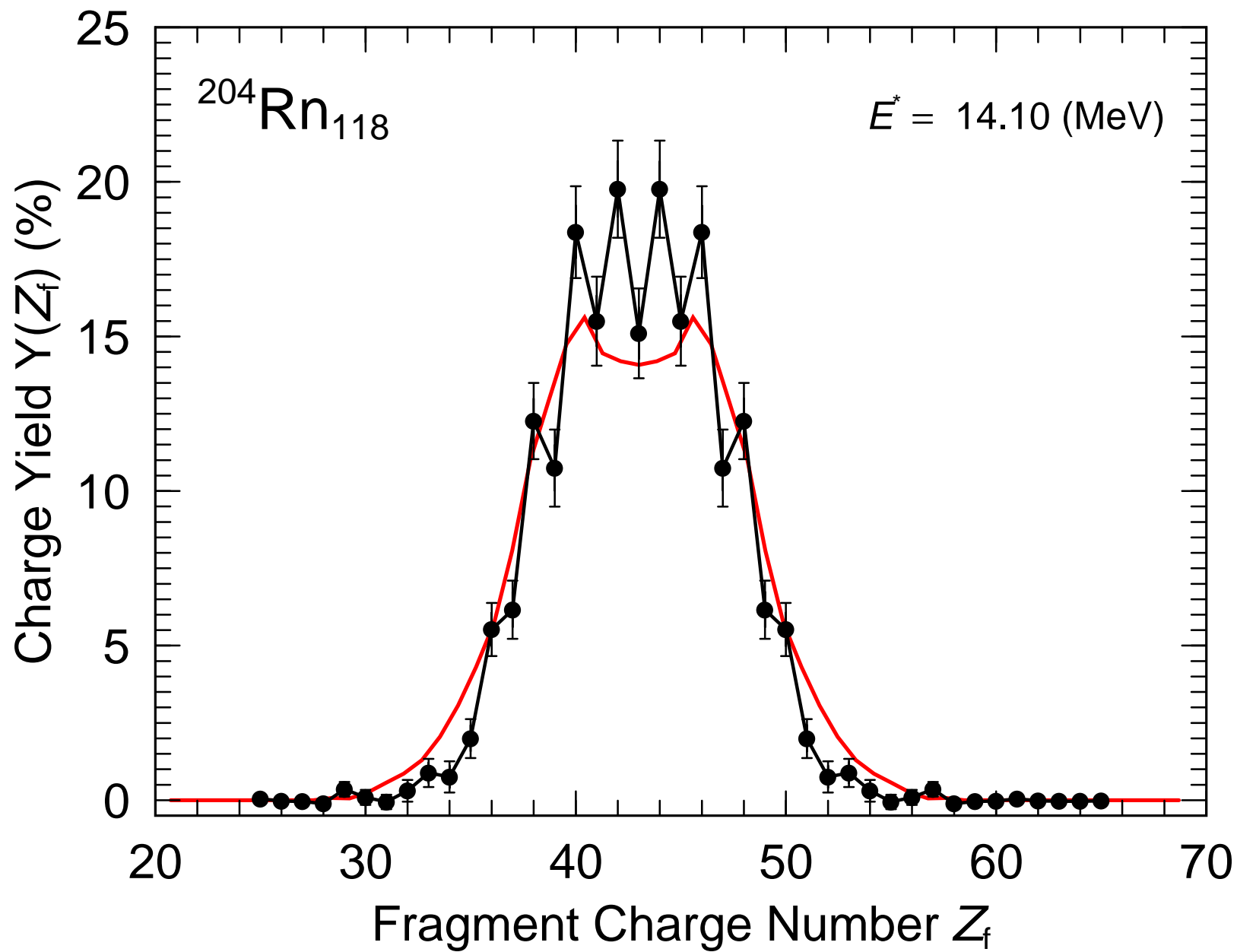
P. Möller *et al*, Nature 409 (2001) 785

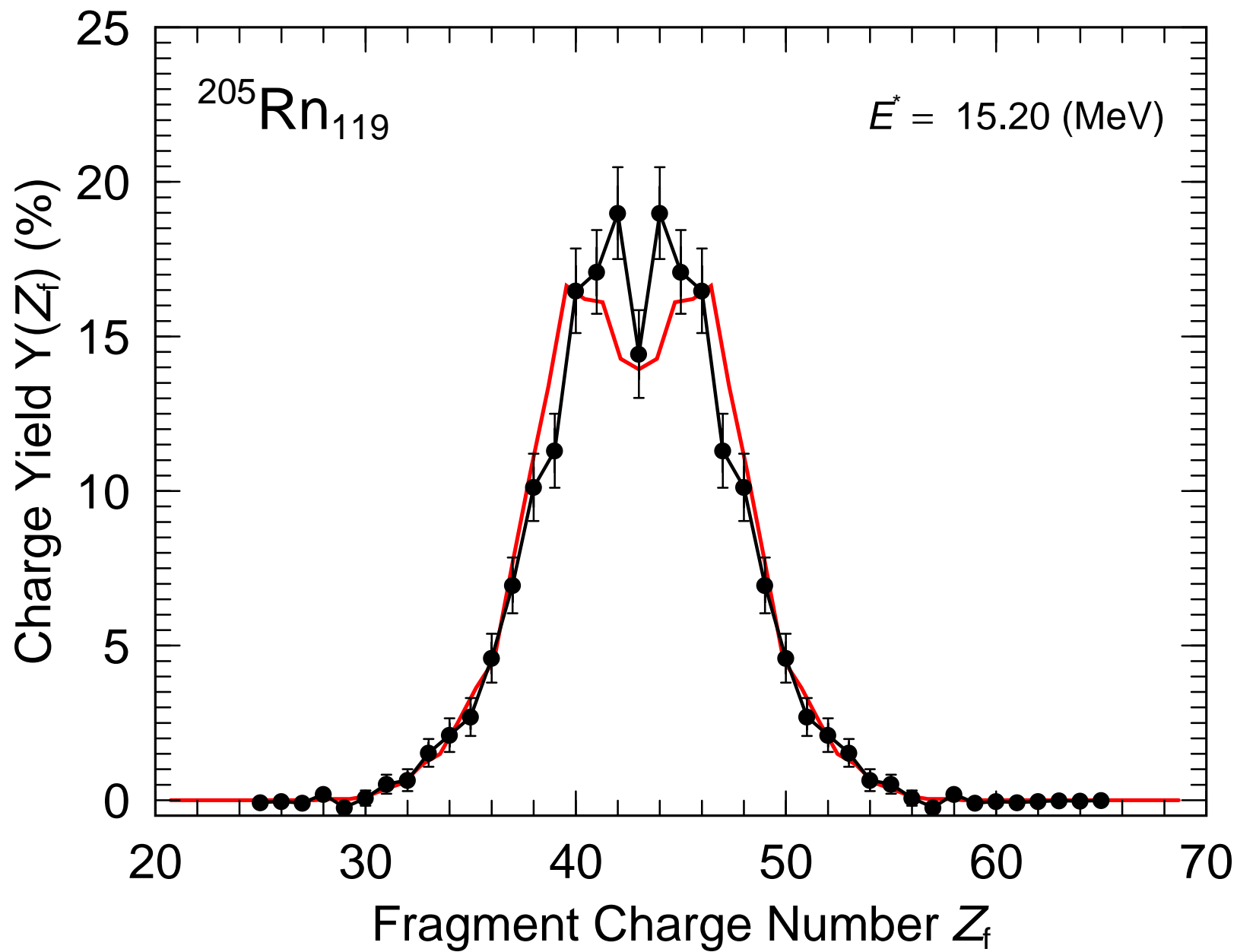
N. Metropolis *et al*, J Chem Phys 26 (1953) 1087

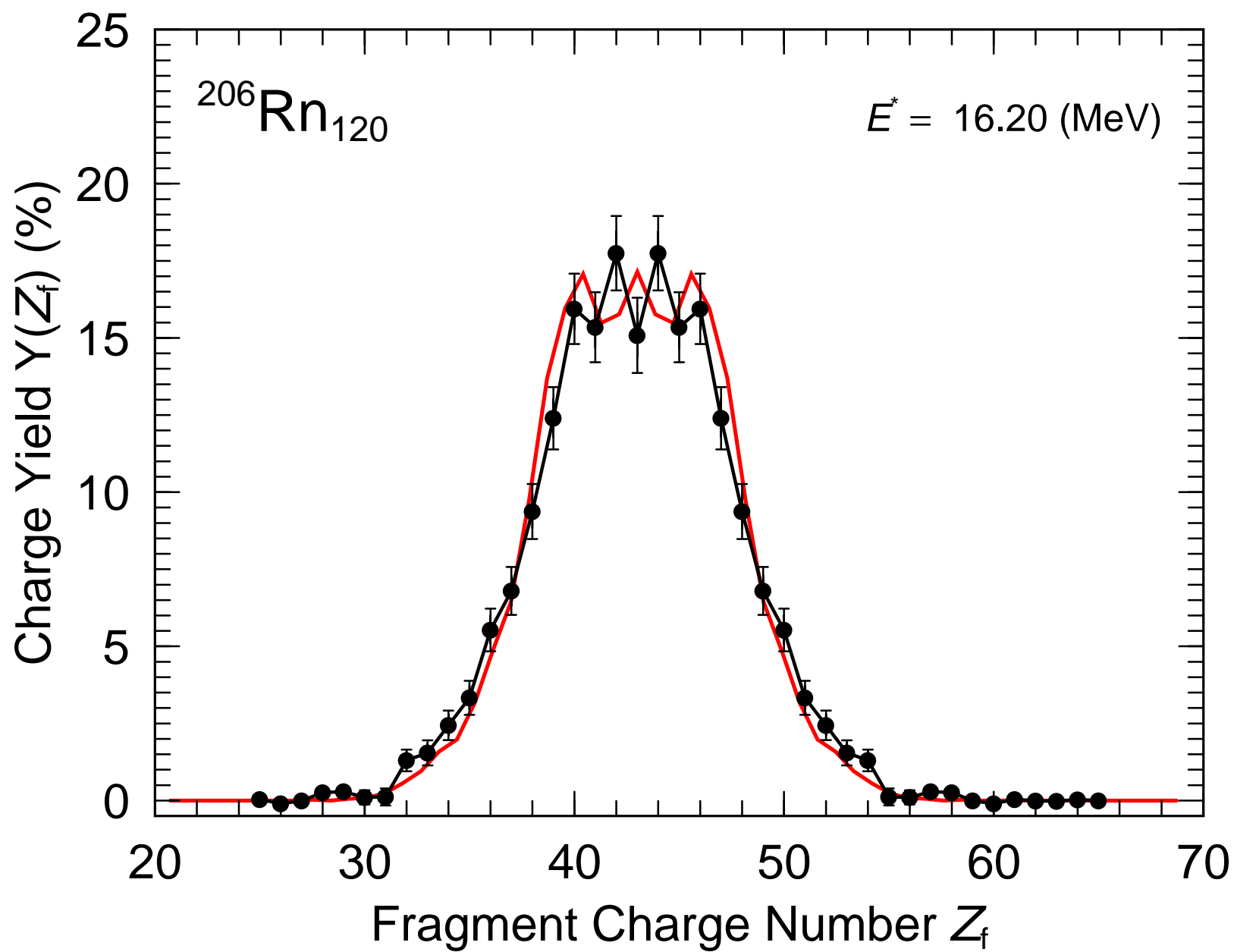


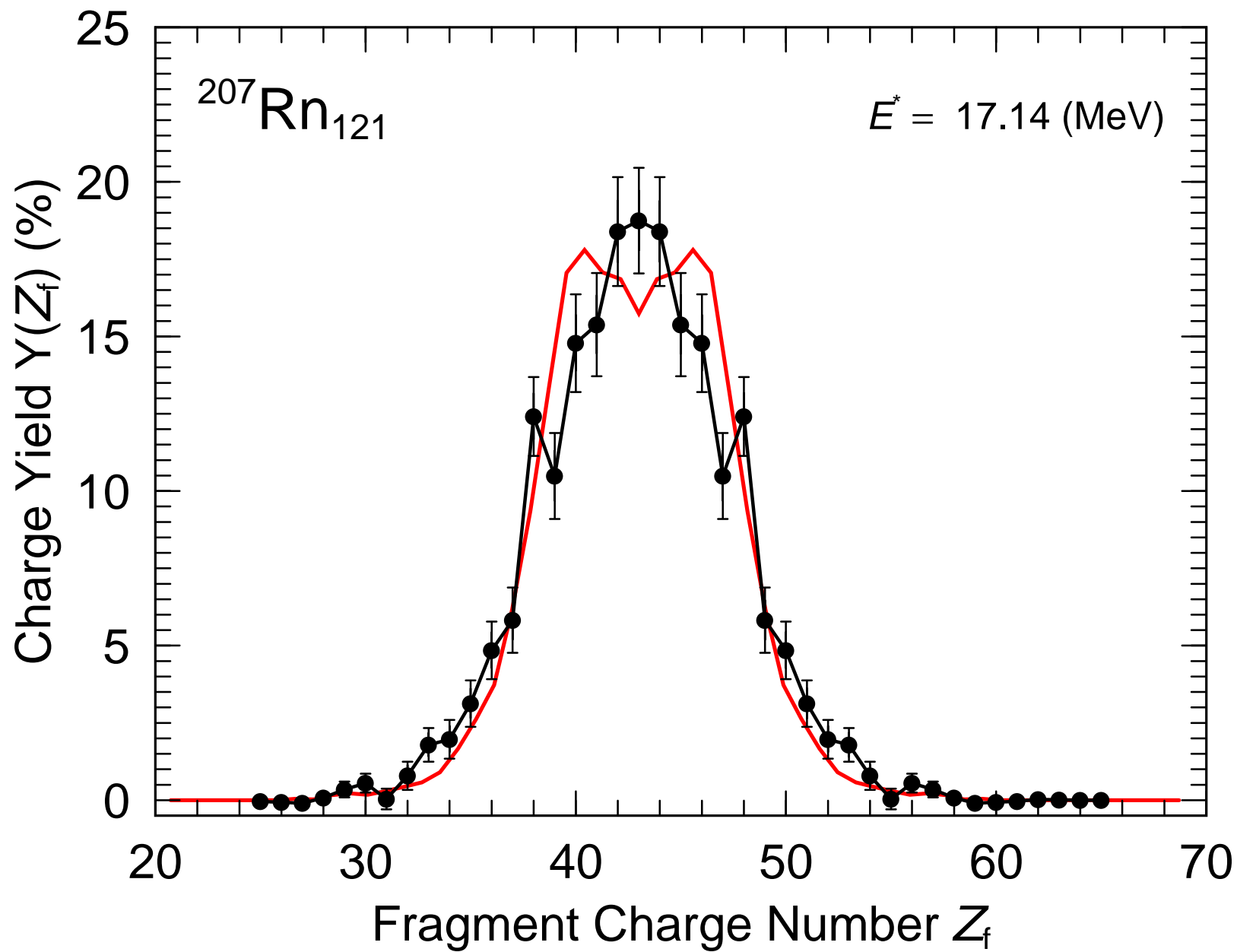




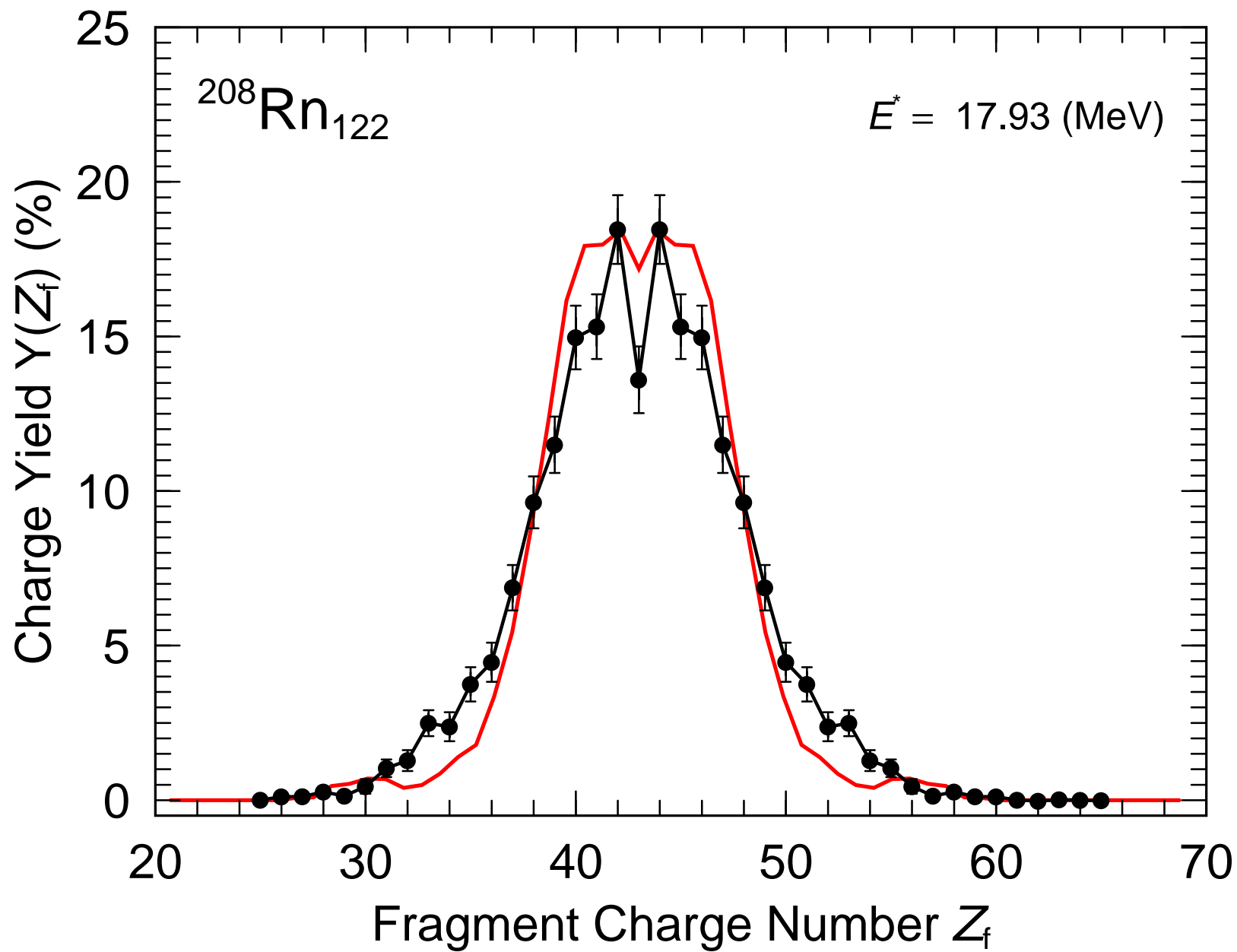


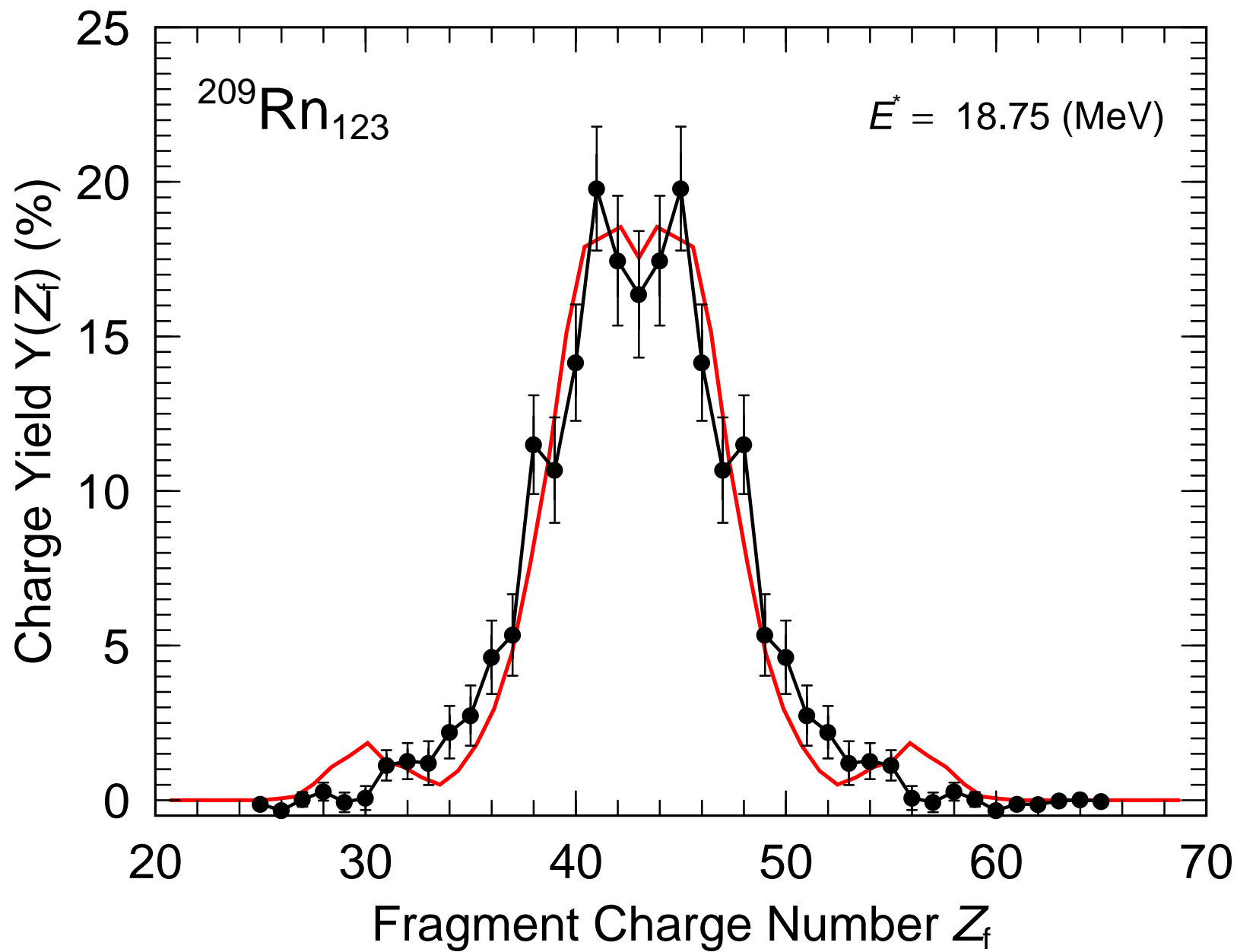


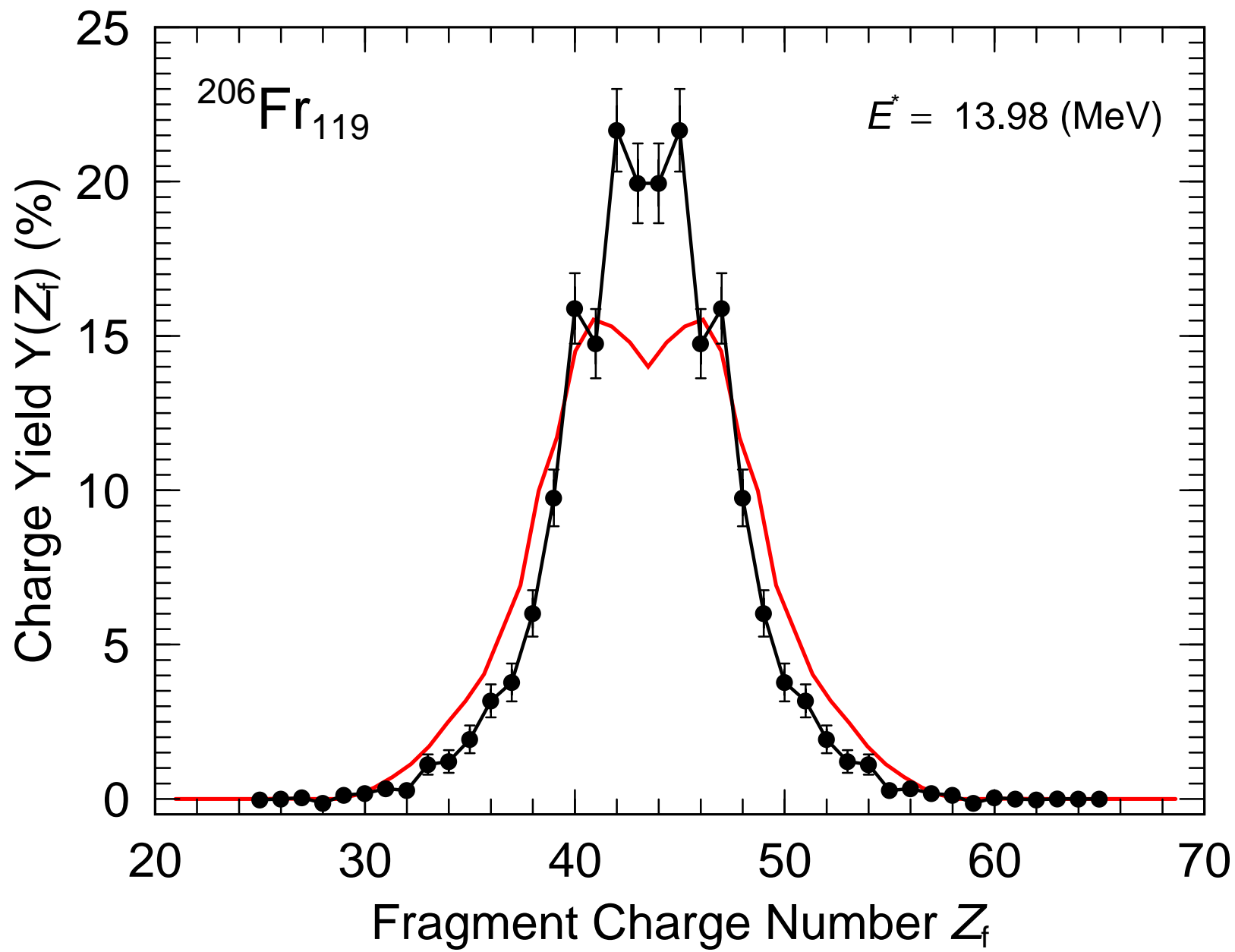


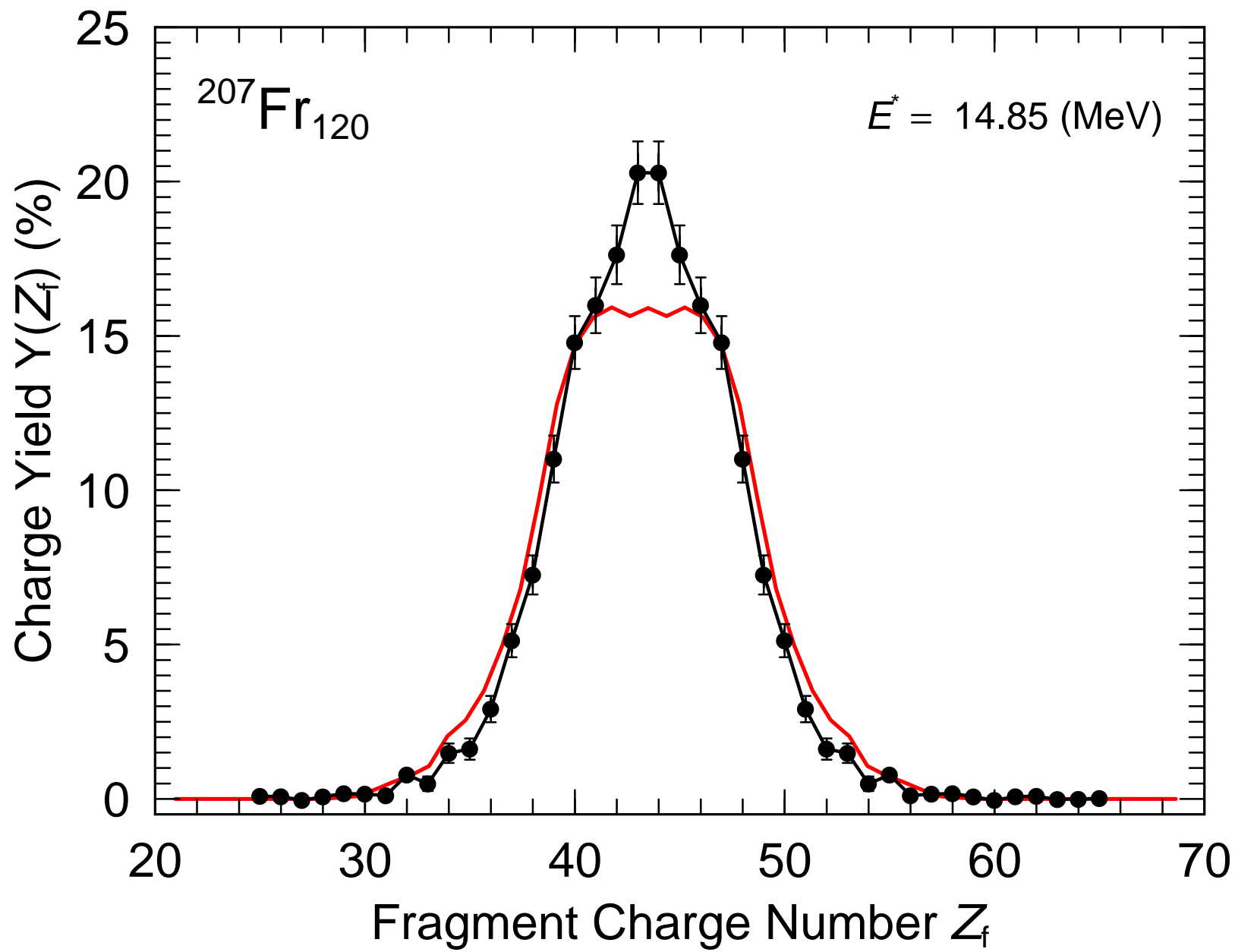


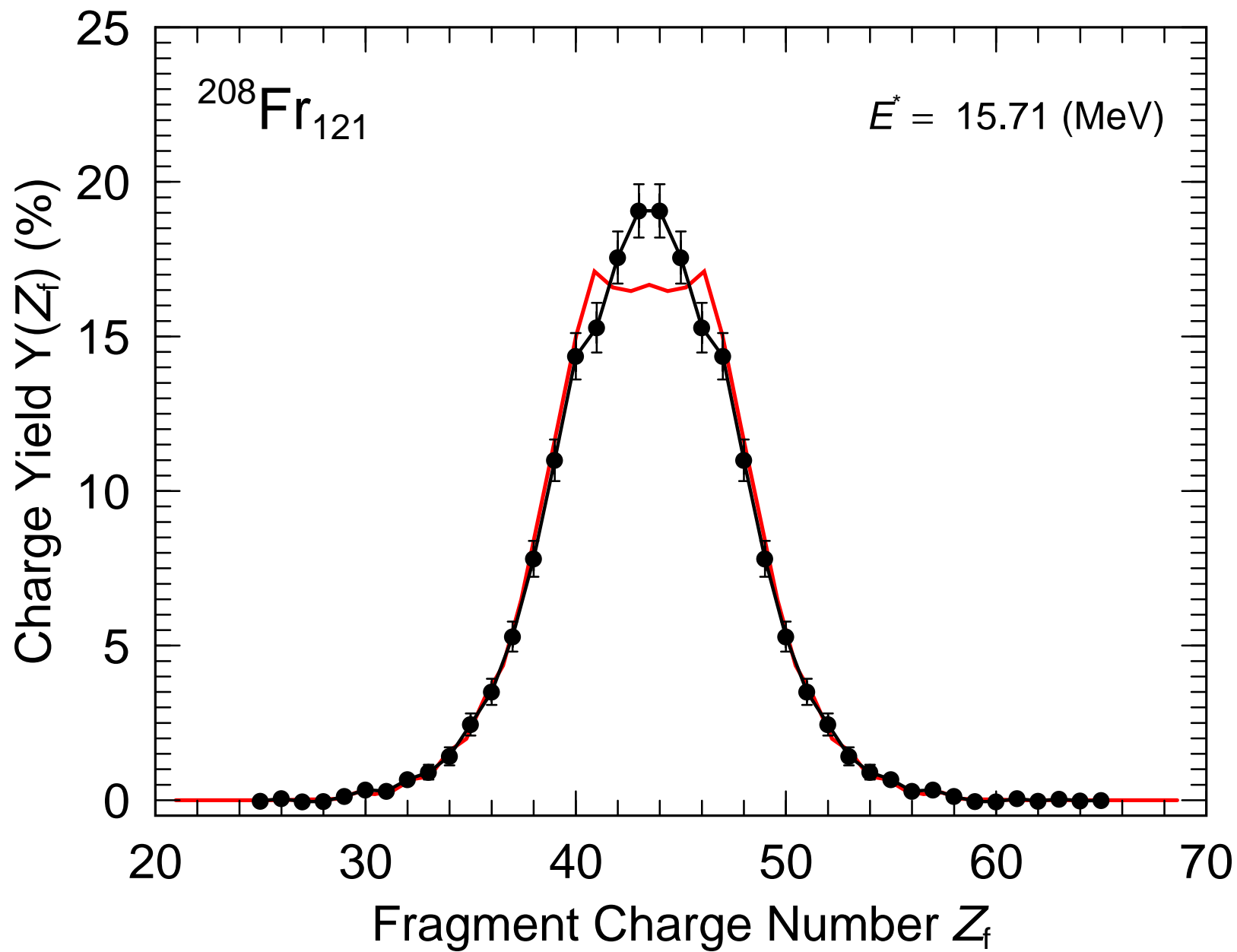


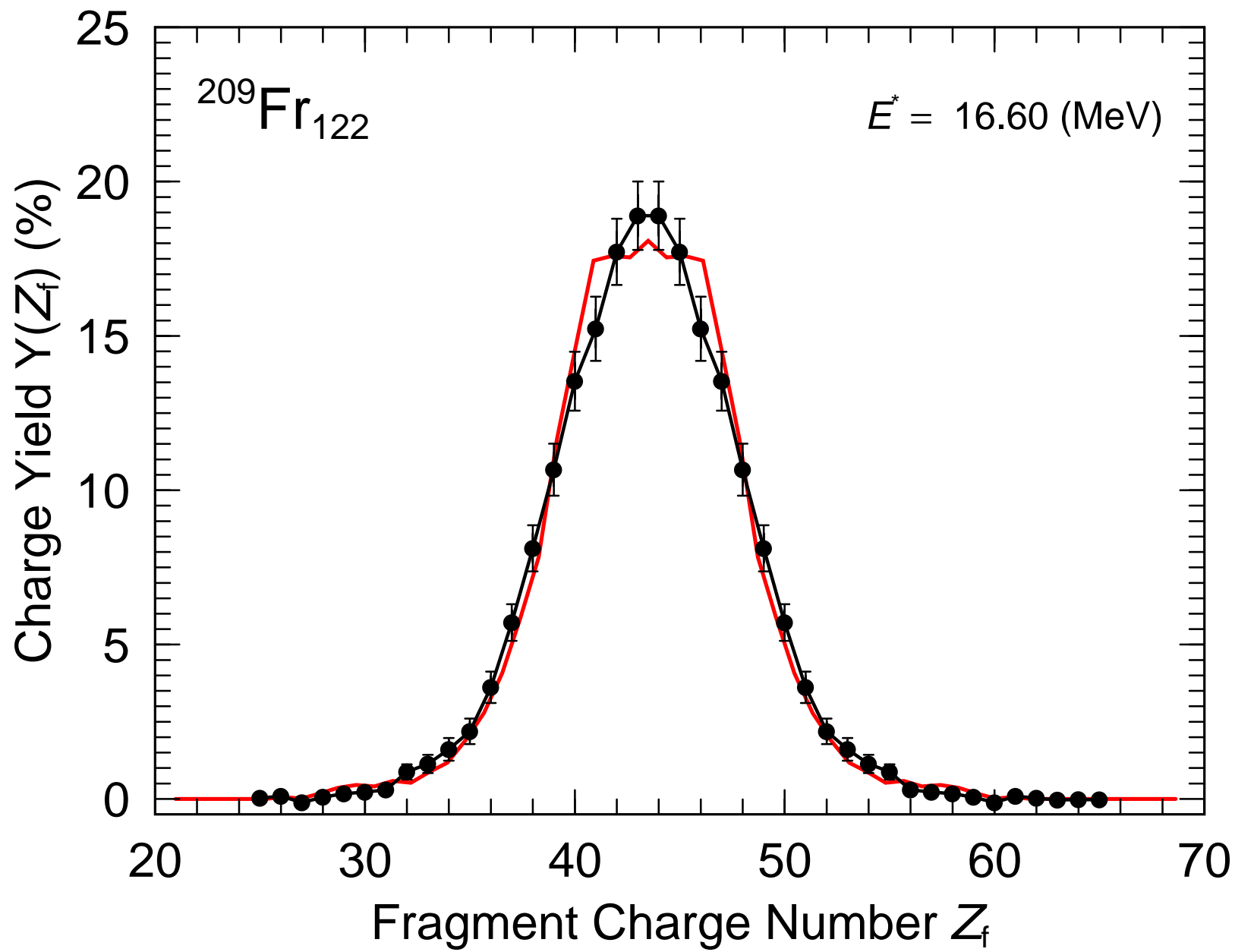


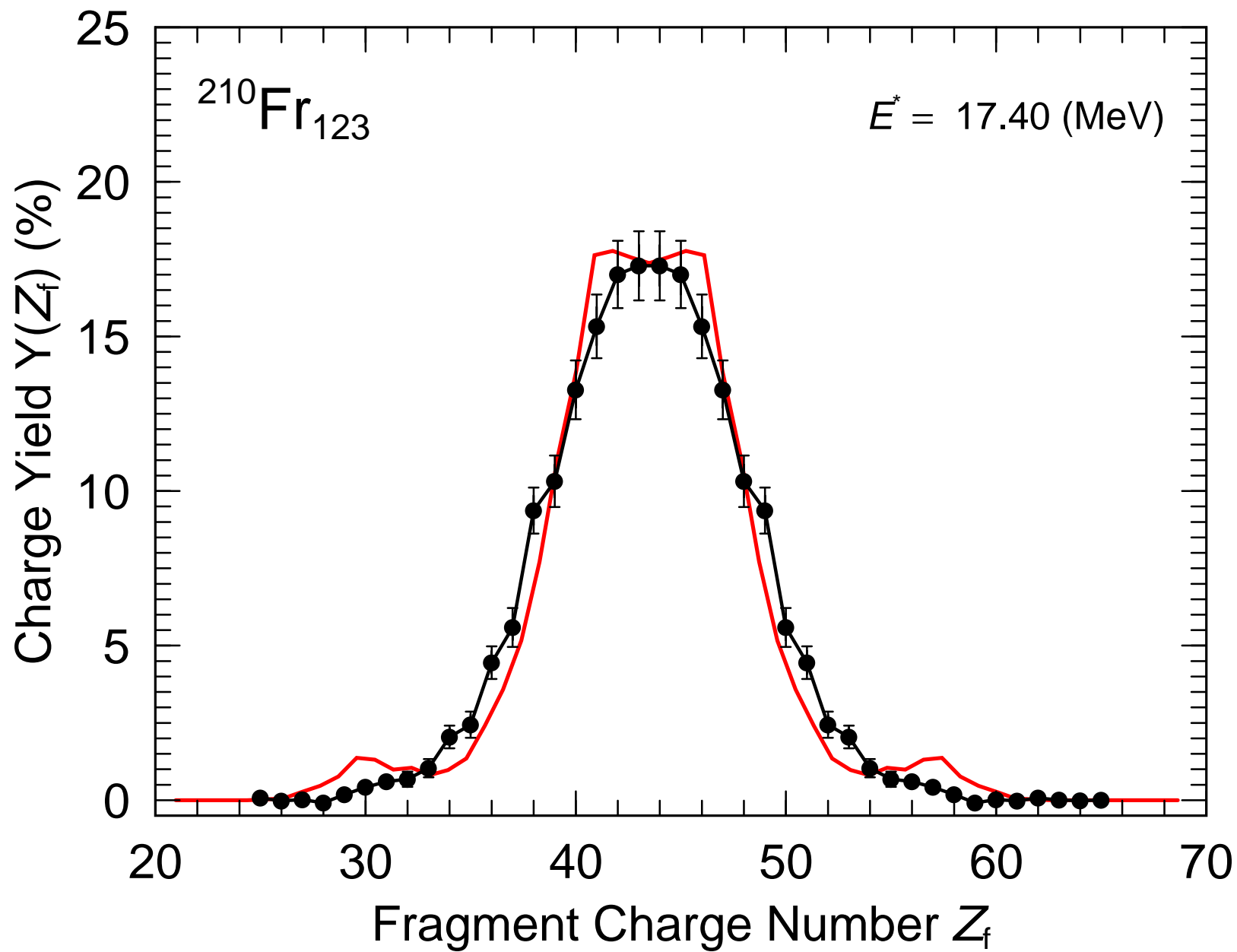


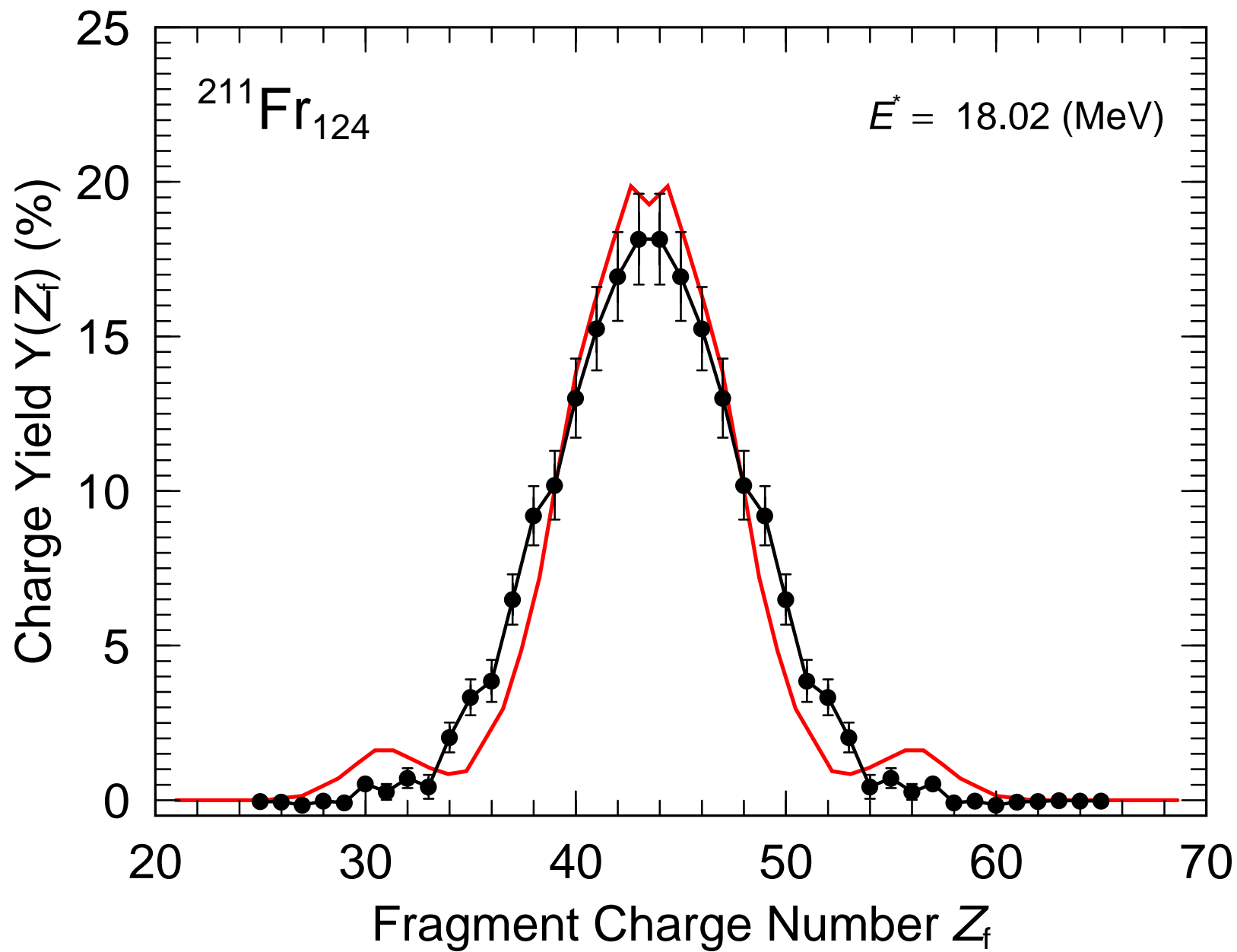




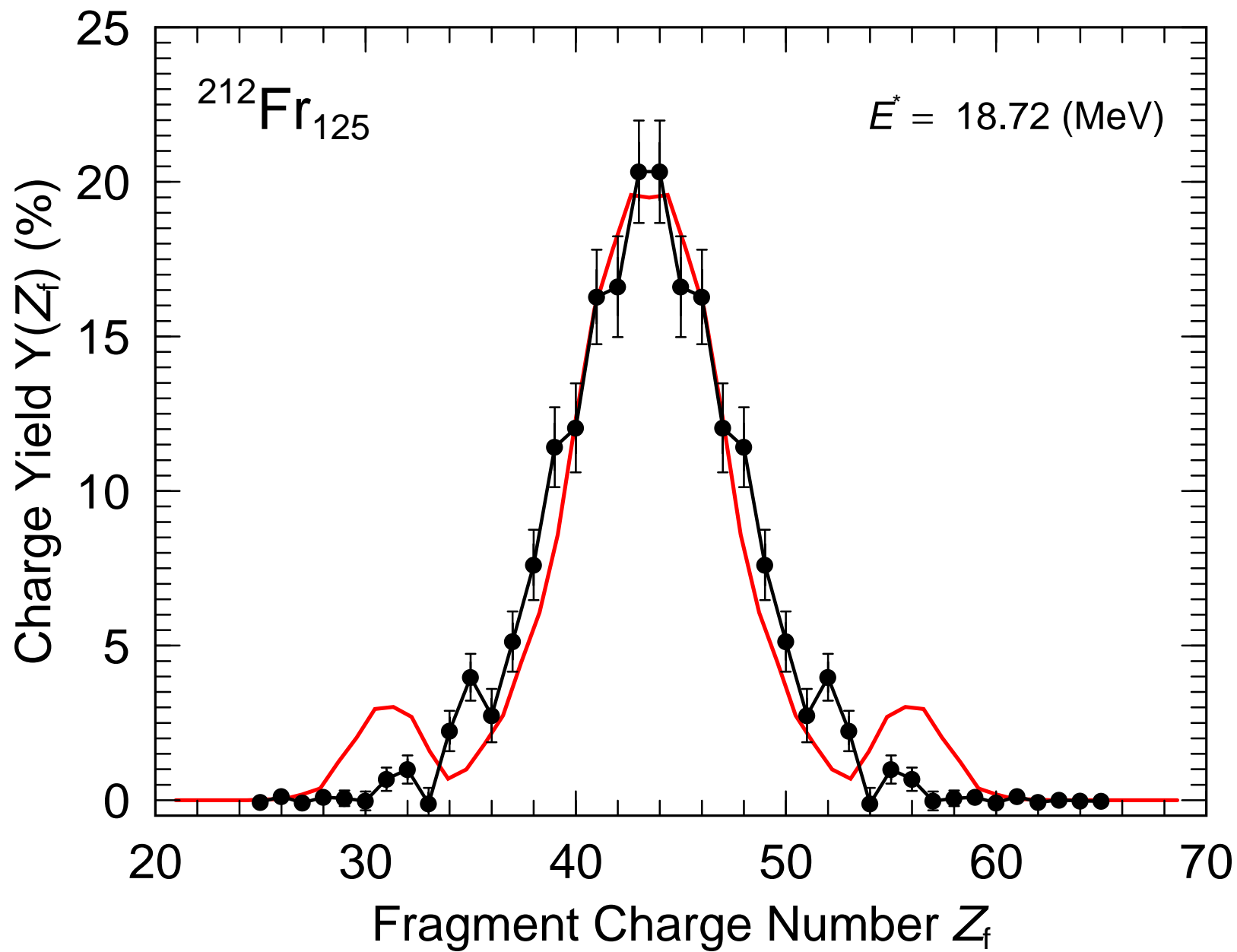


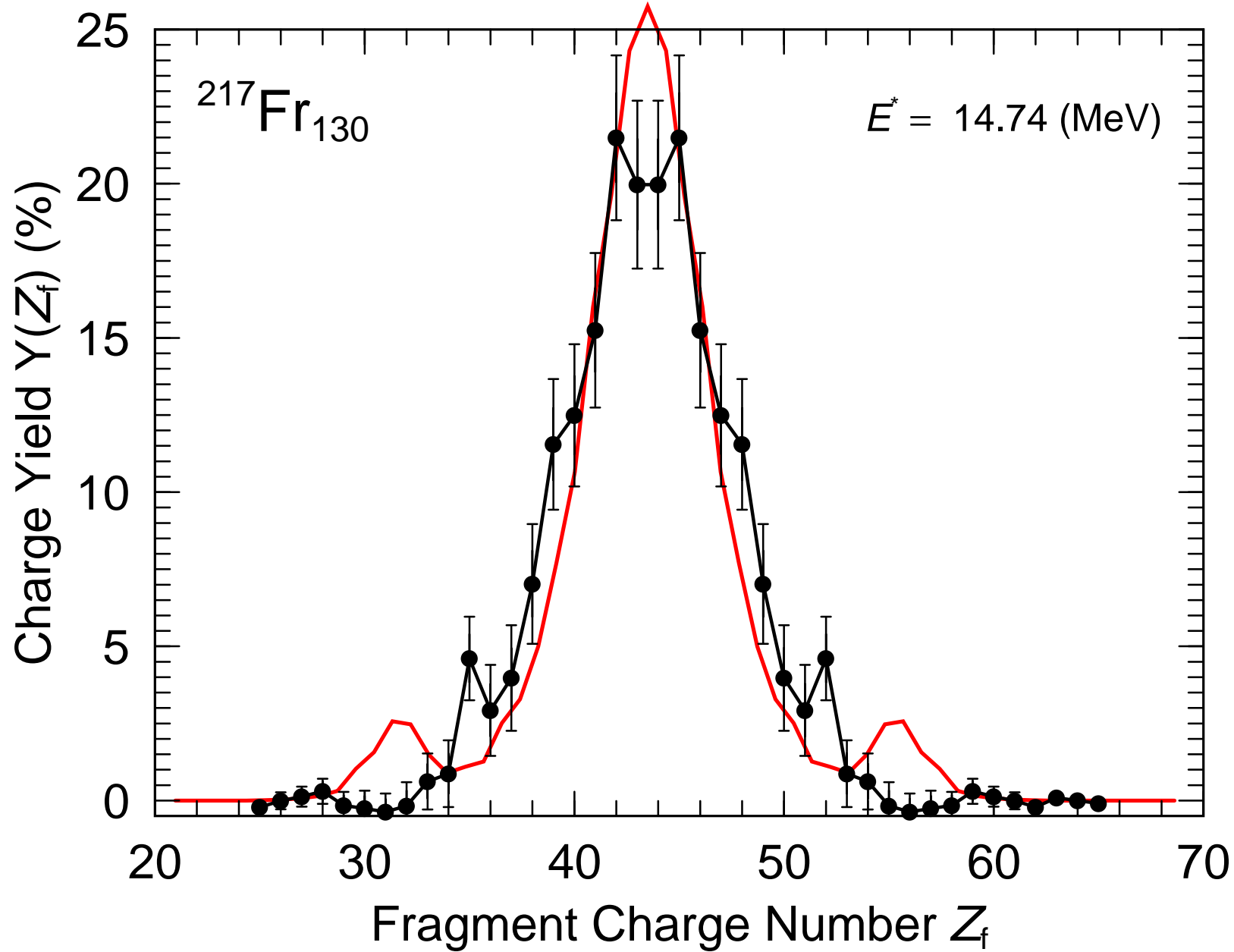


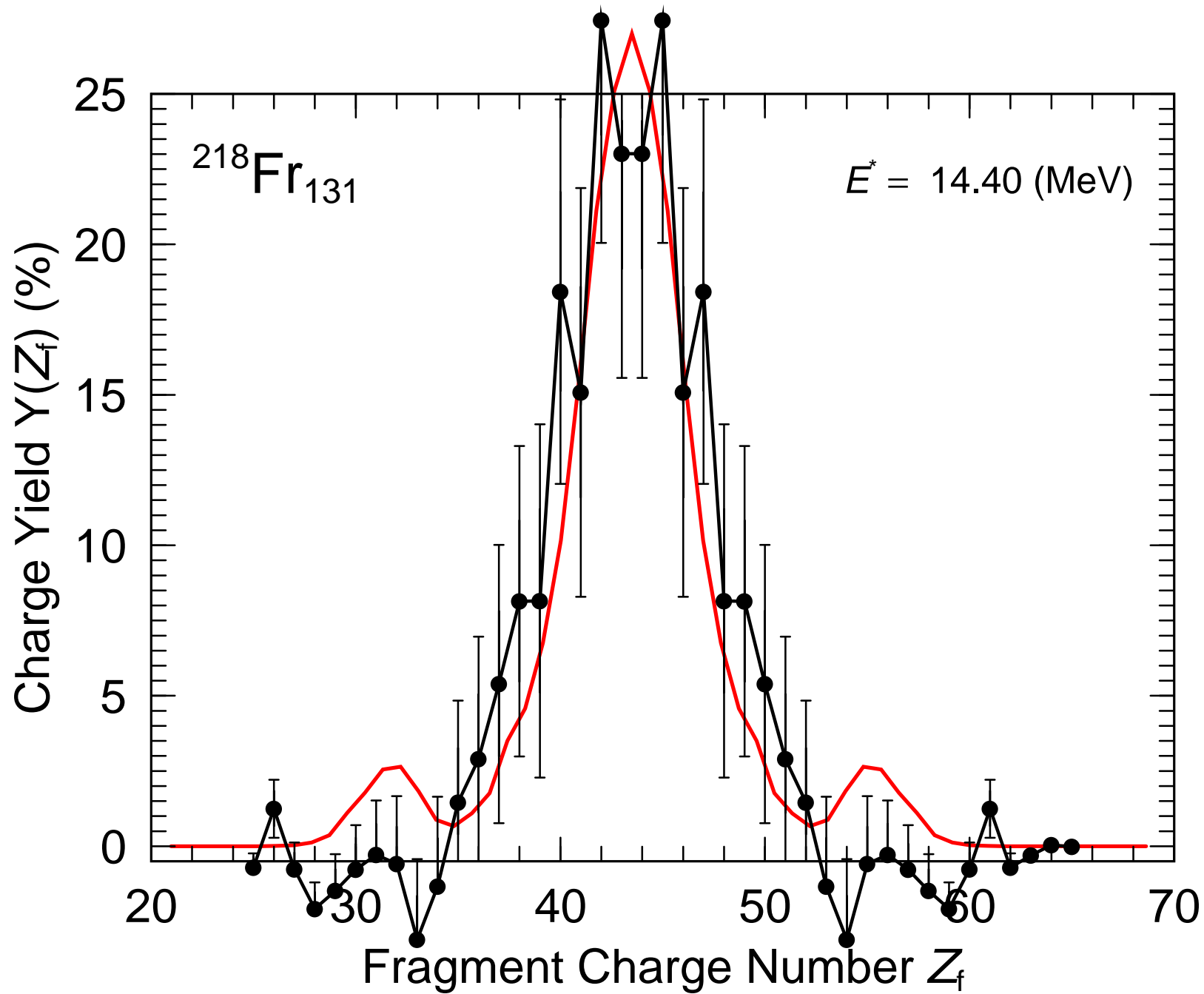


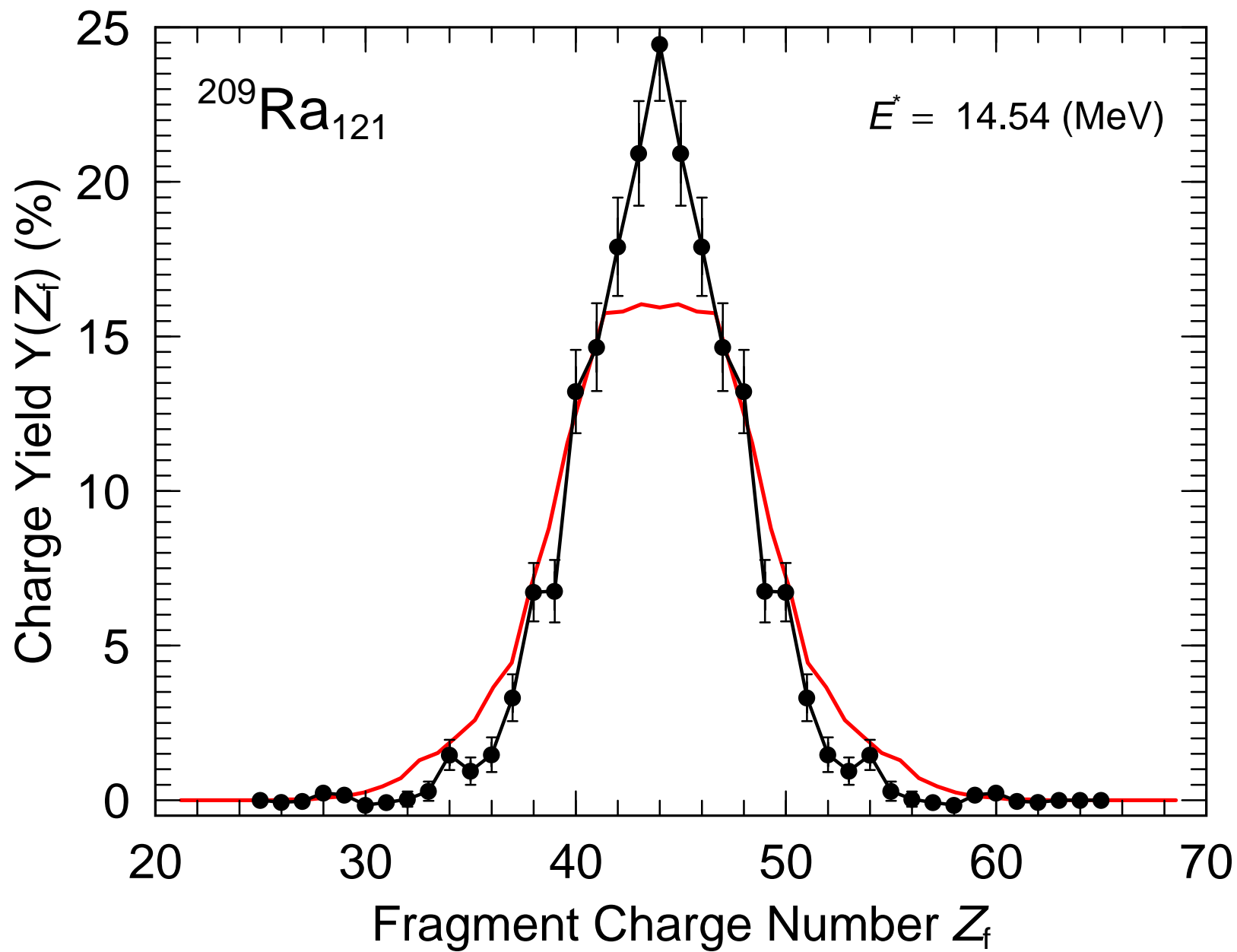


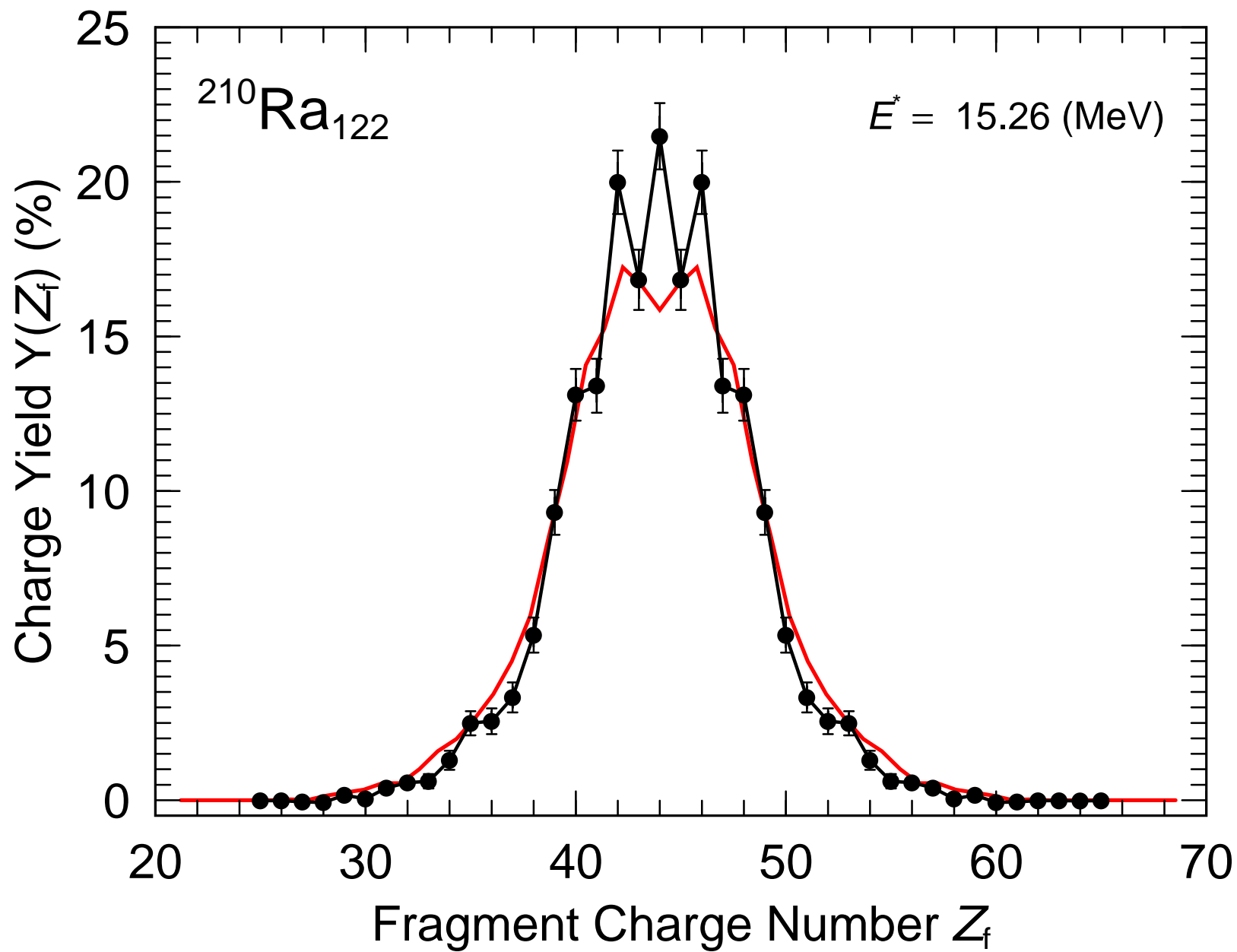


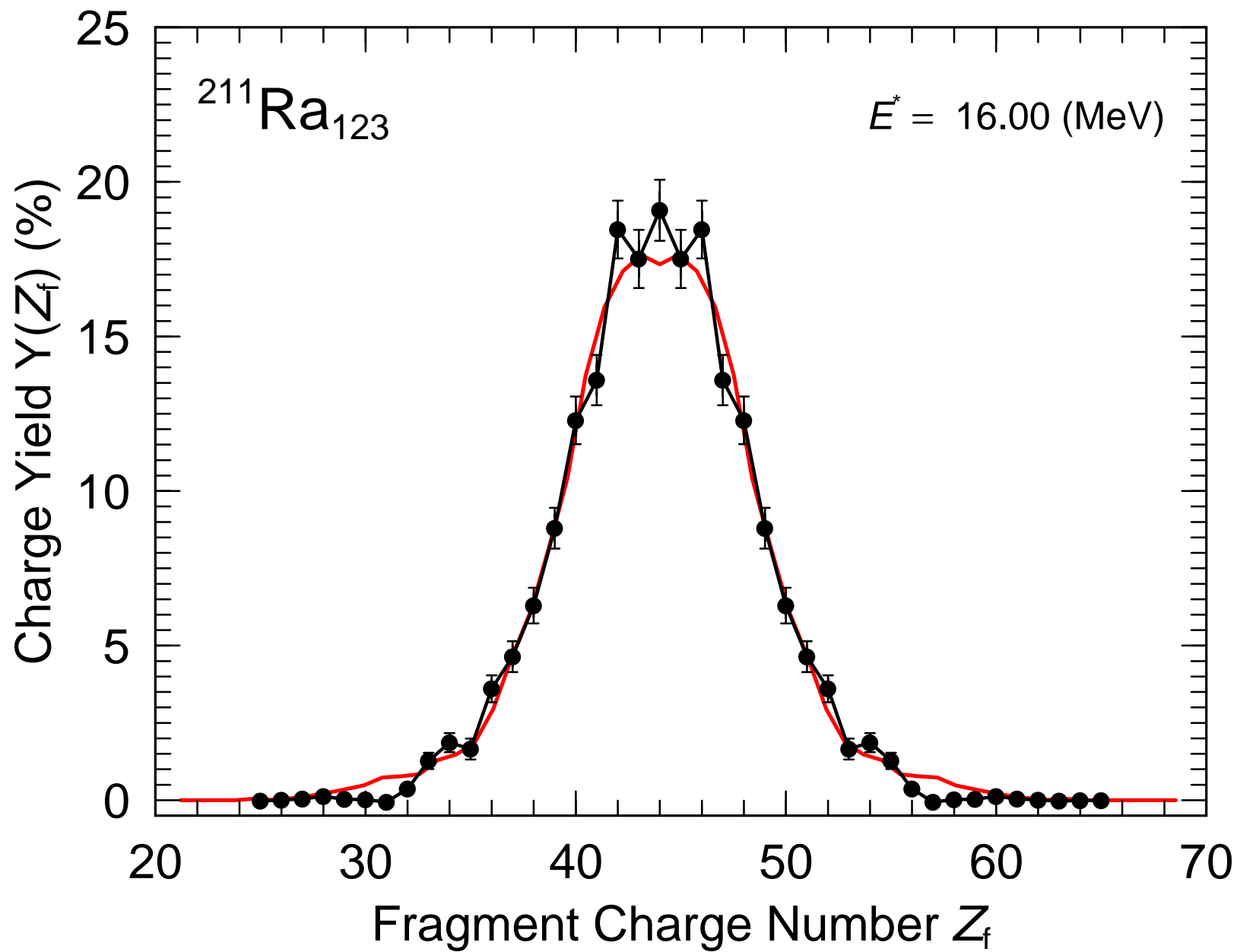


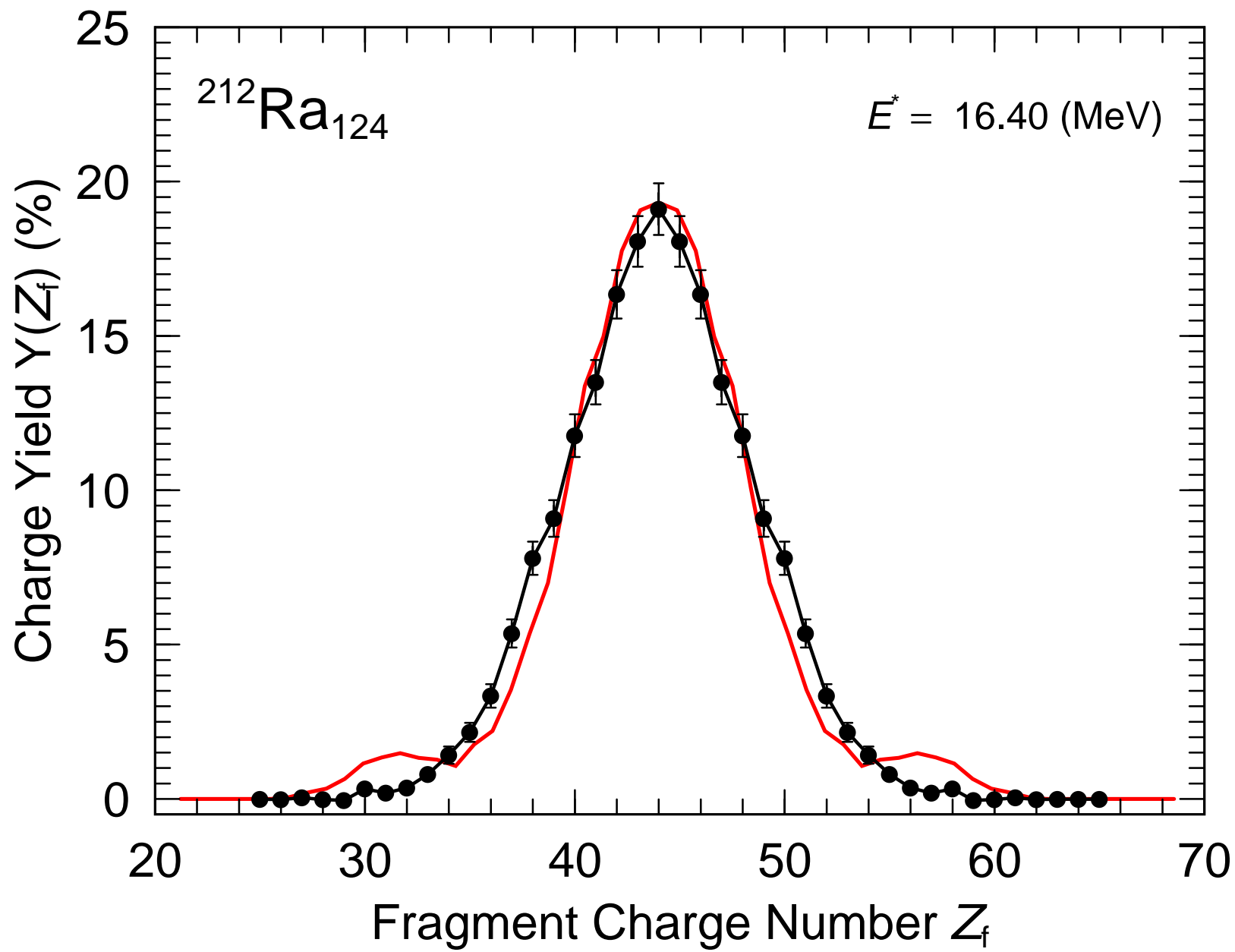


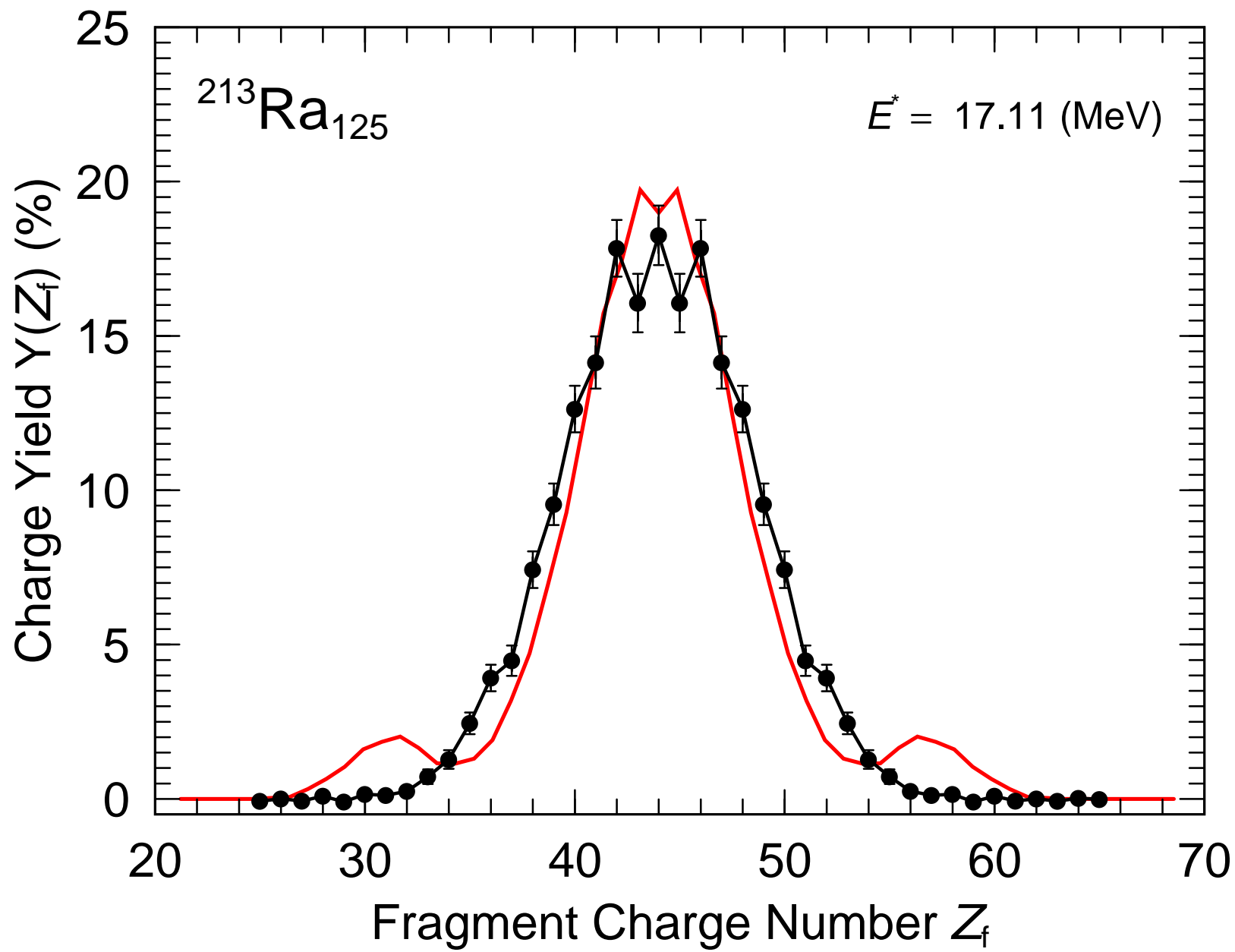




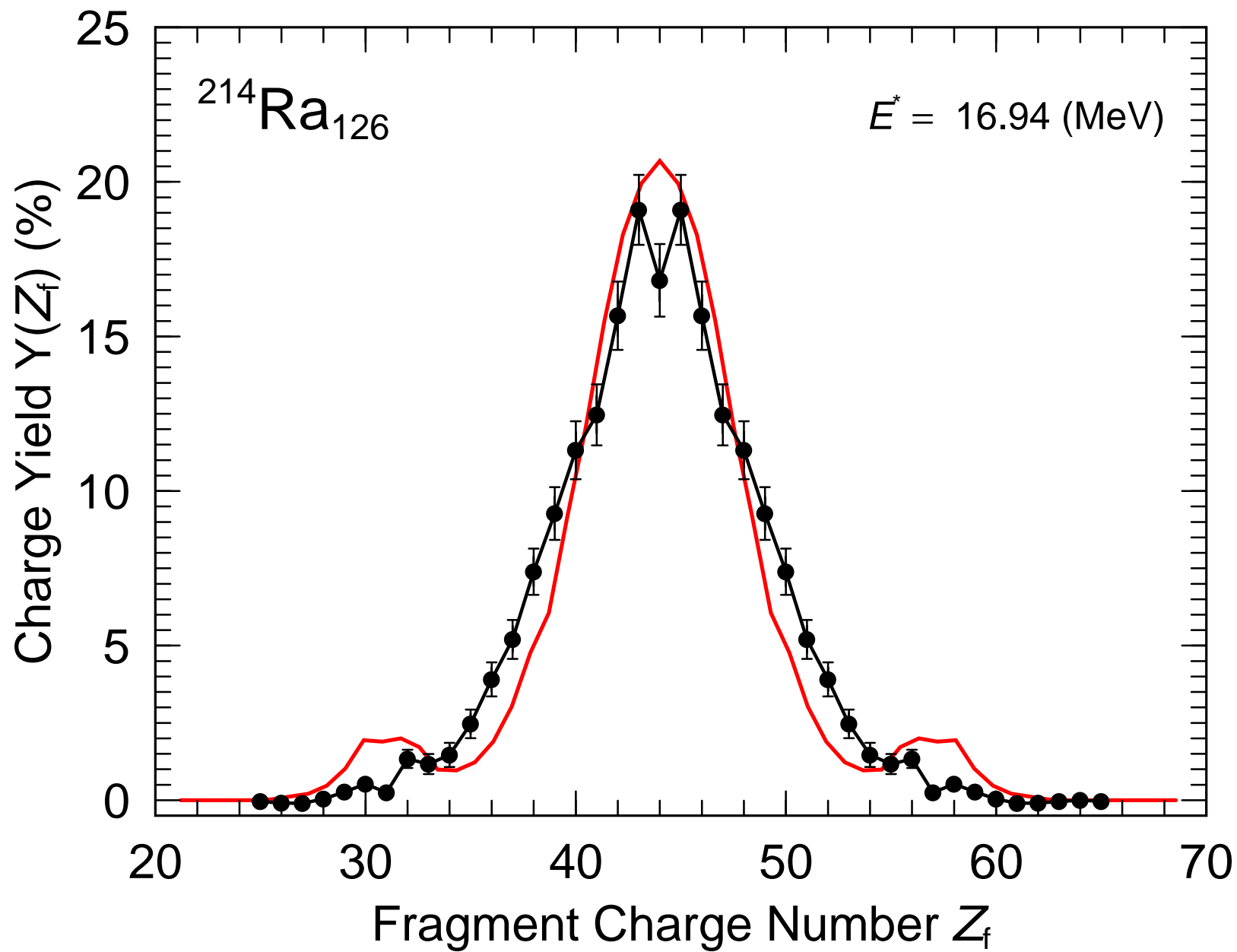


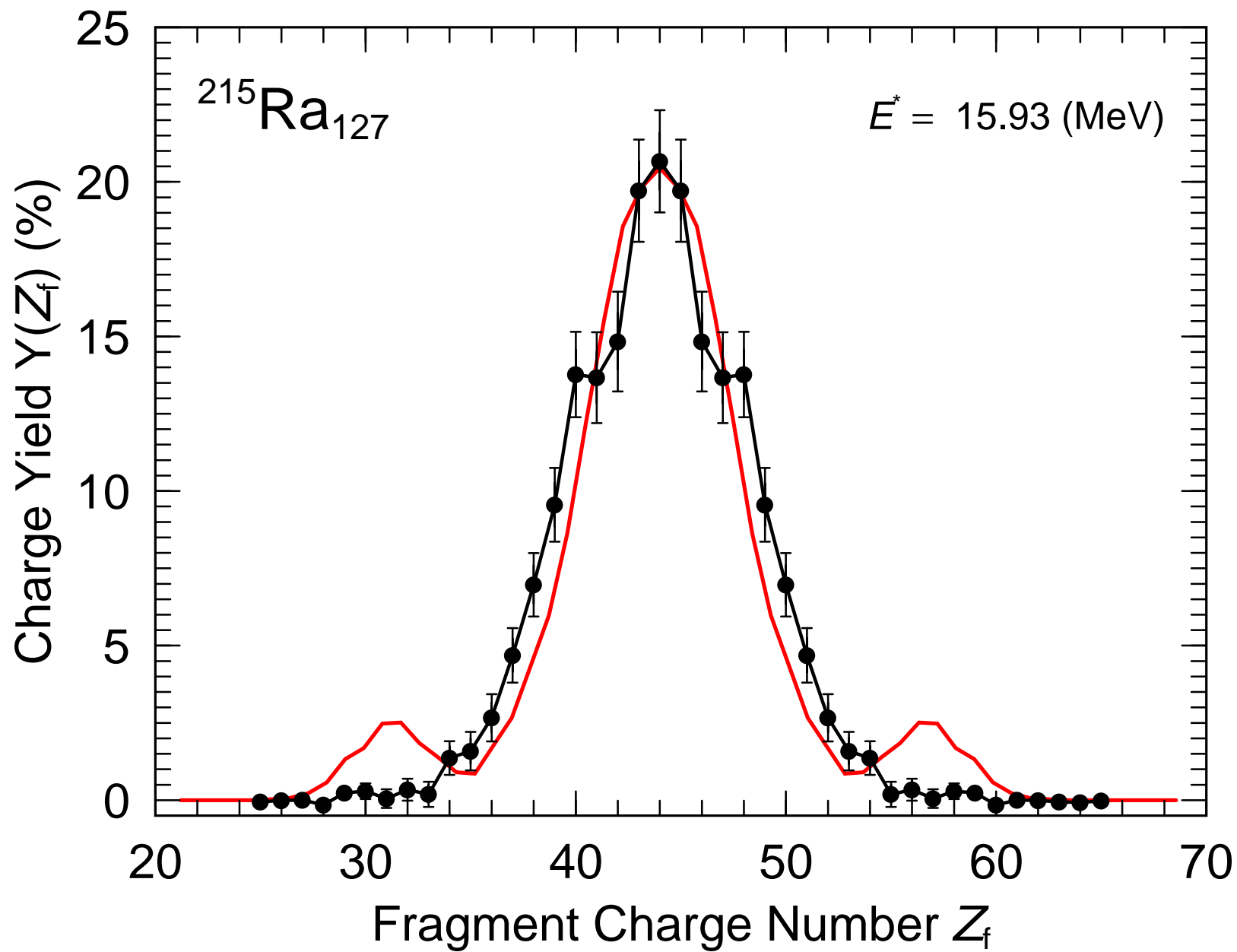


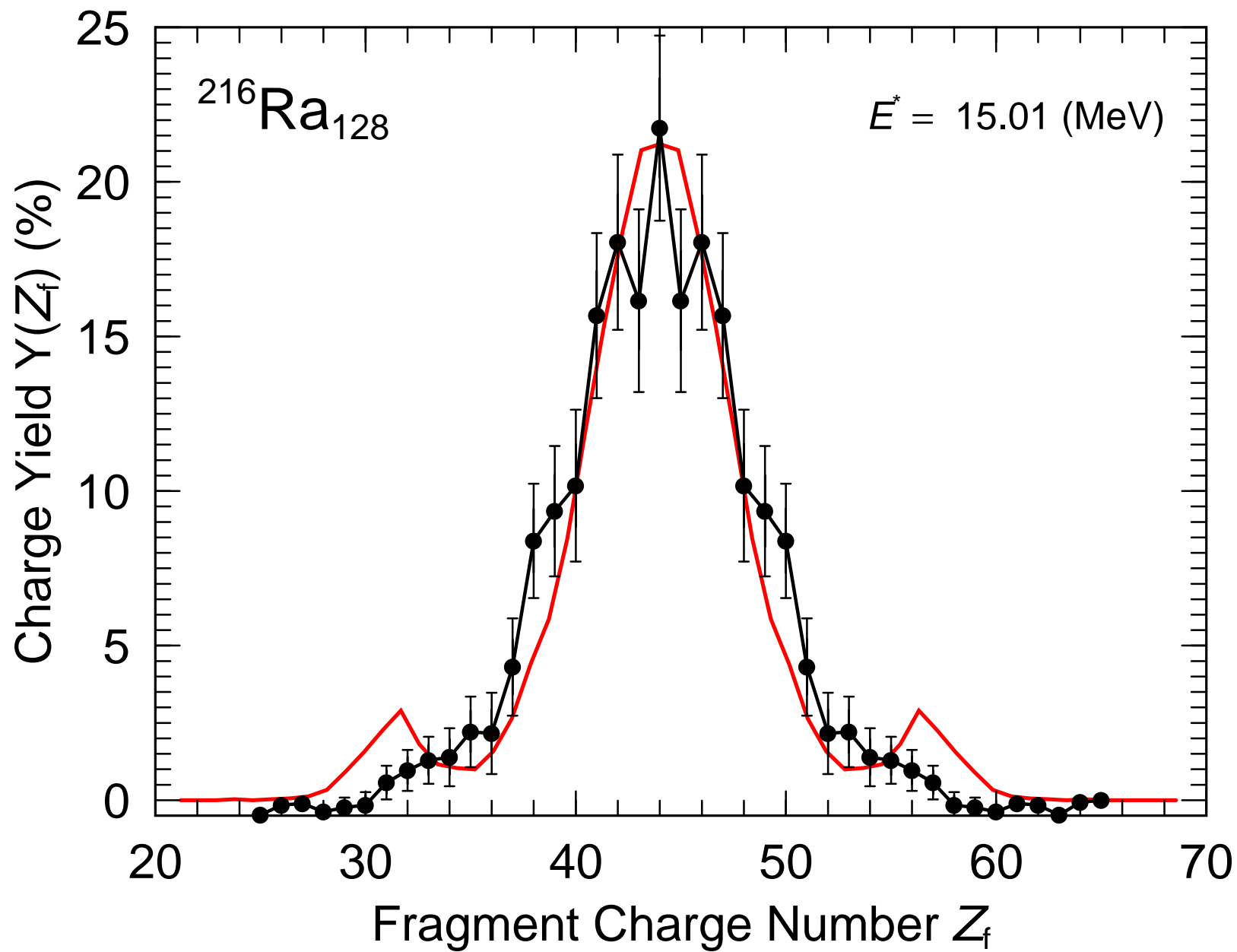


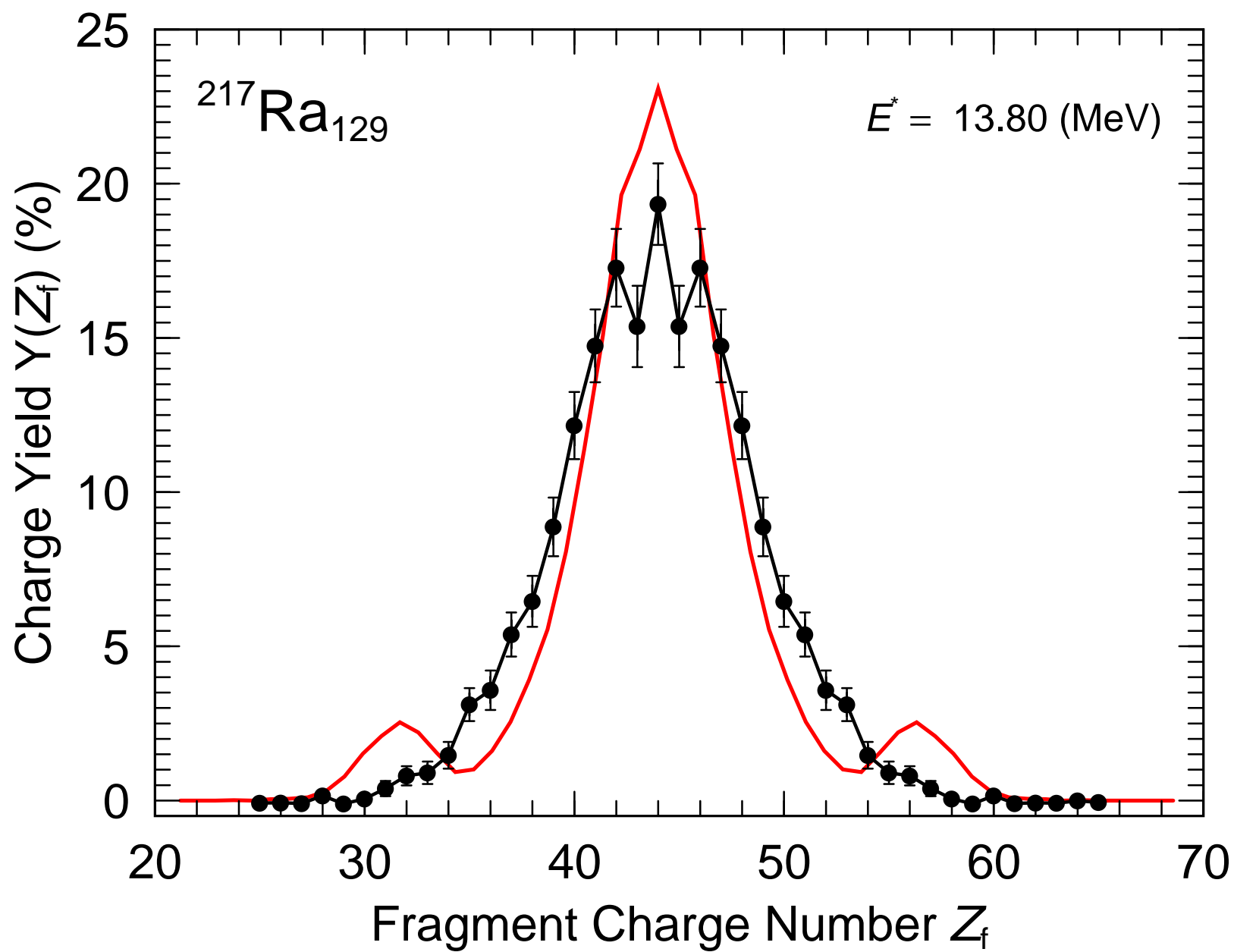


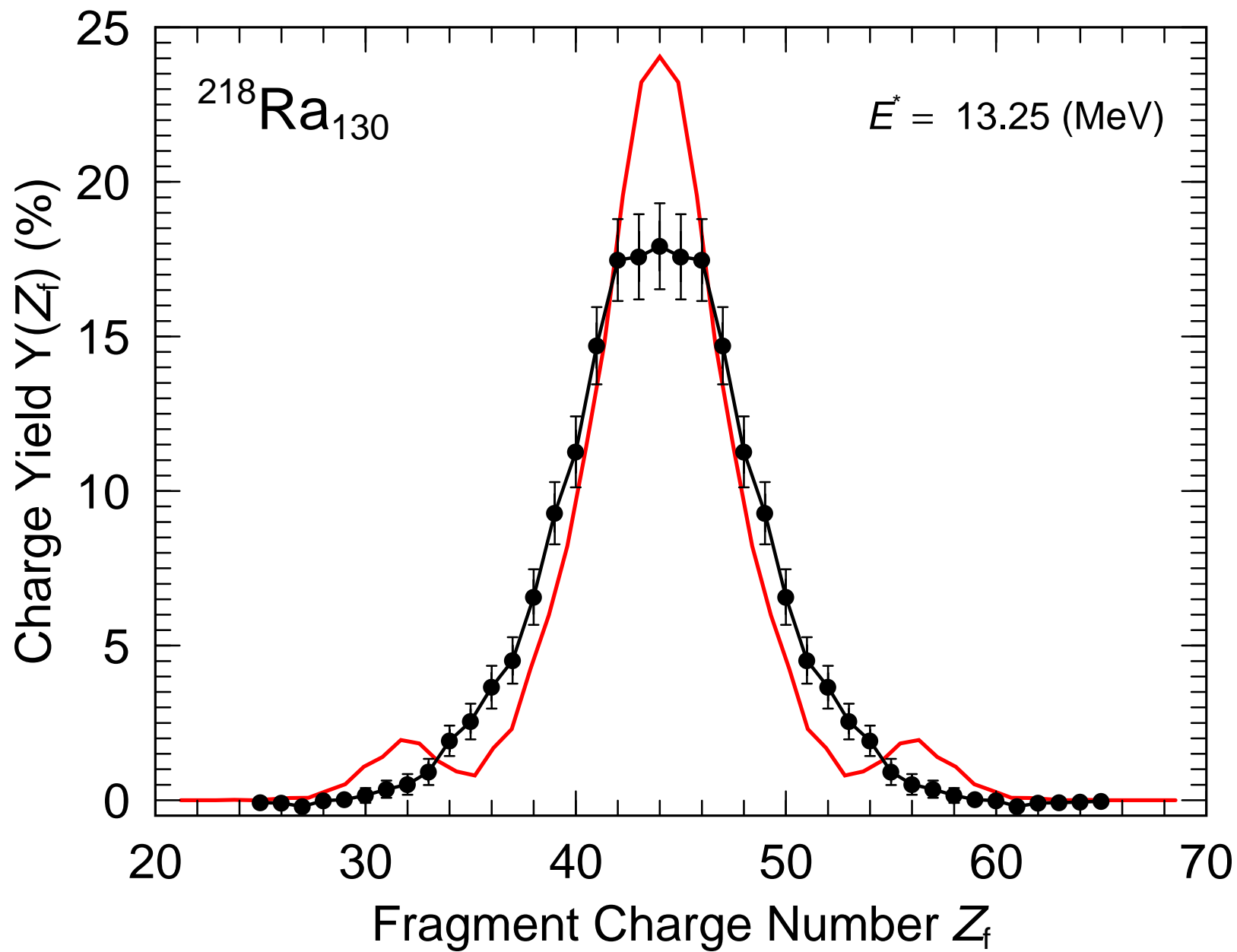


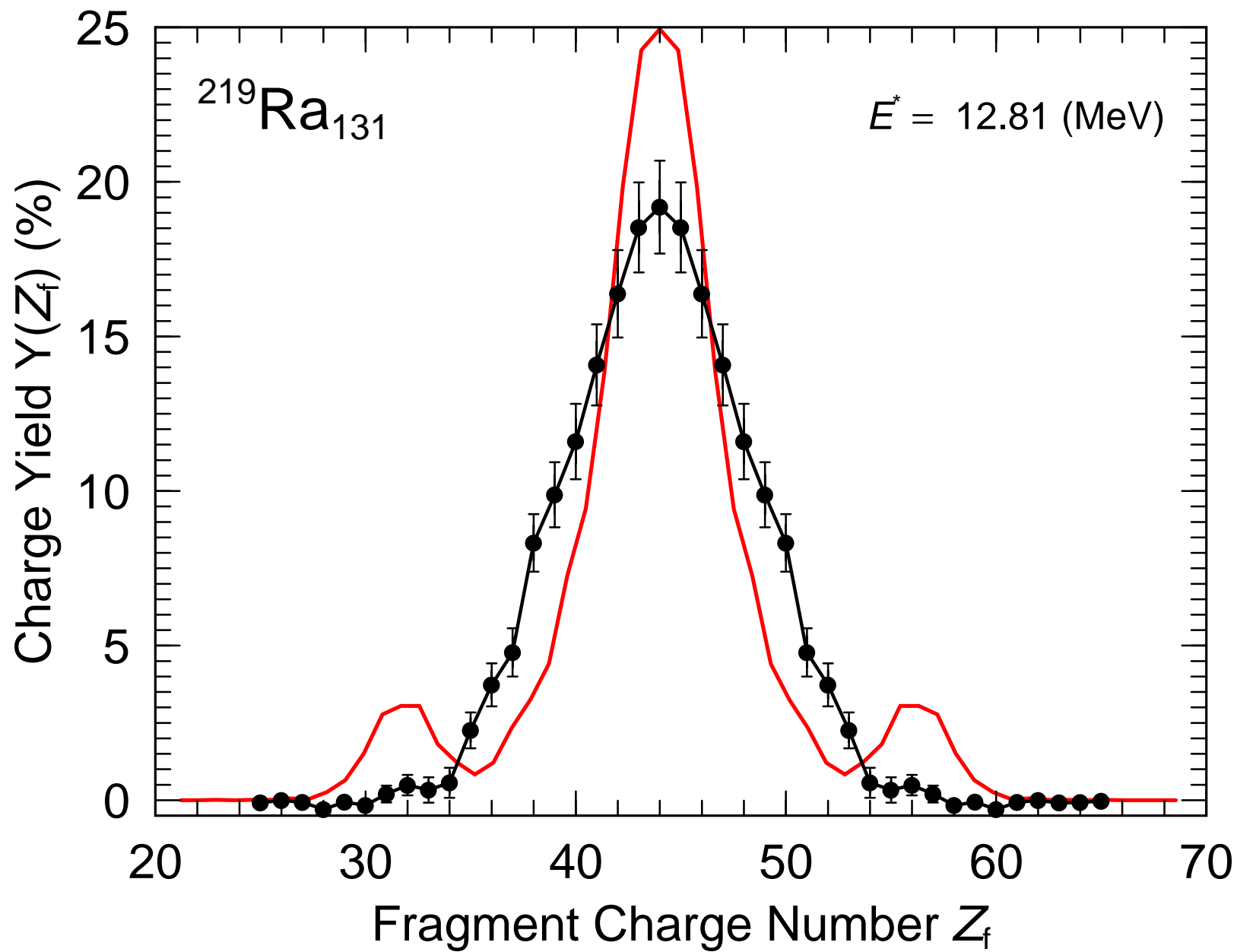


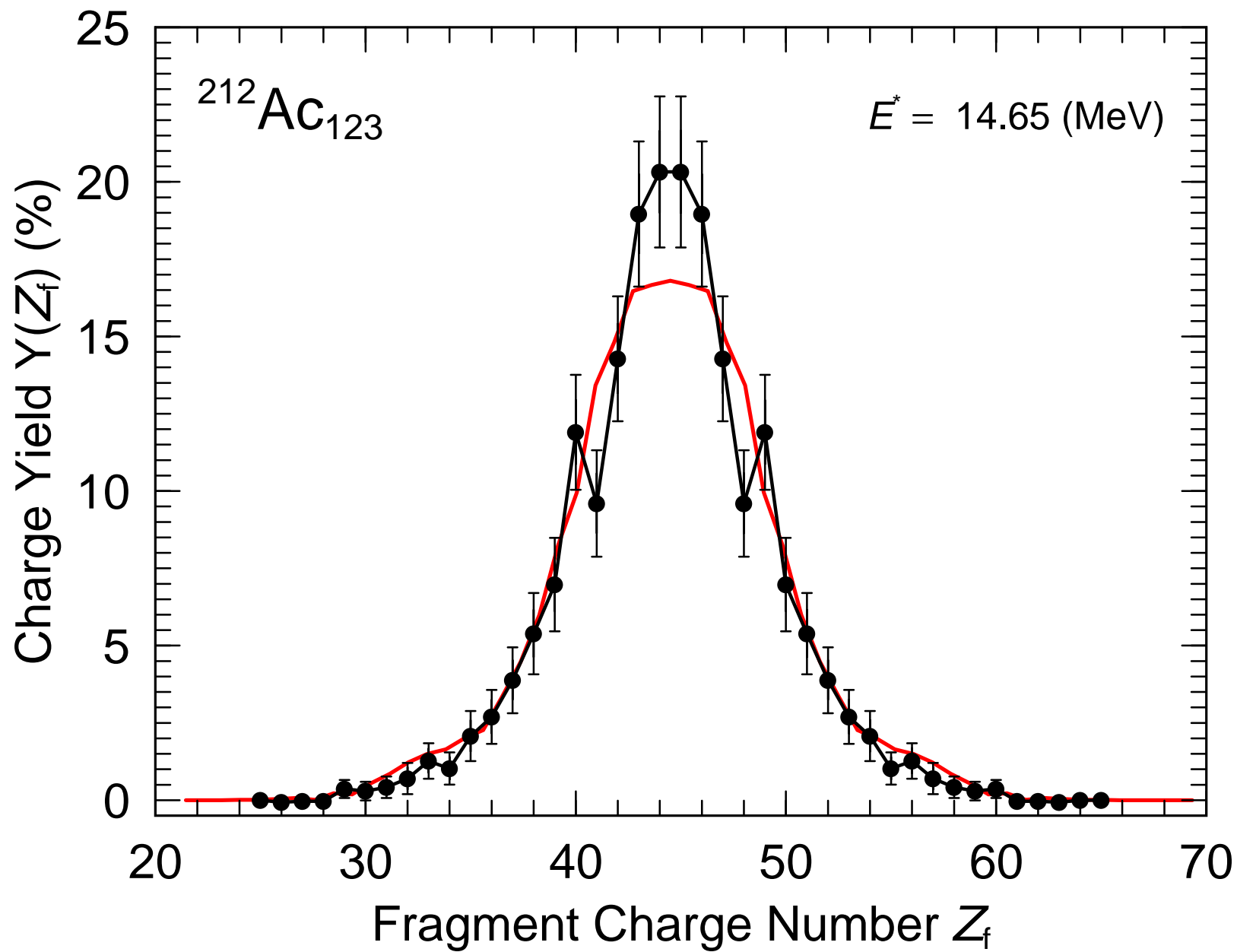


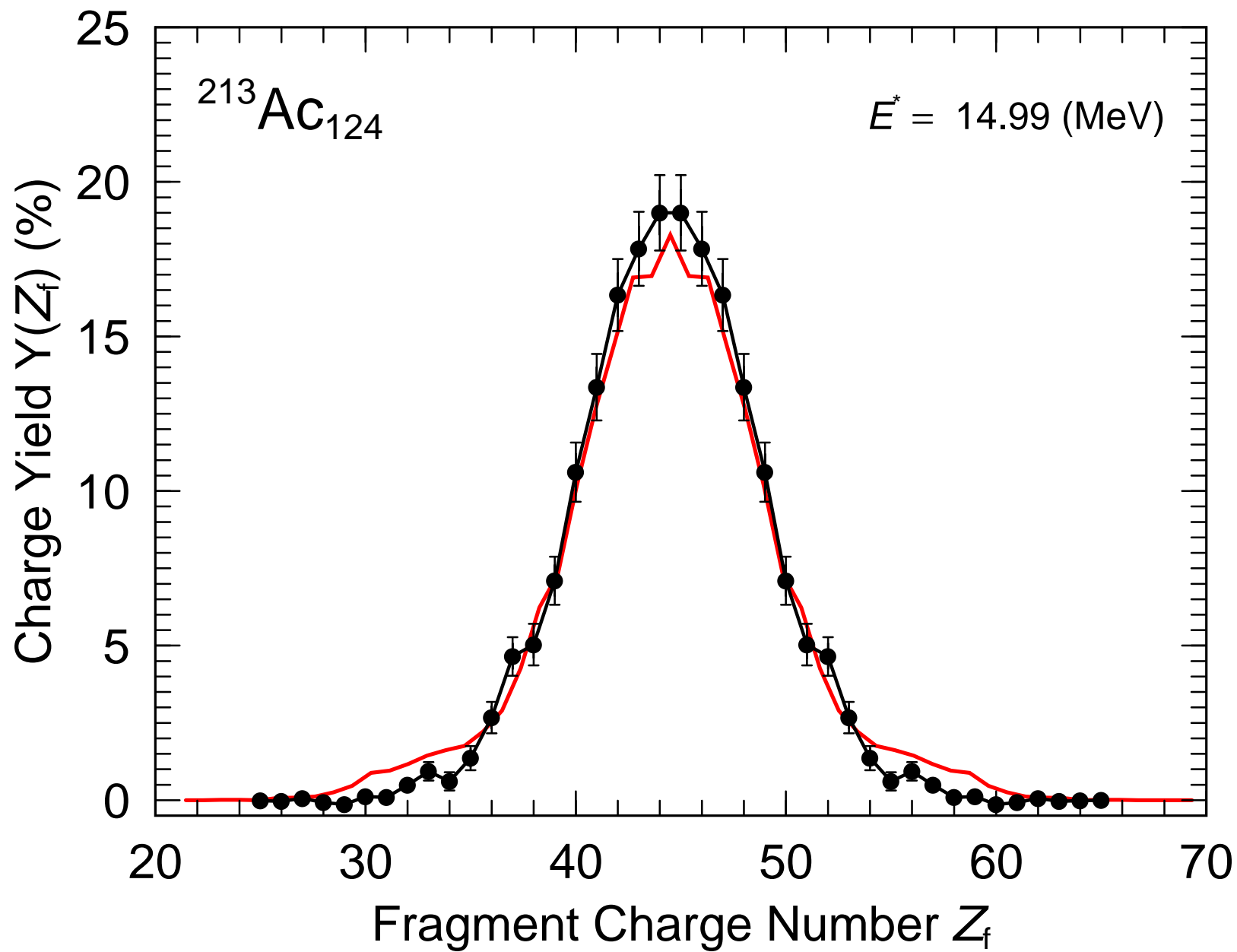




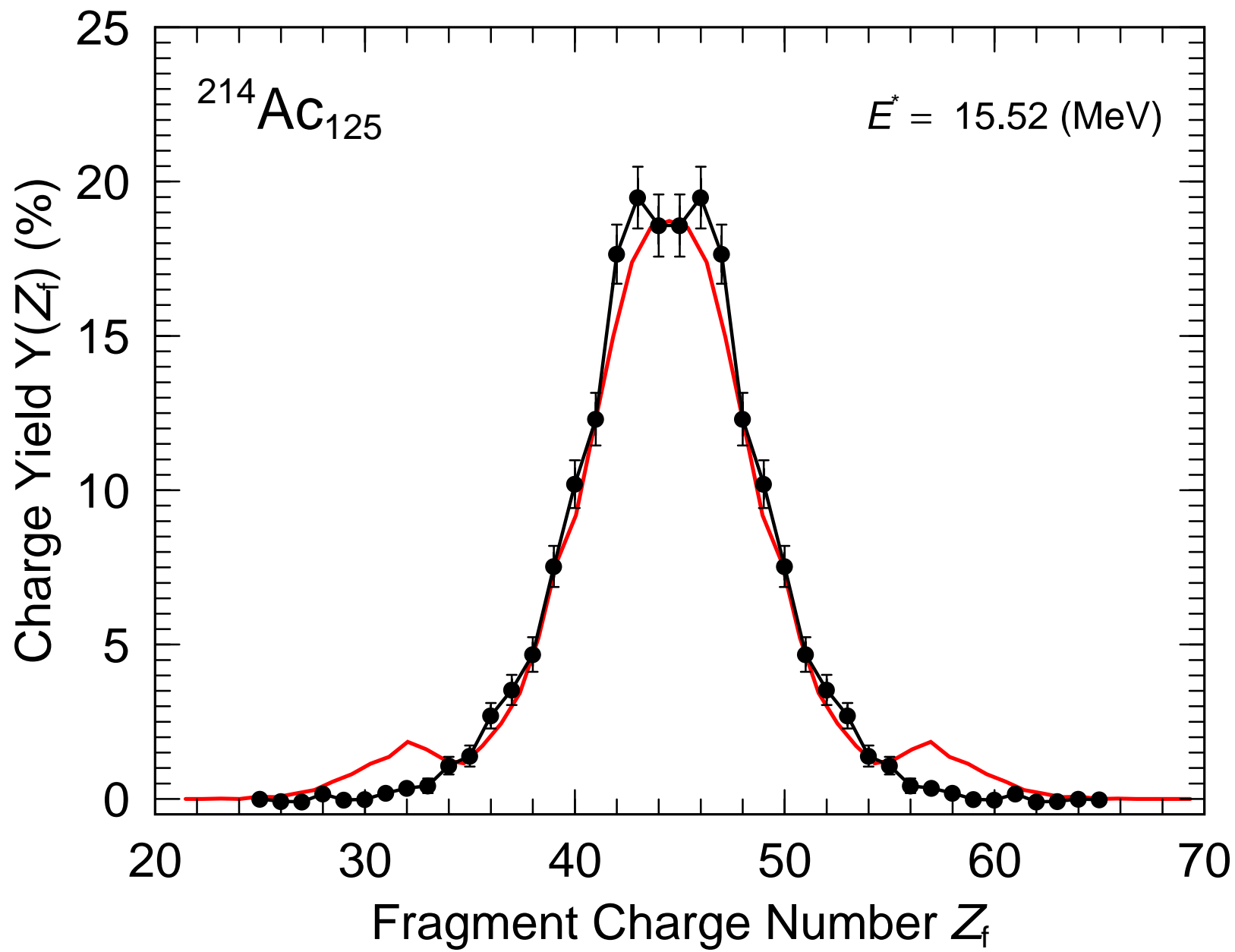


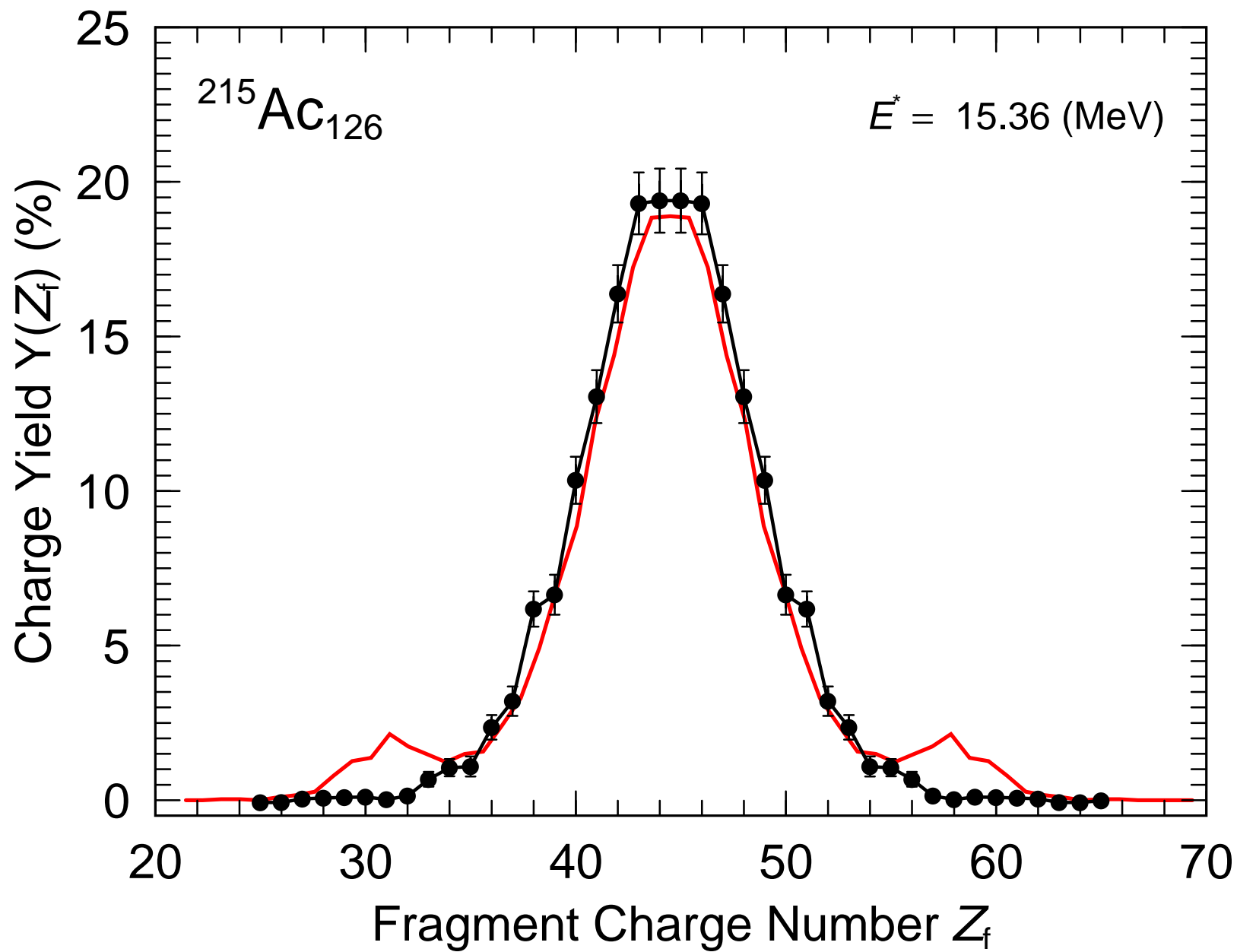


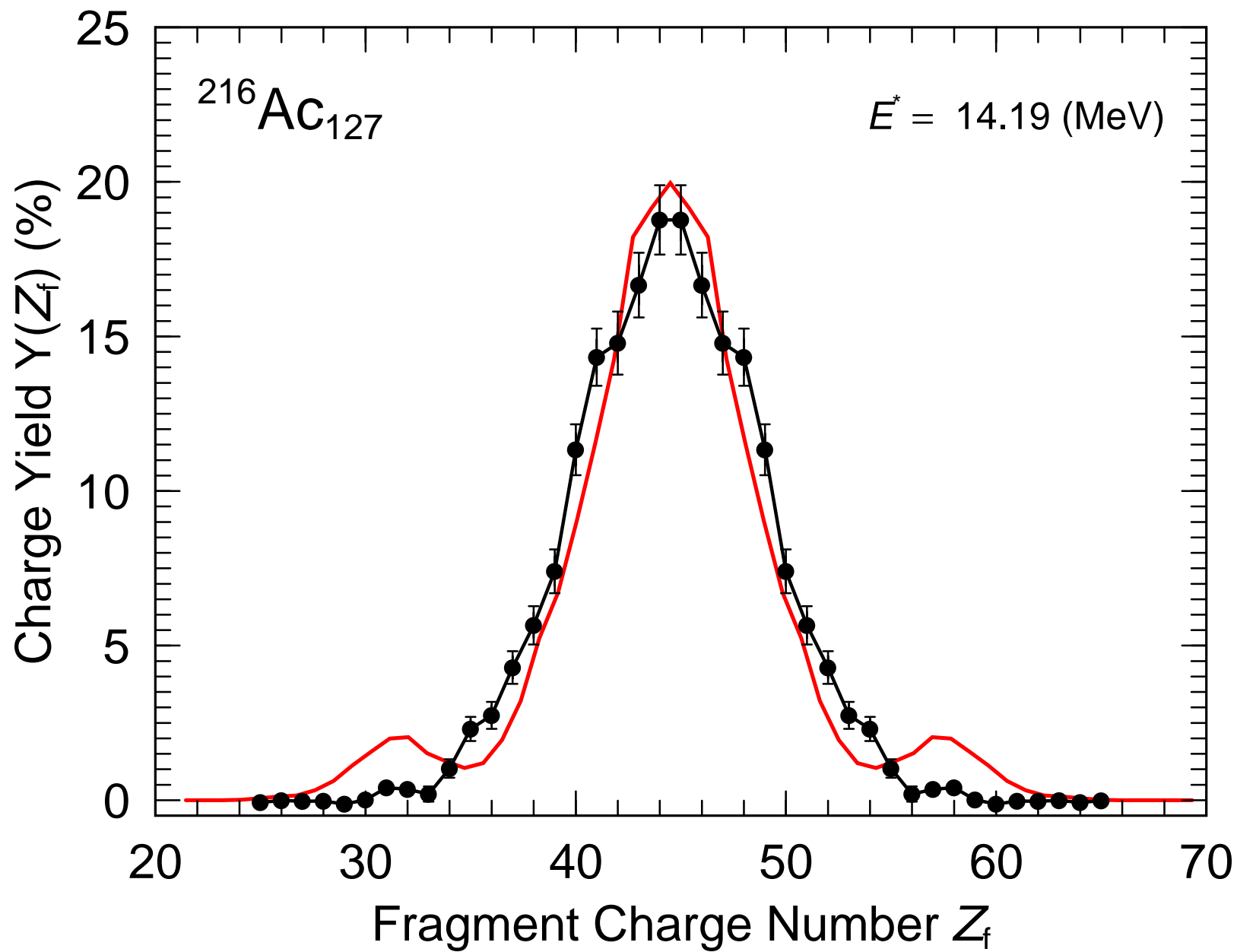


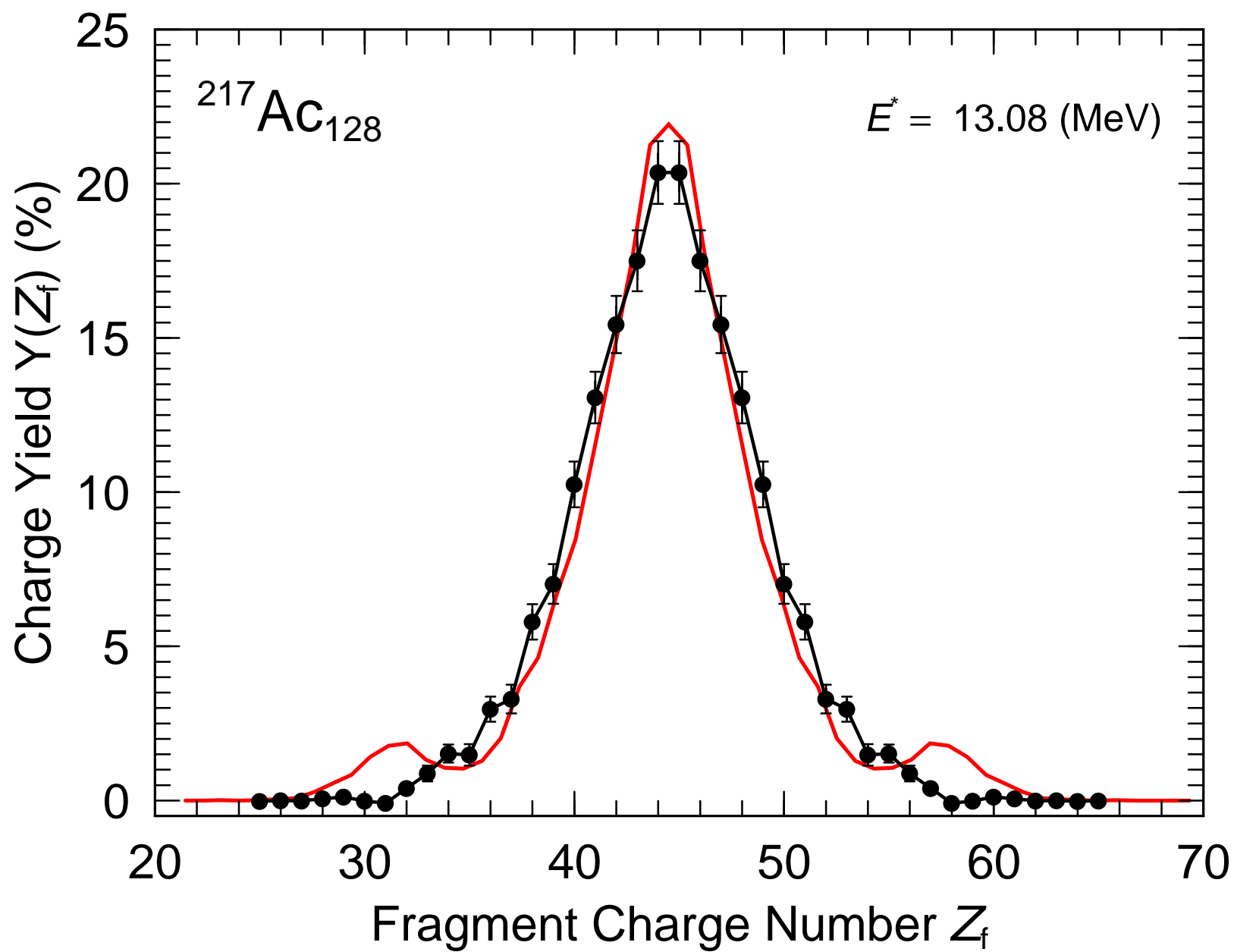


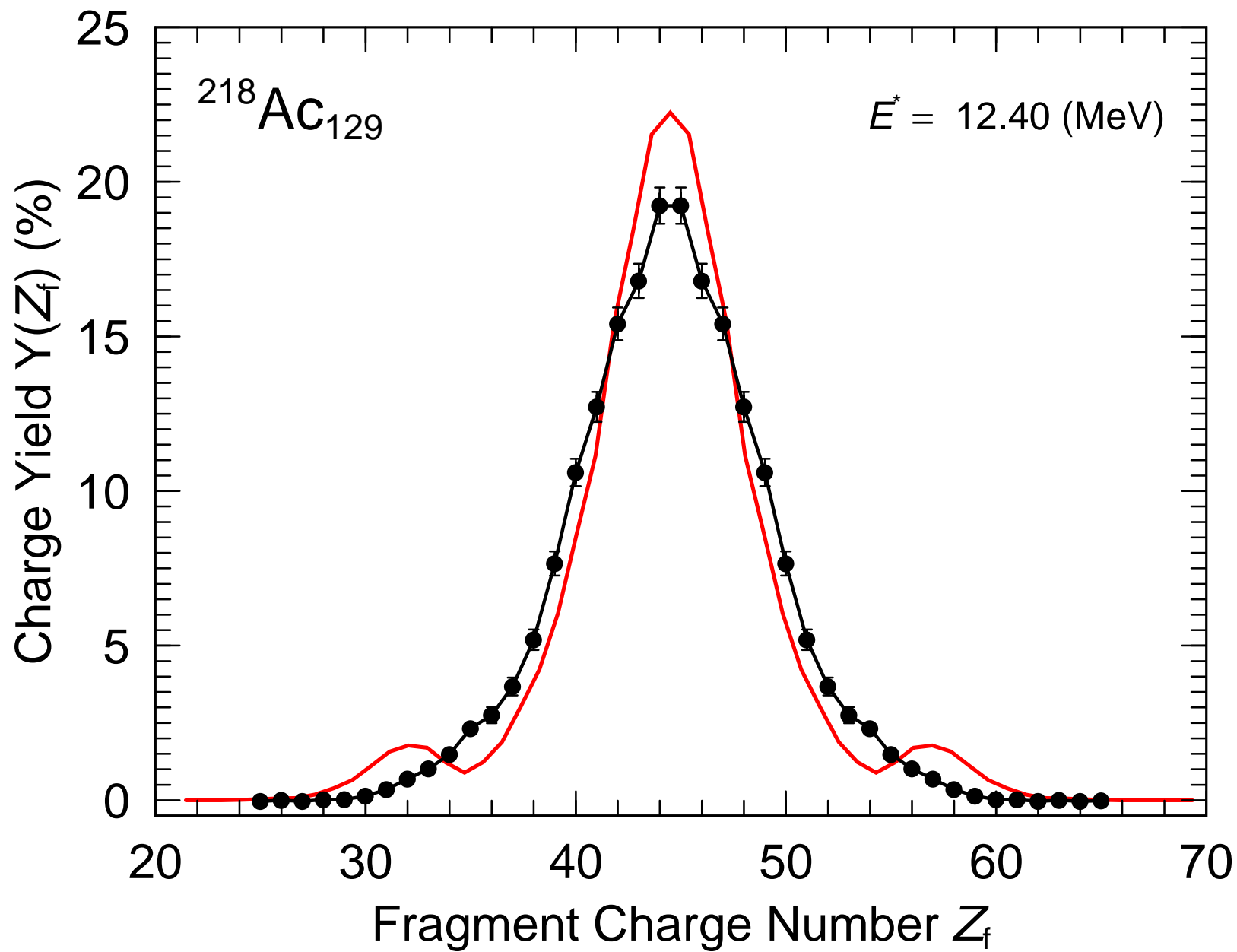


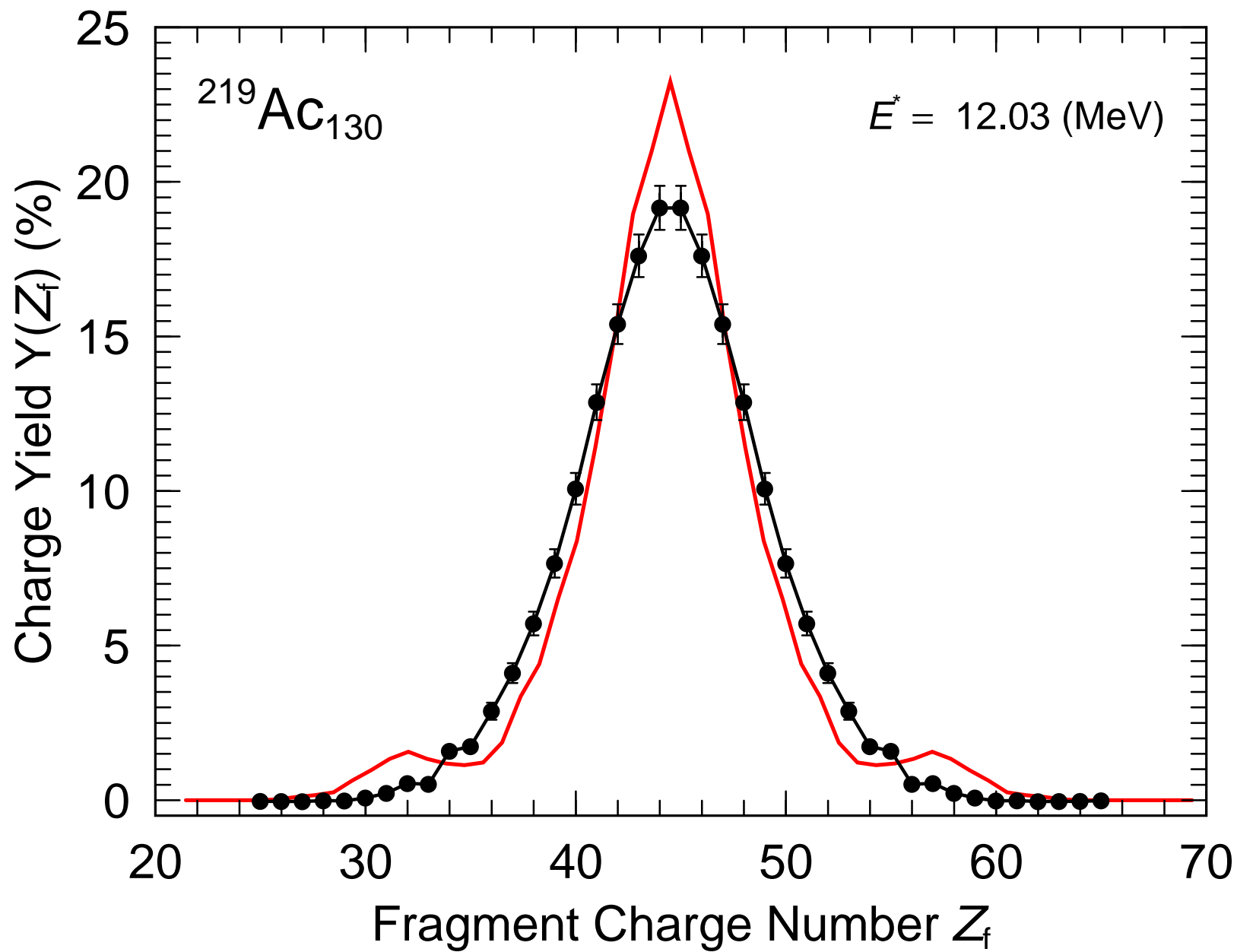


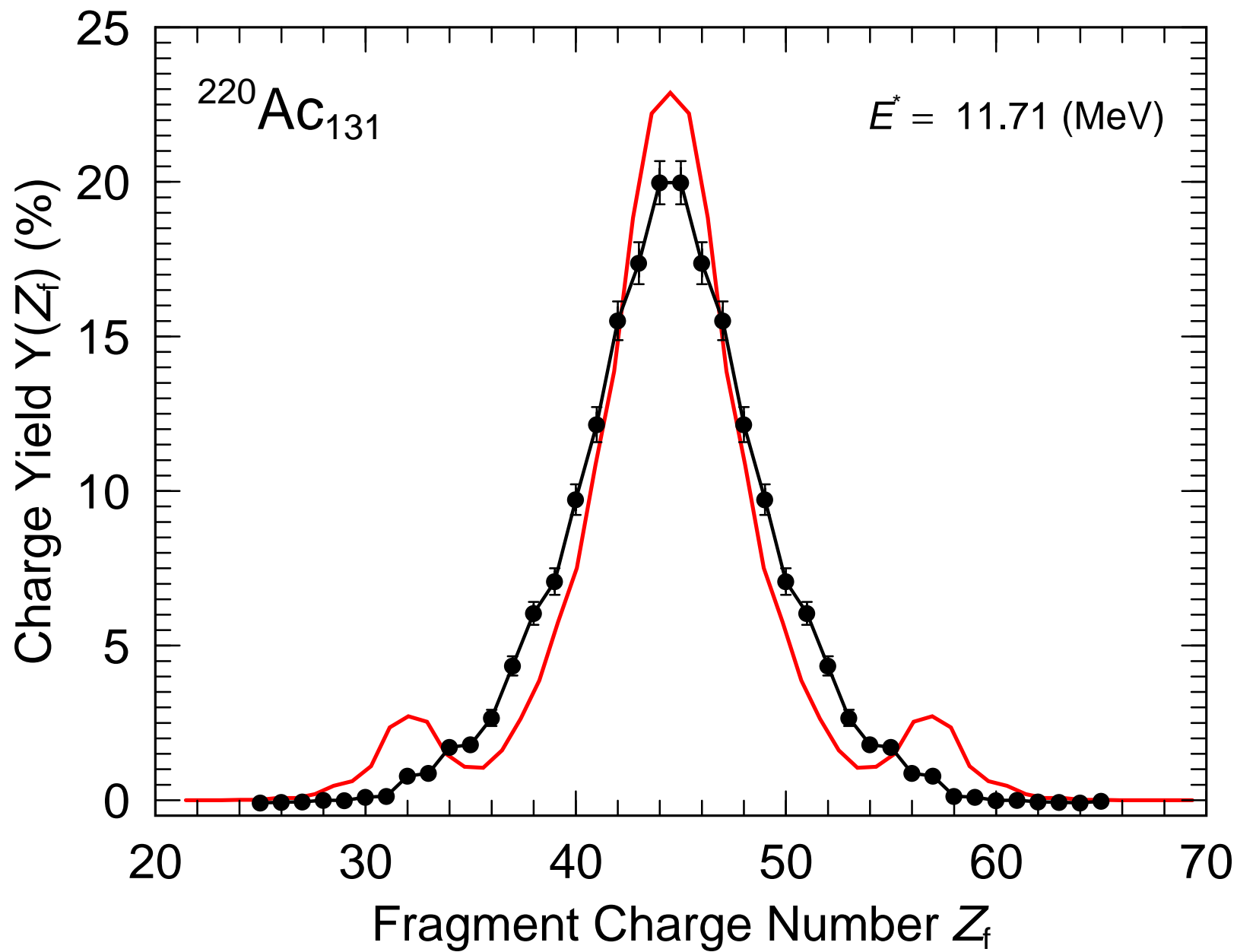


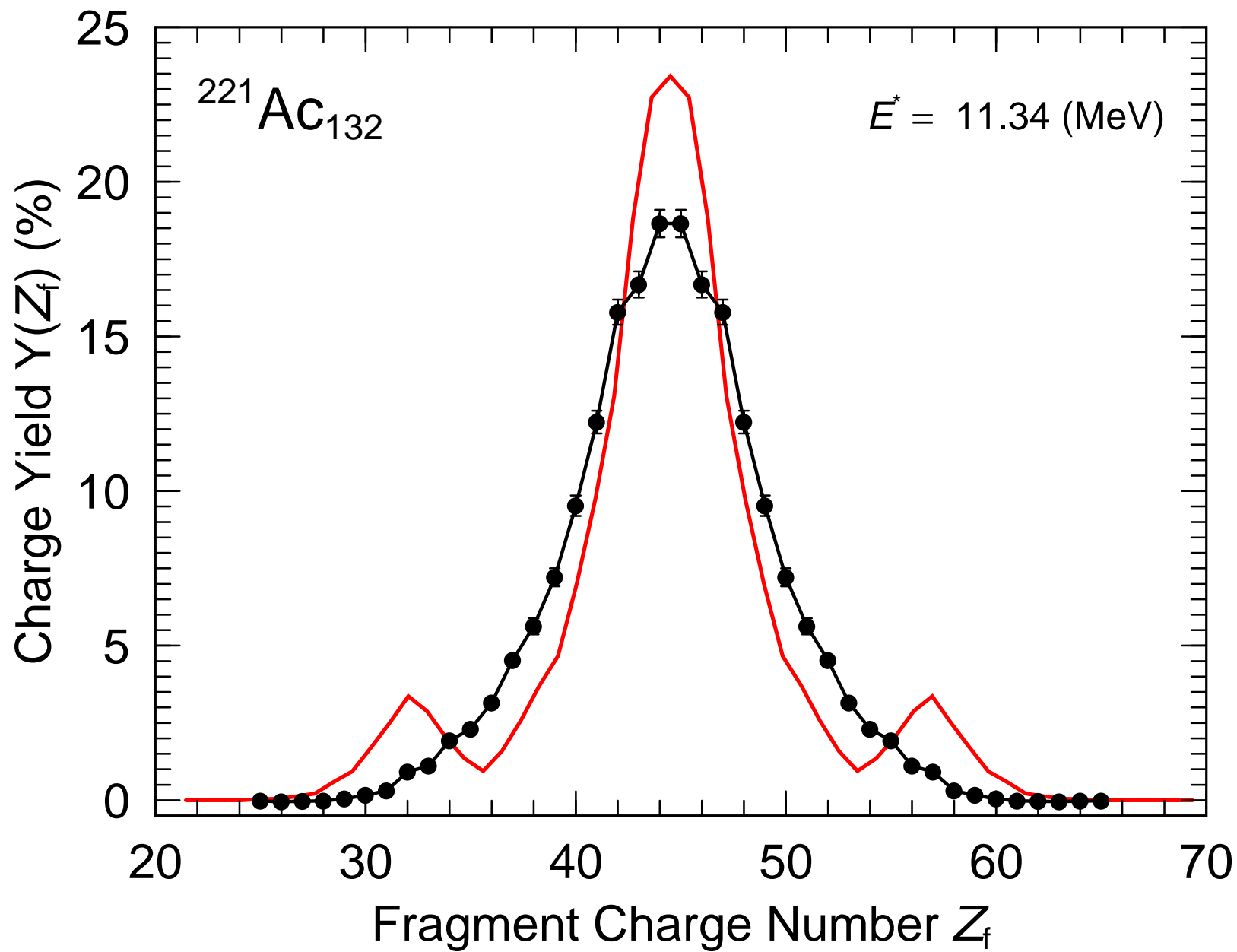




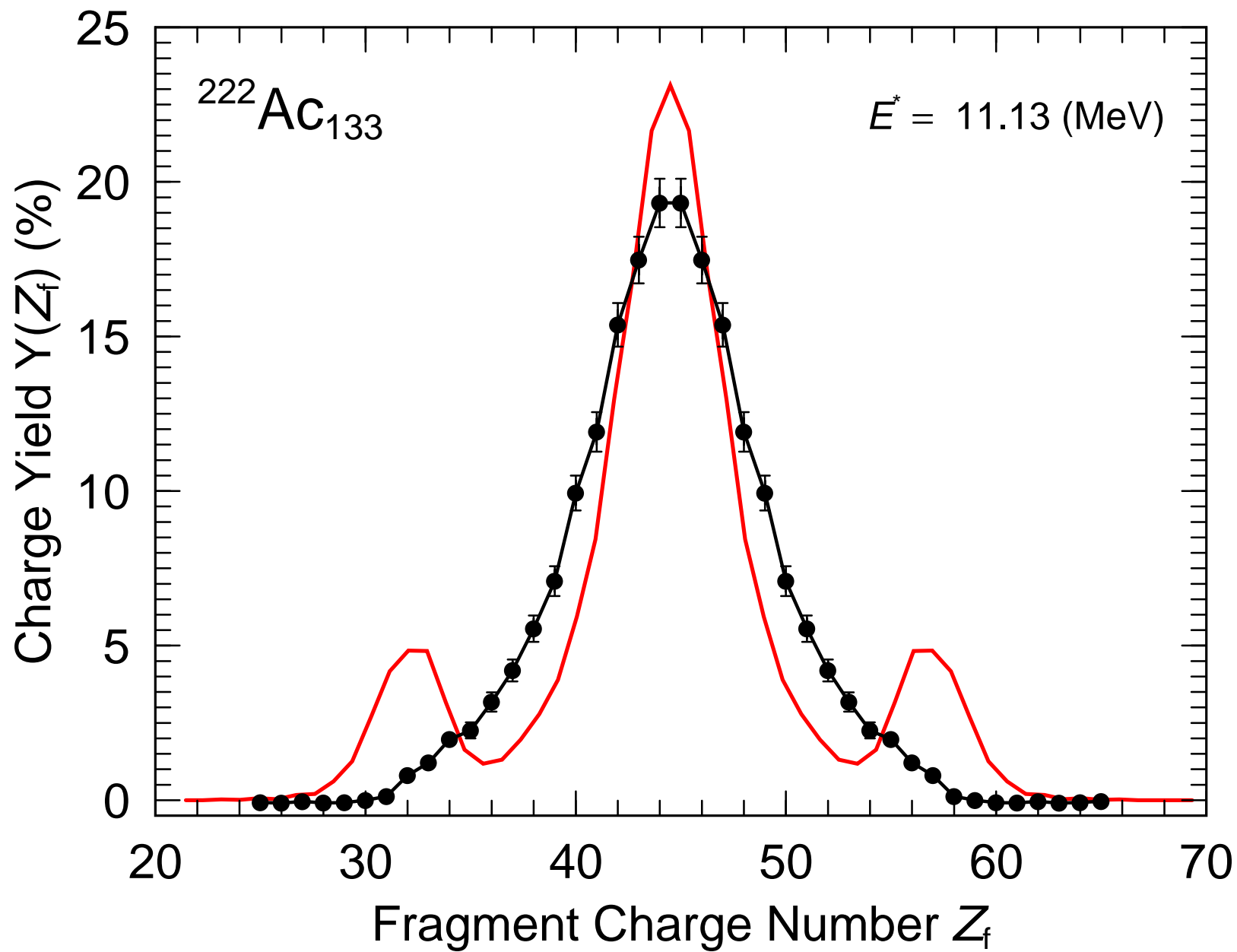


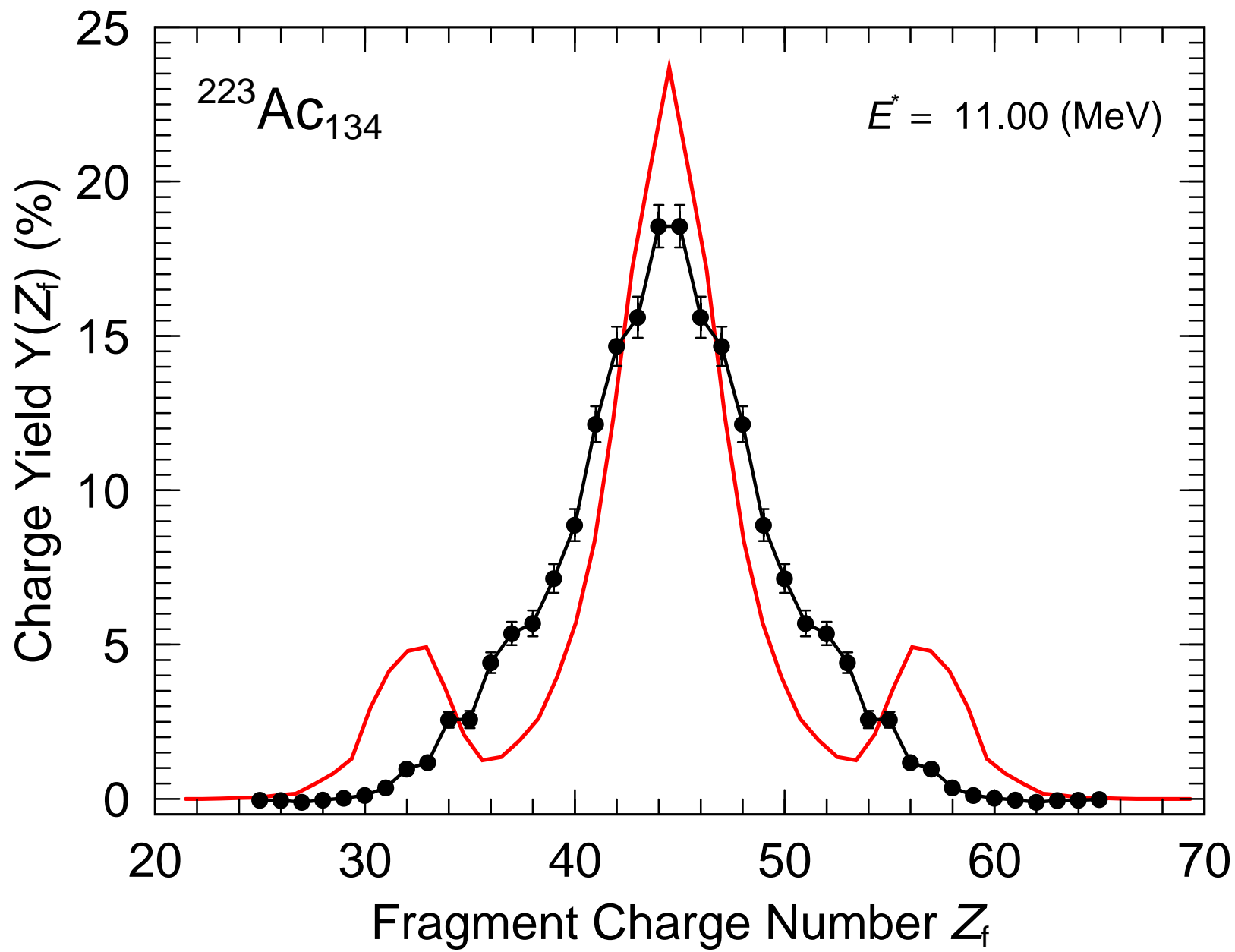


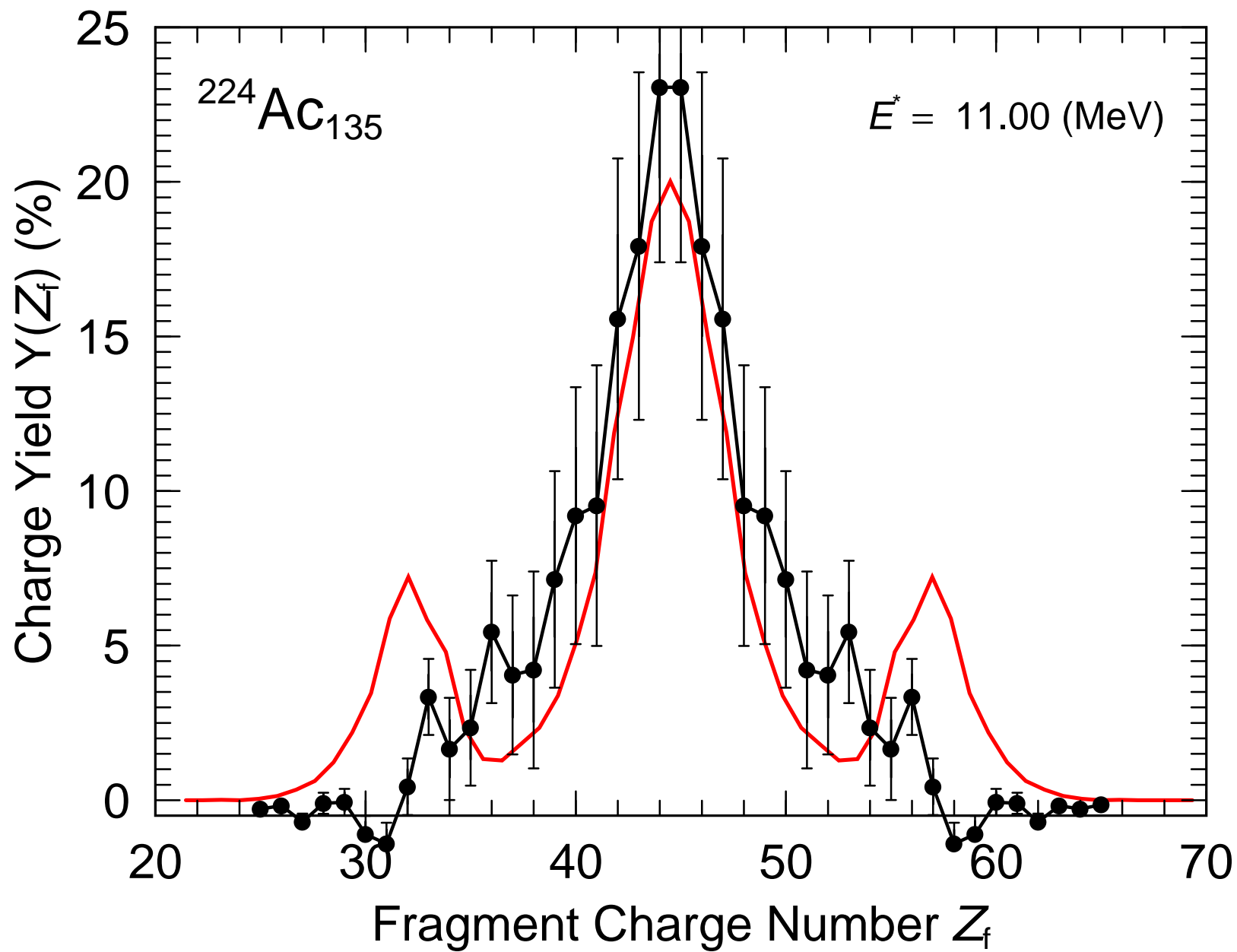


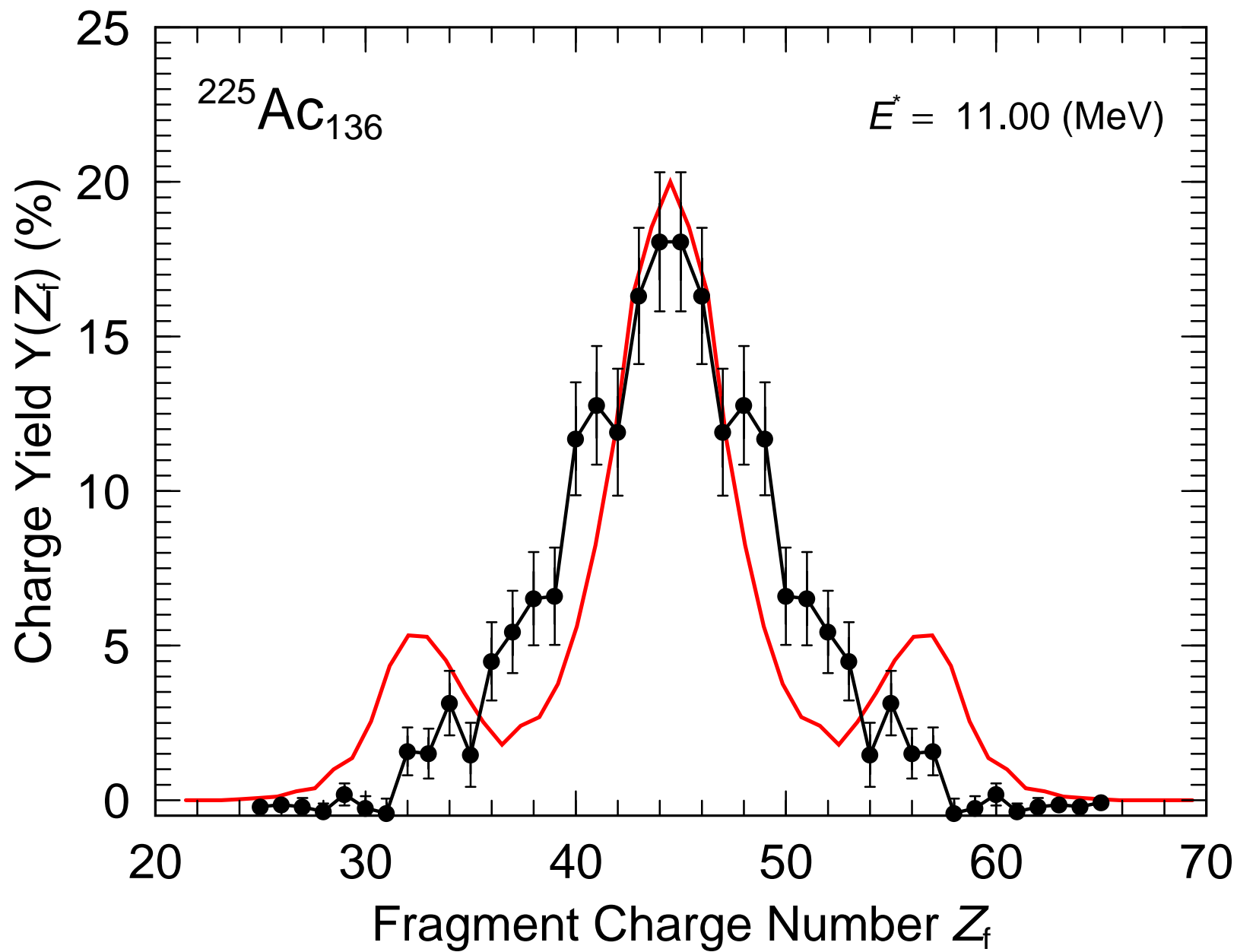


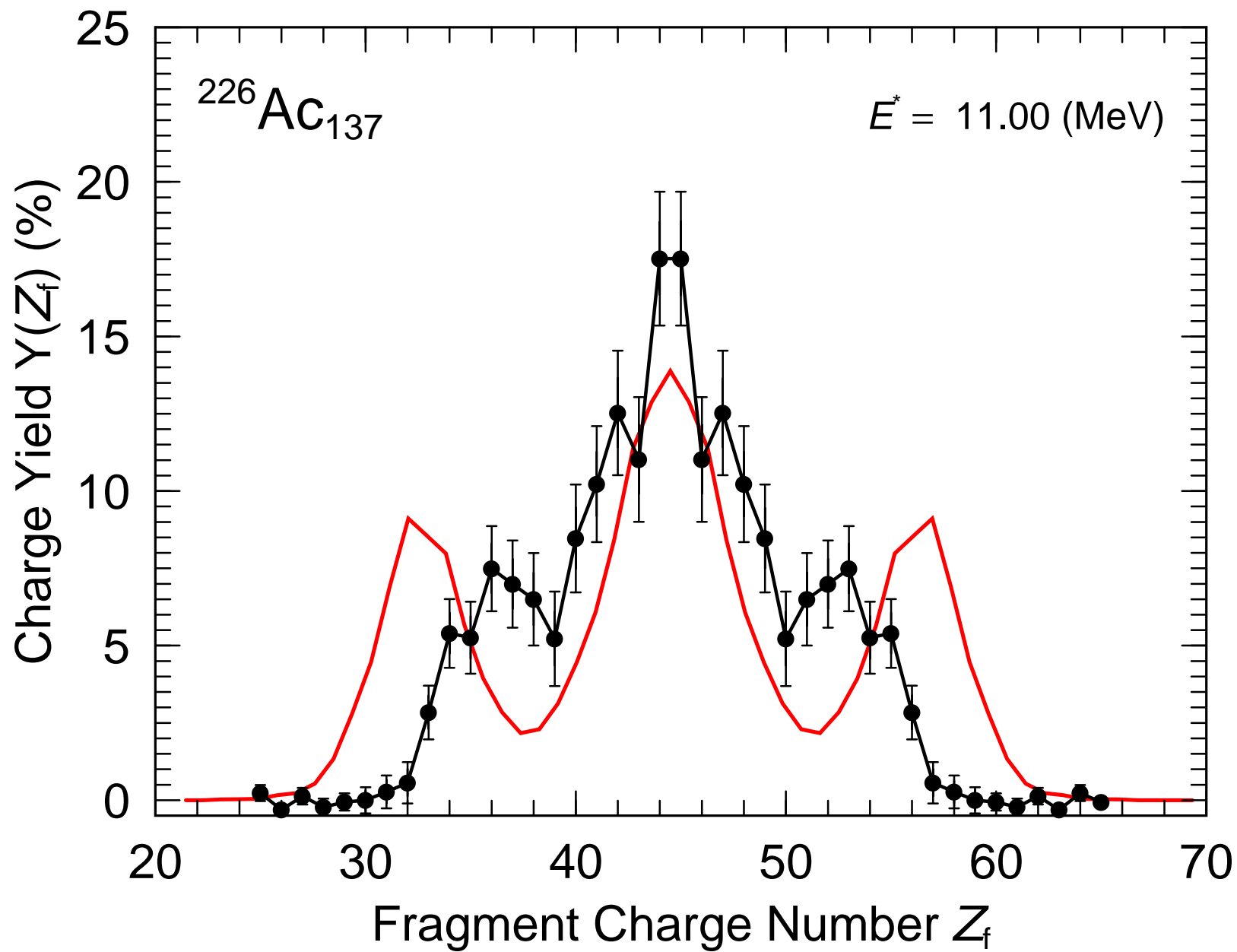


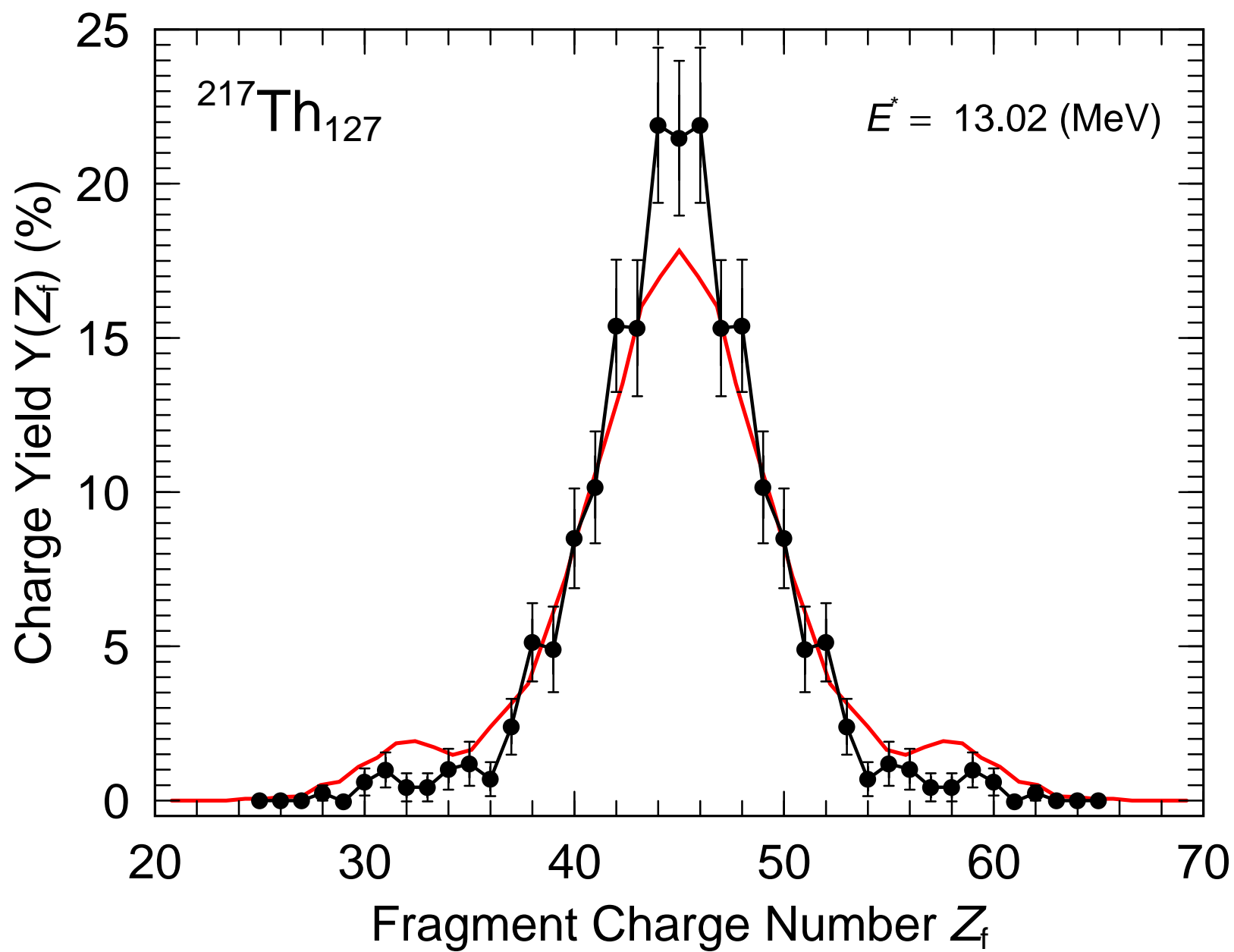


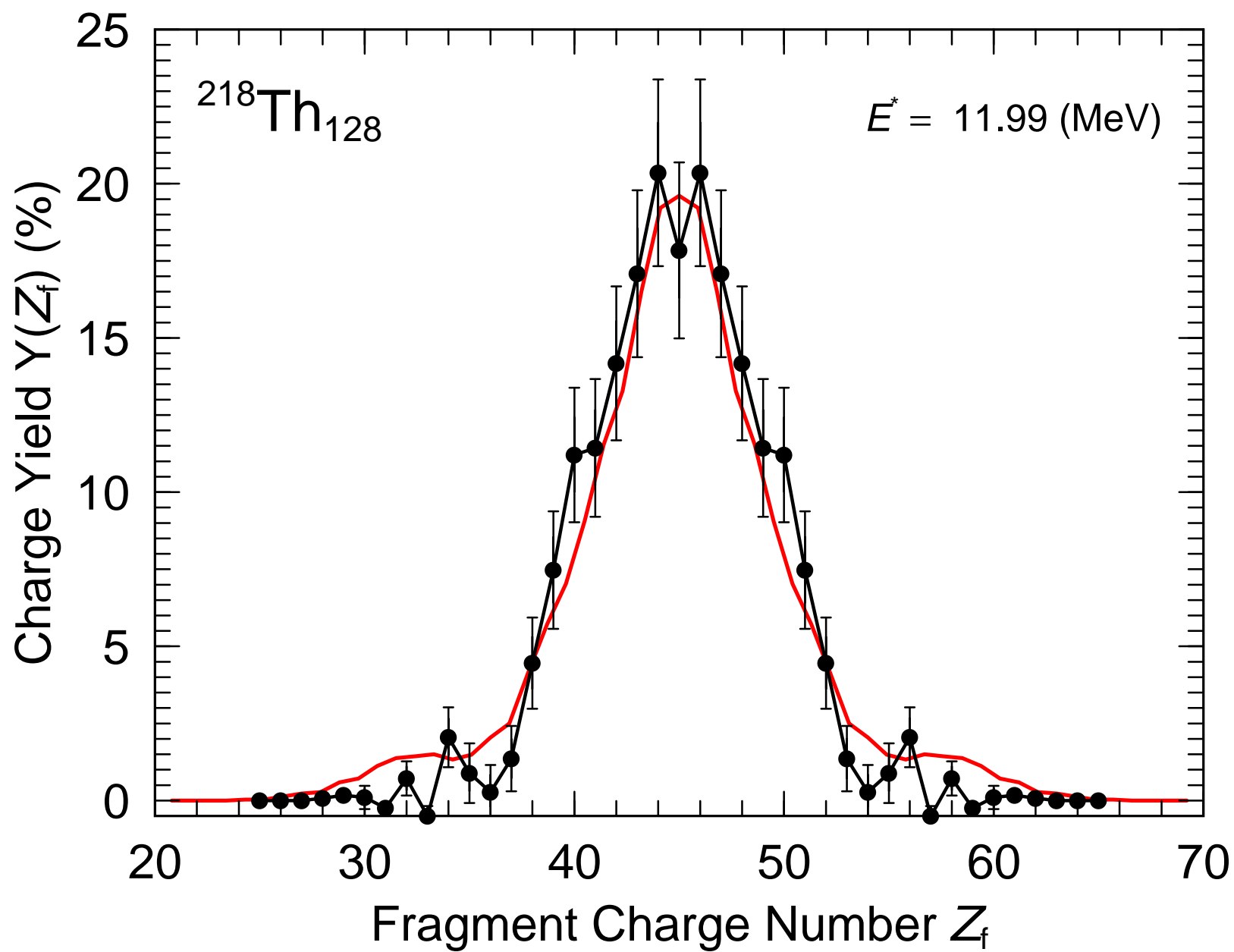


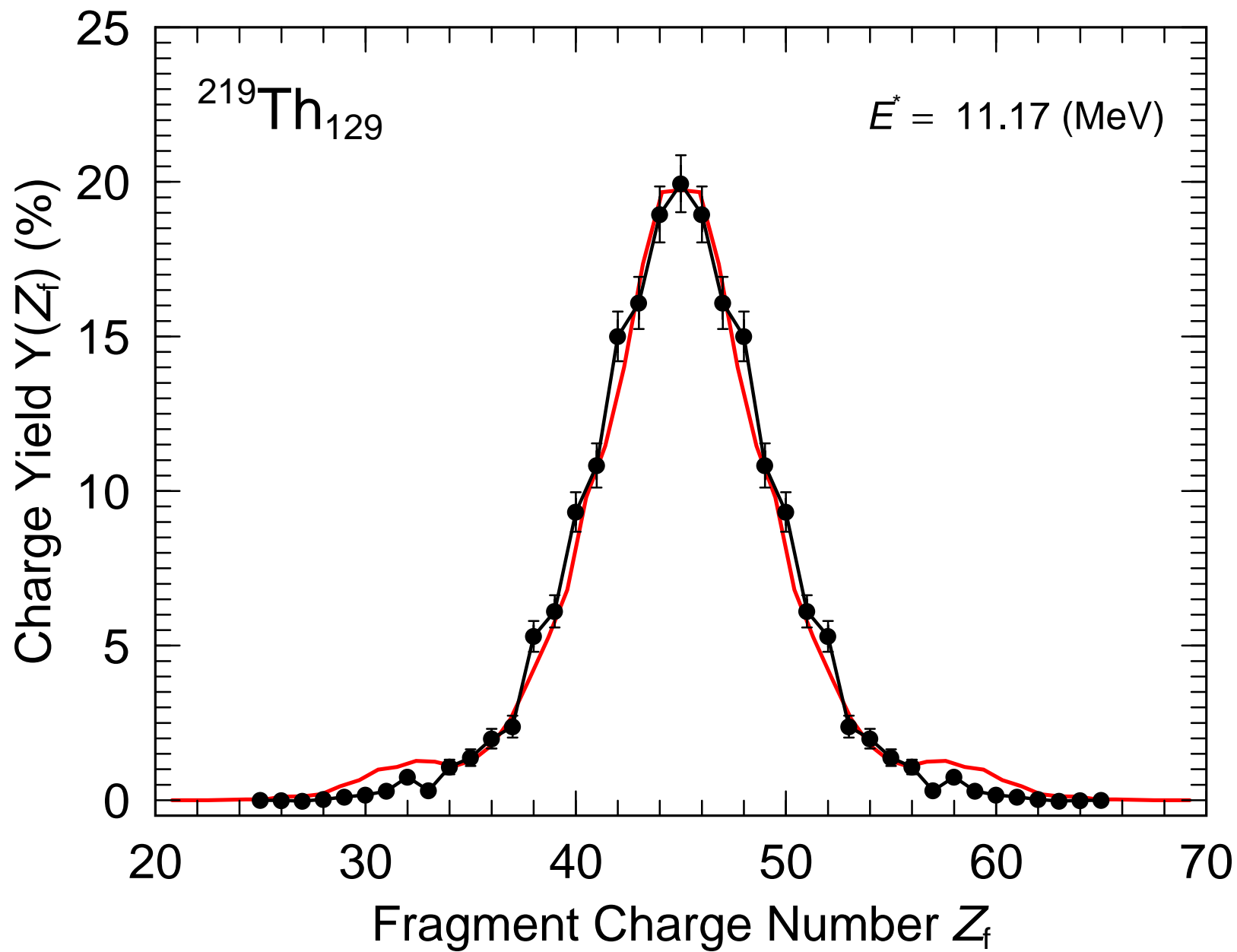




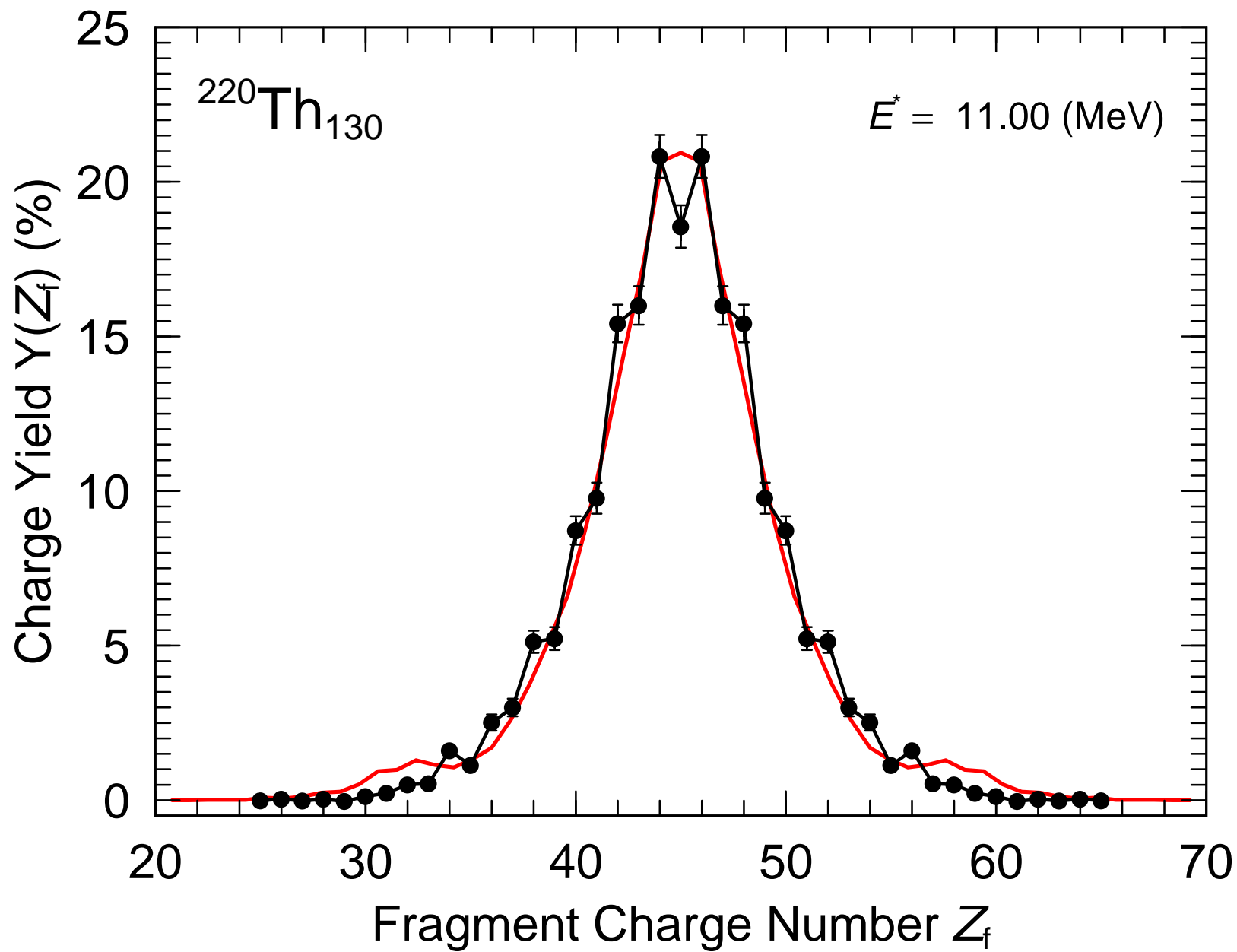


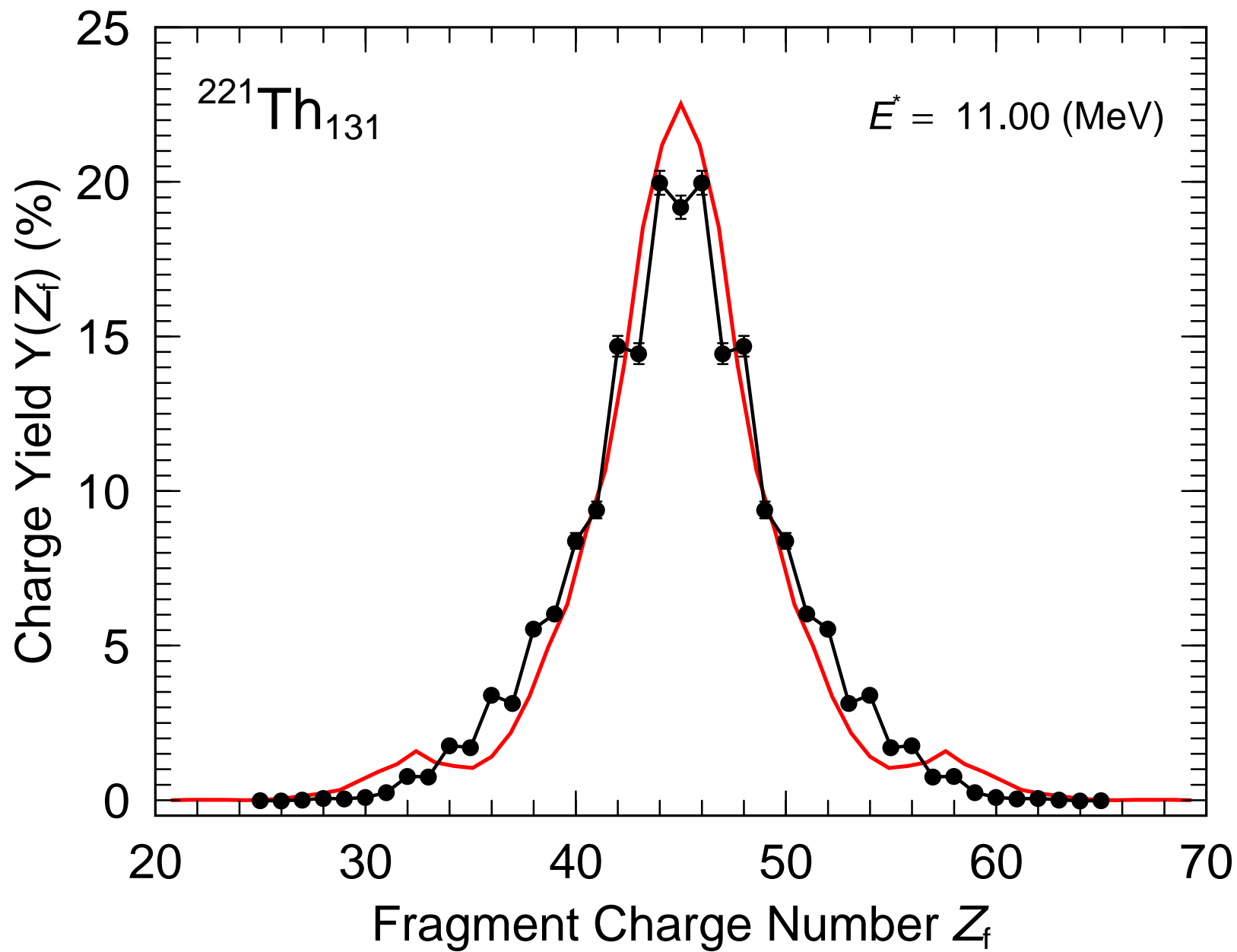


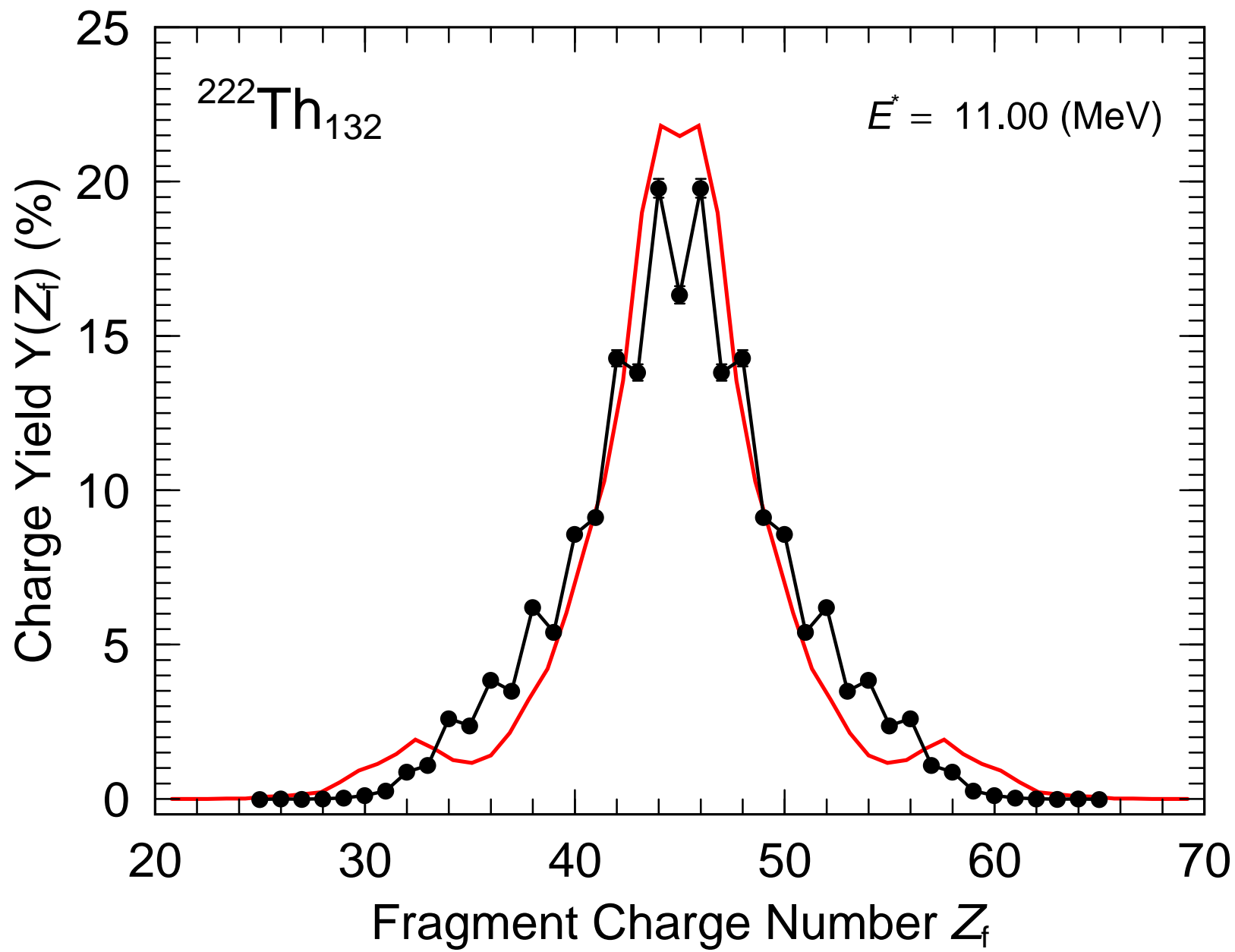


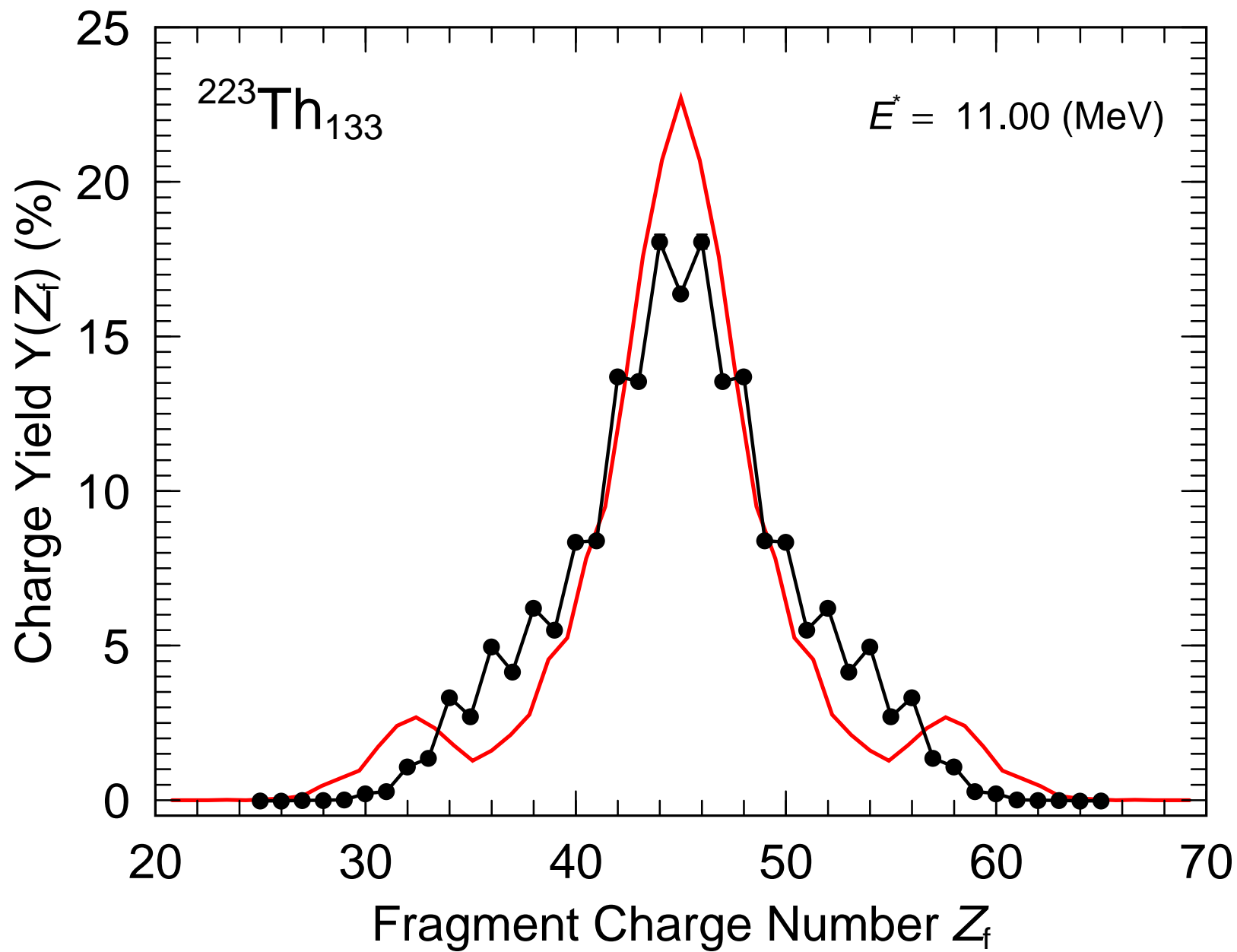


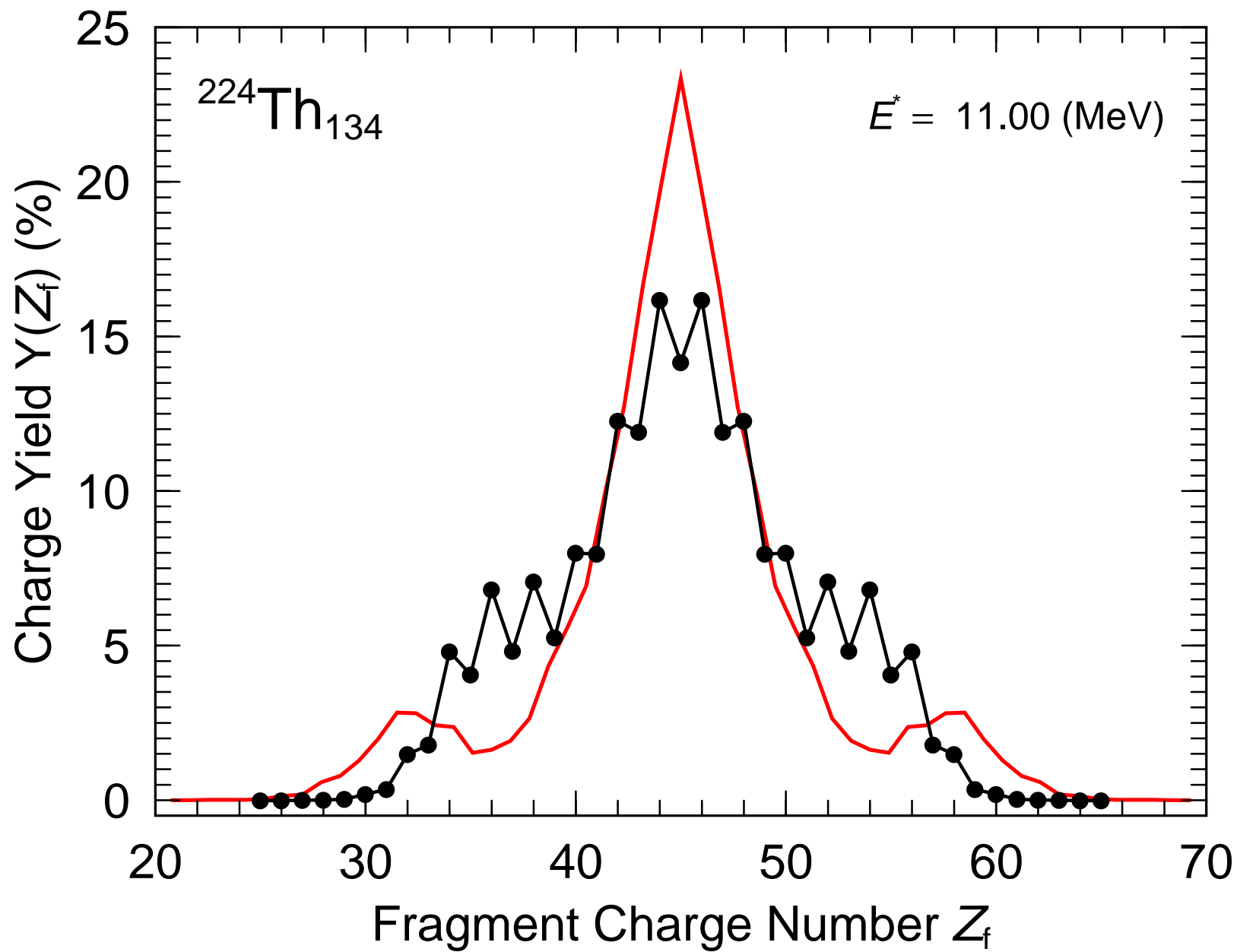


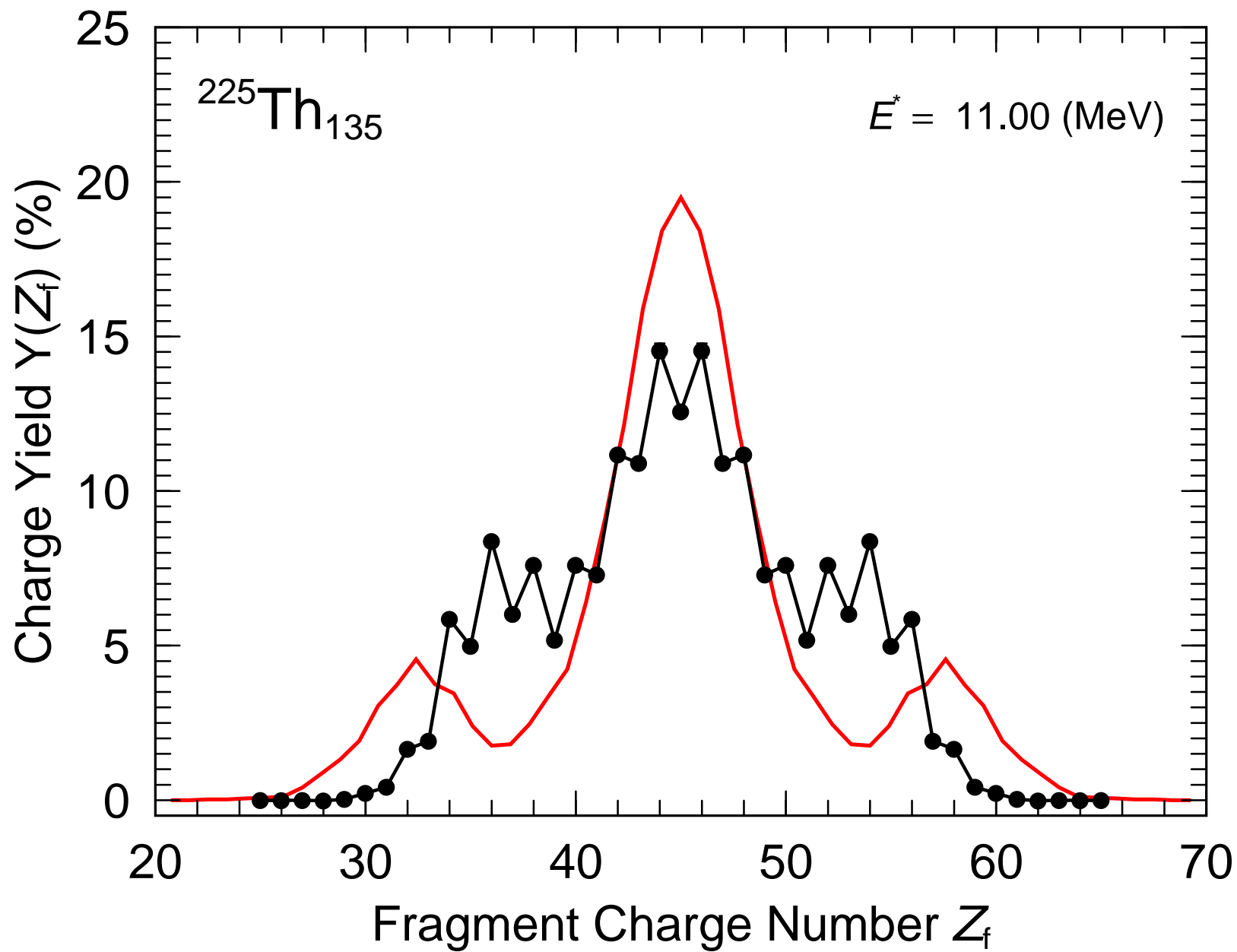


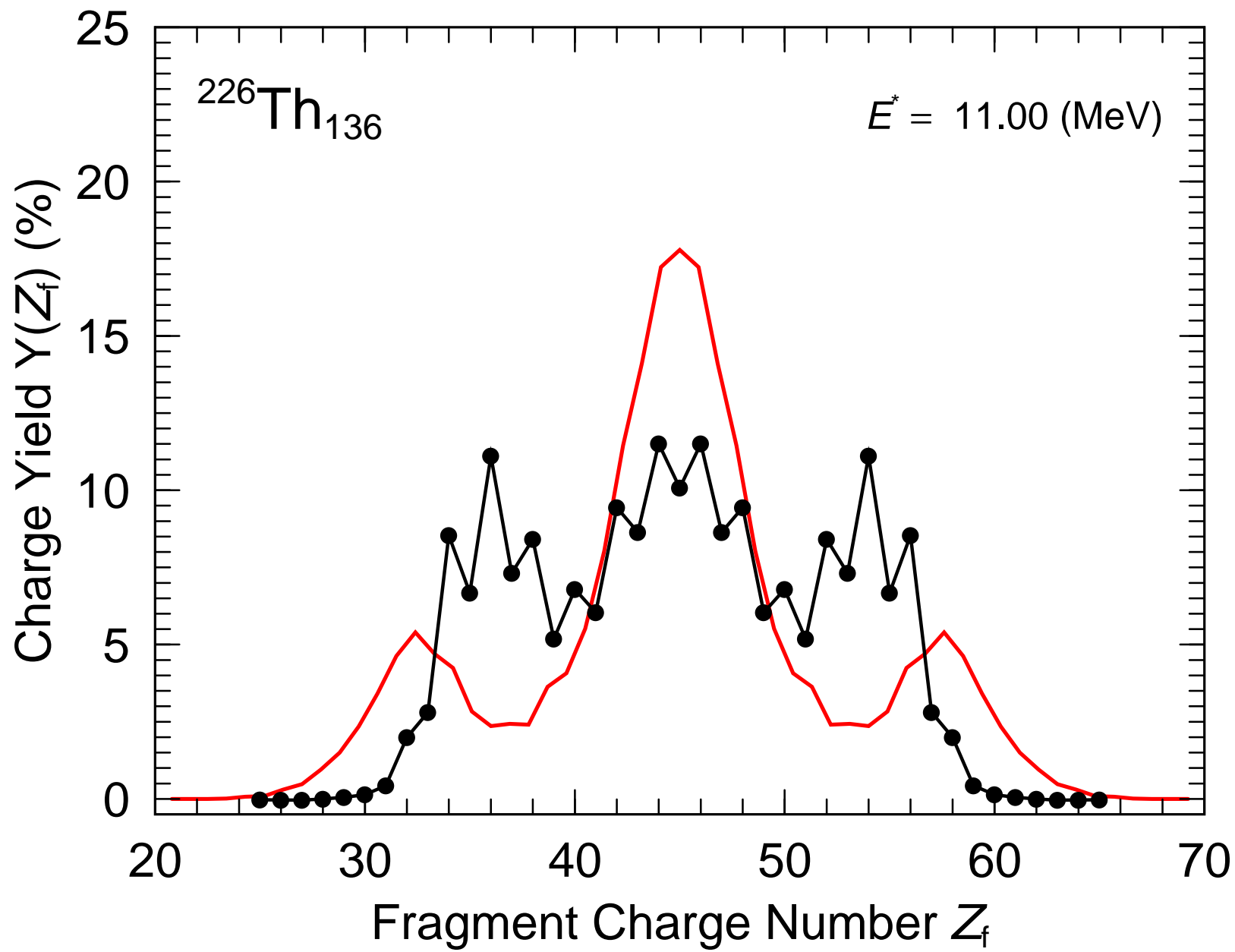


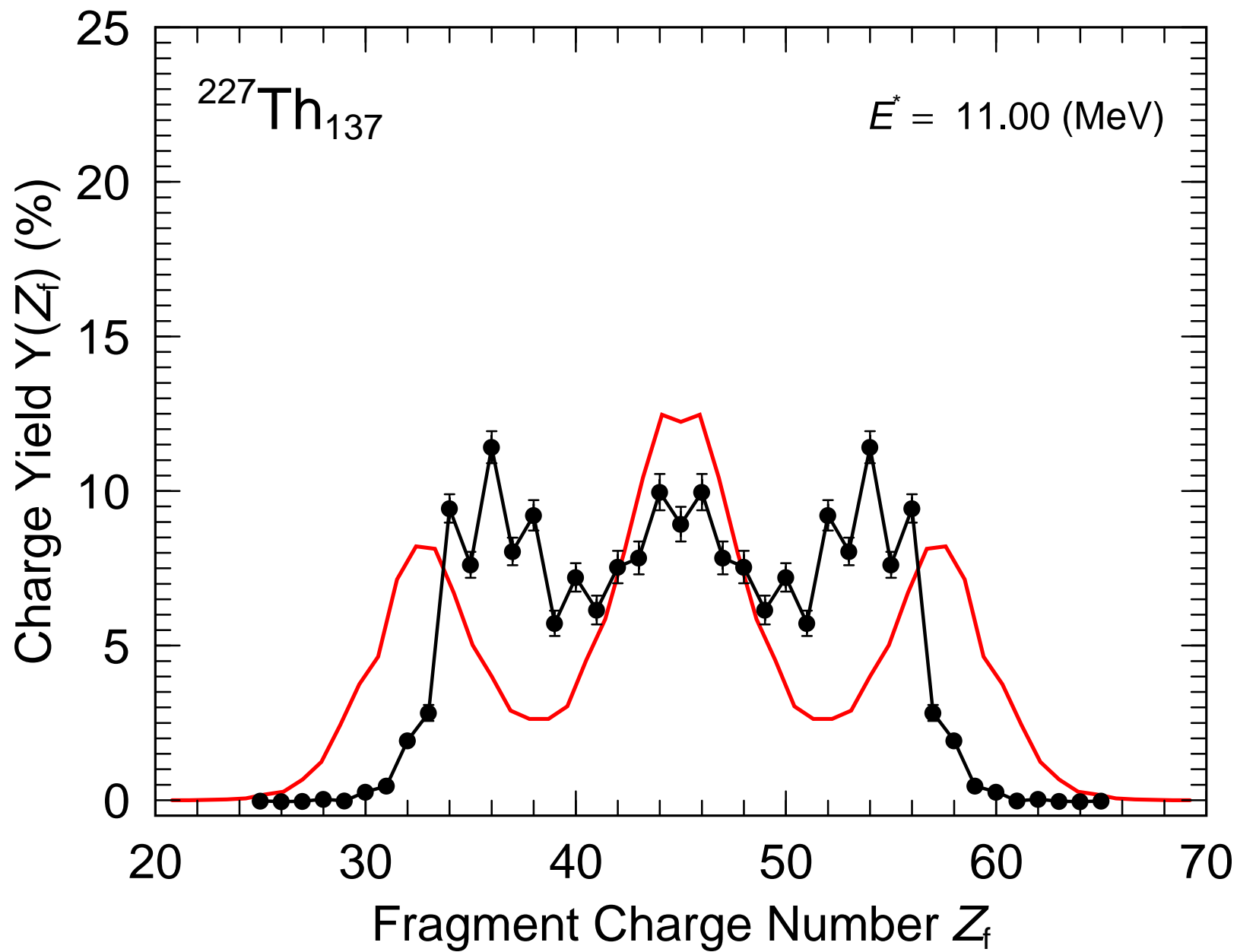




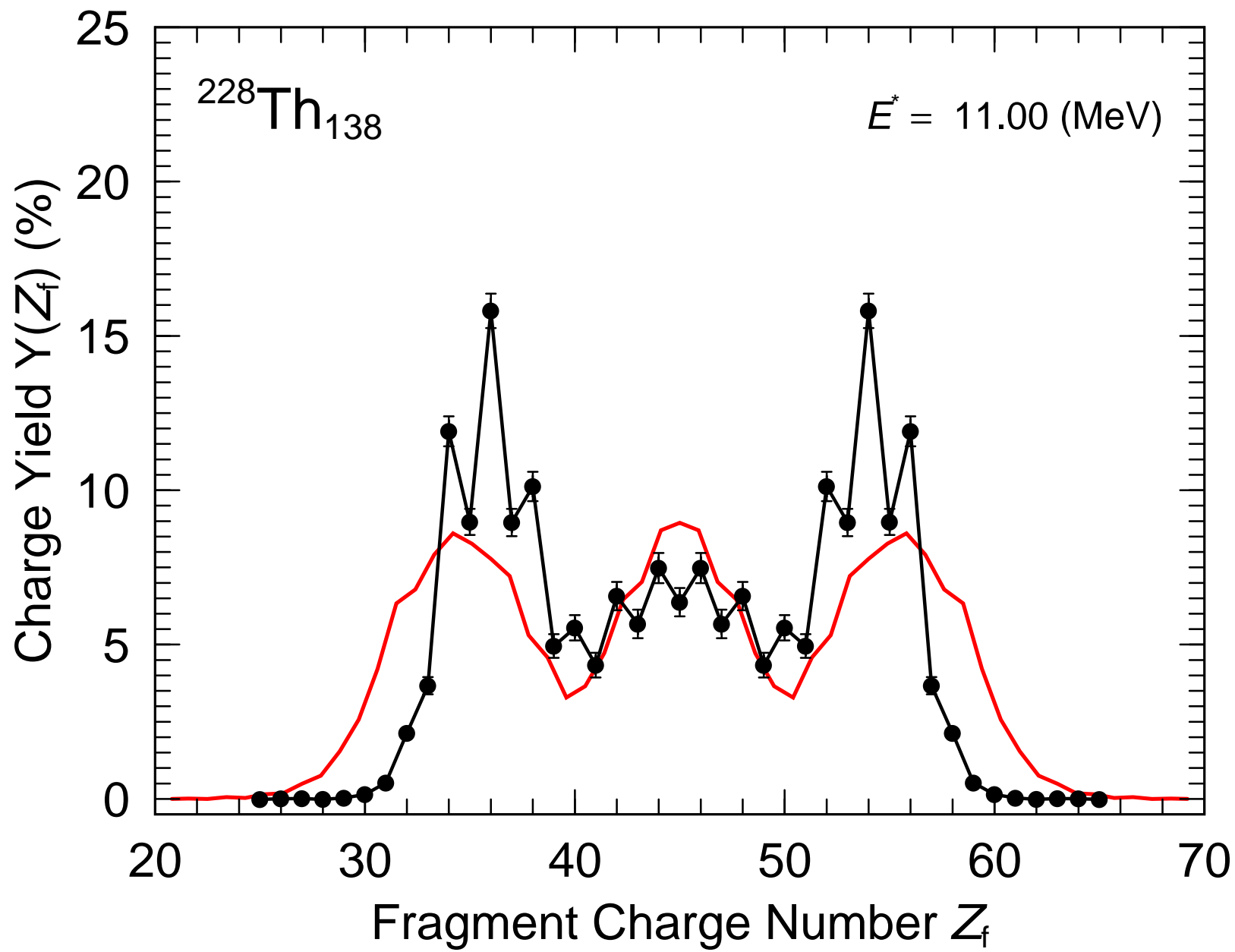


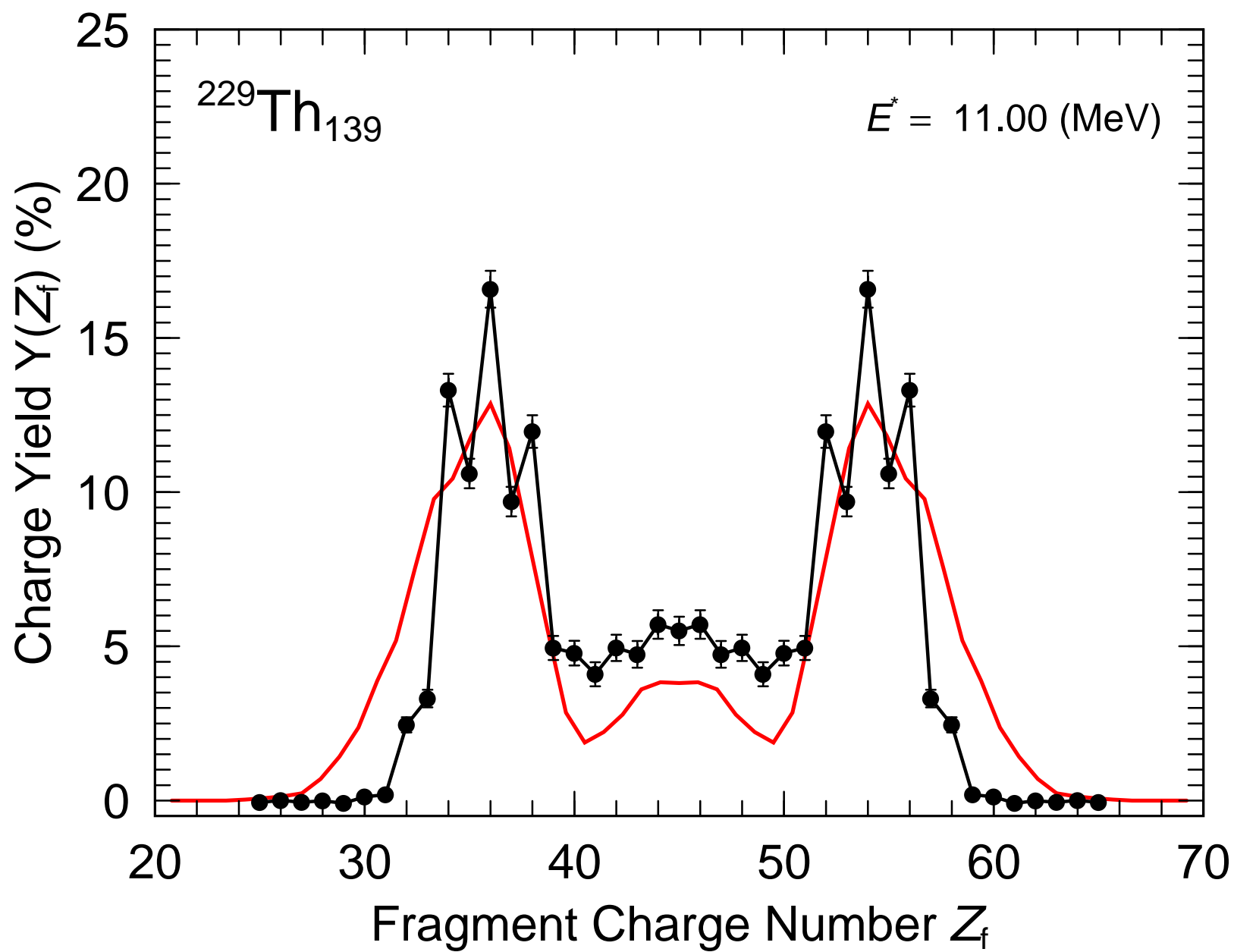


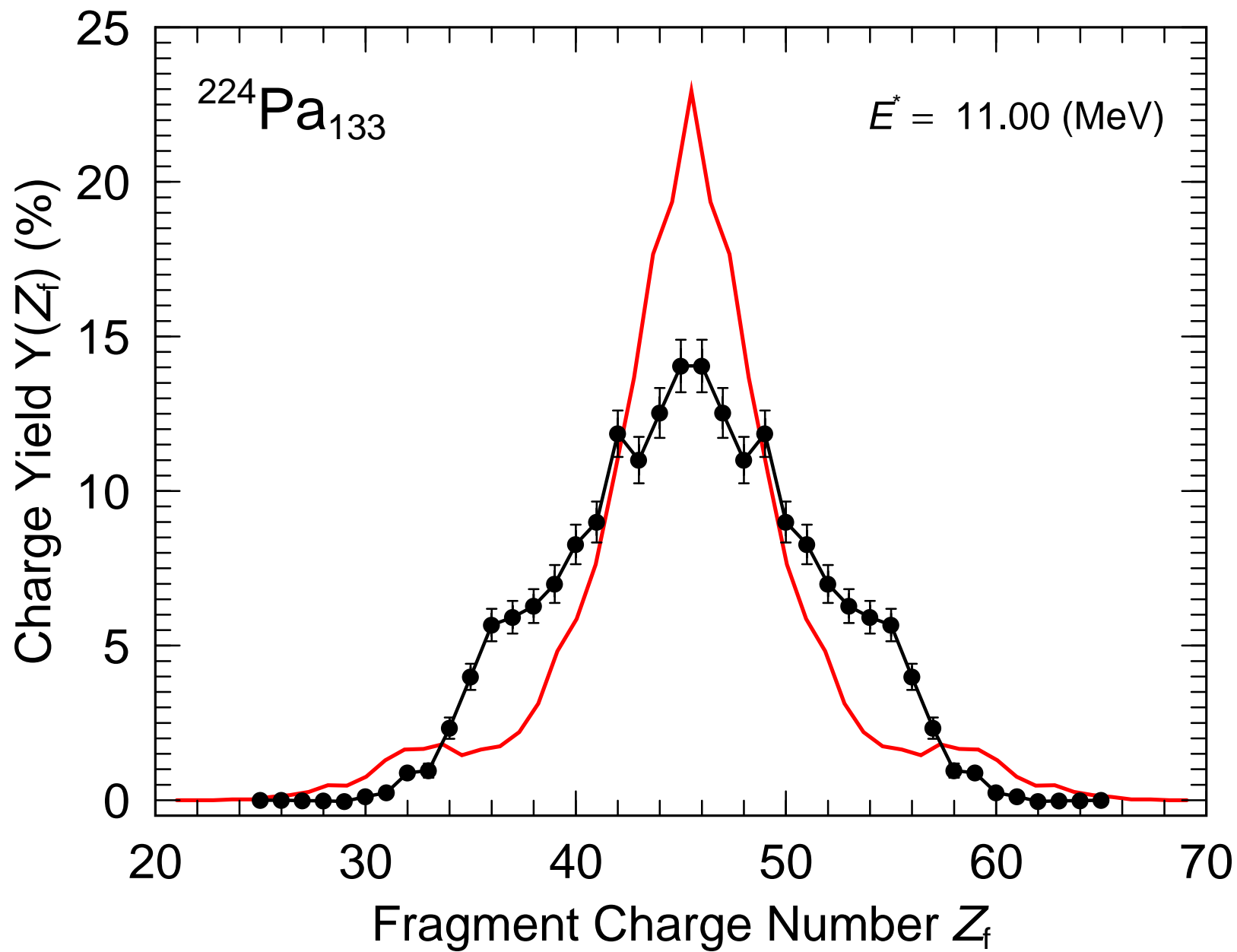


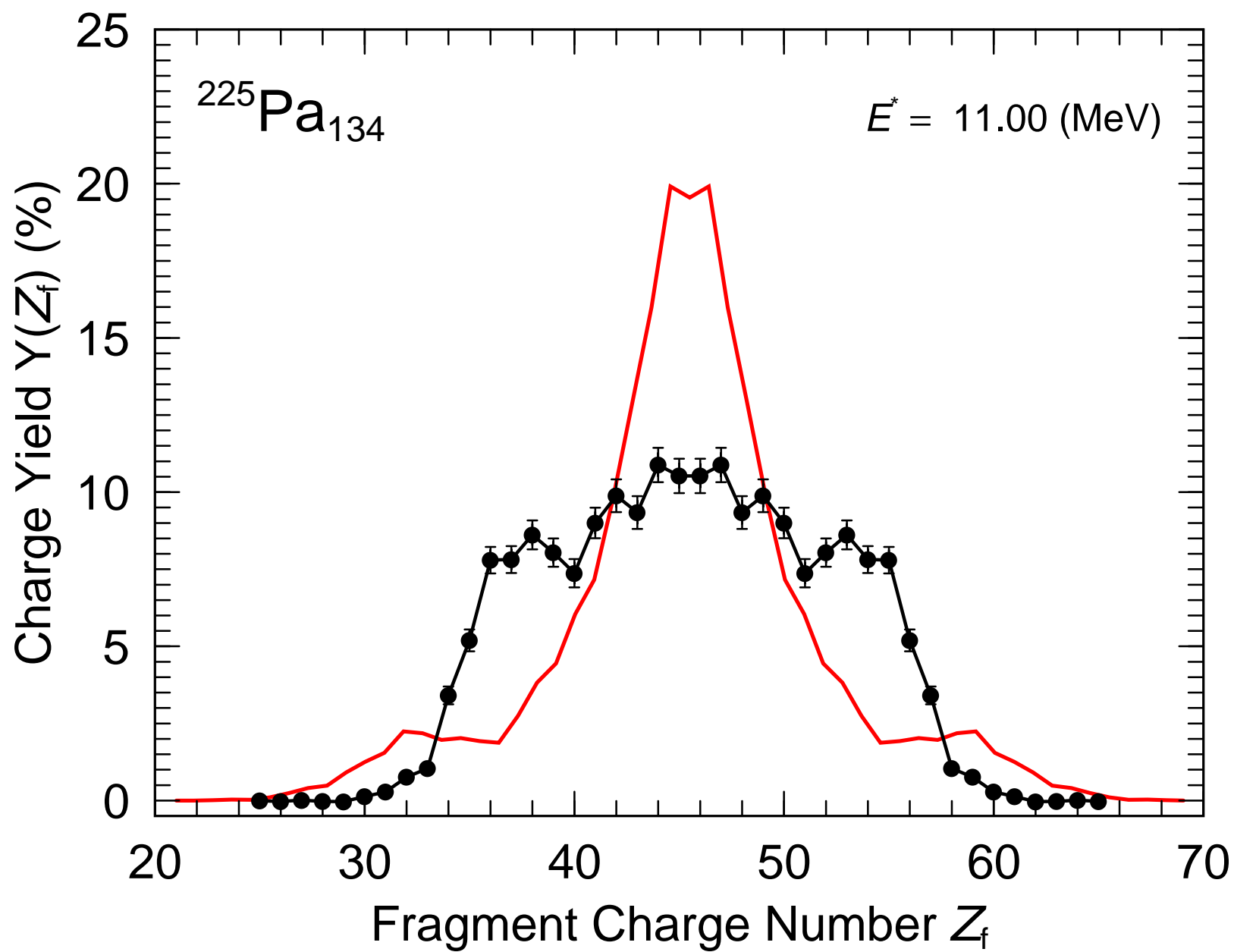


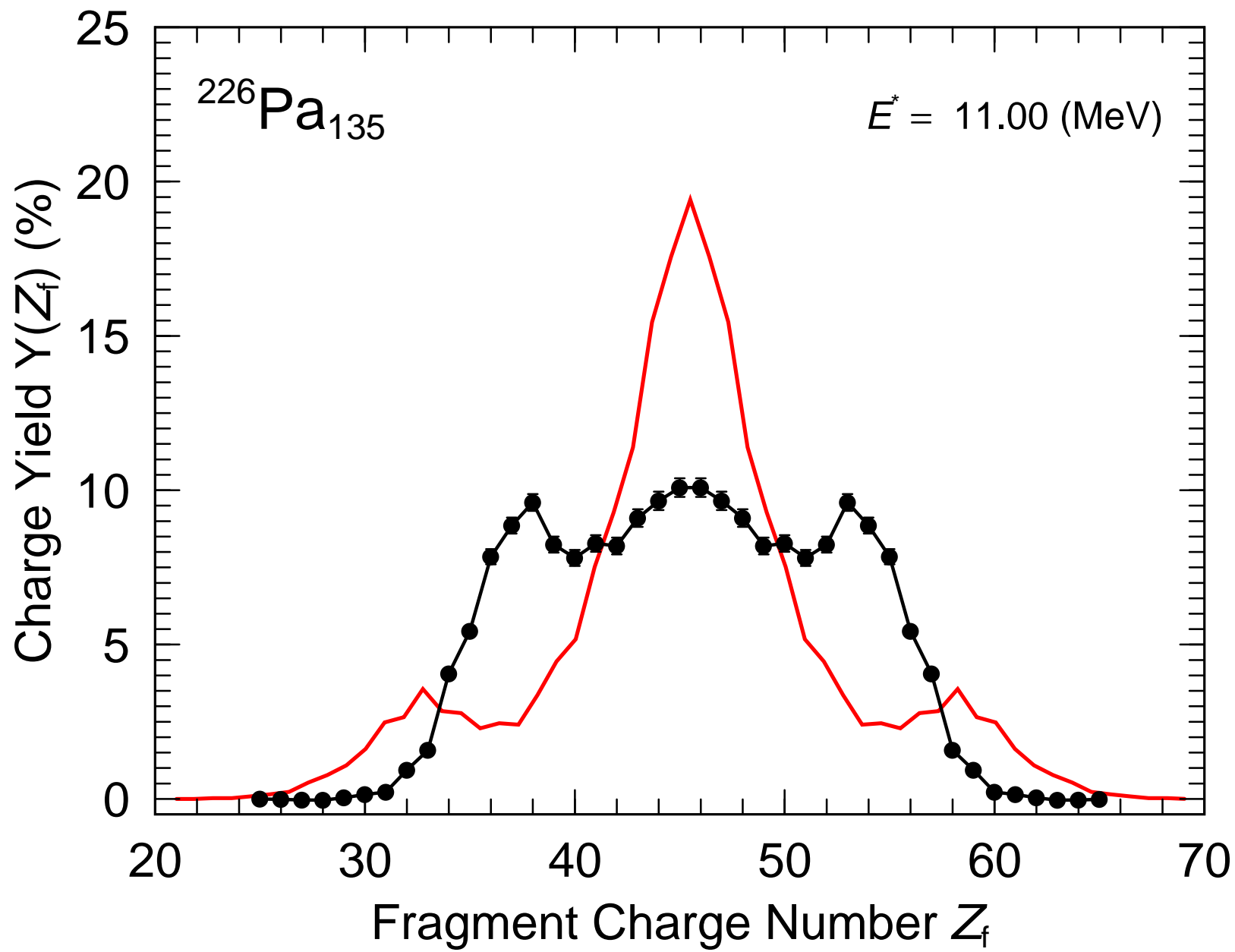


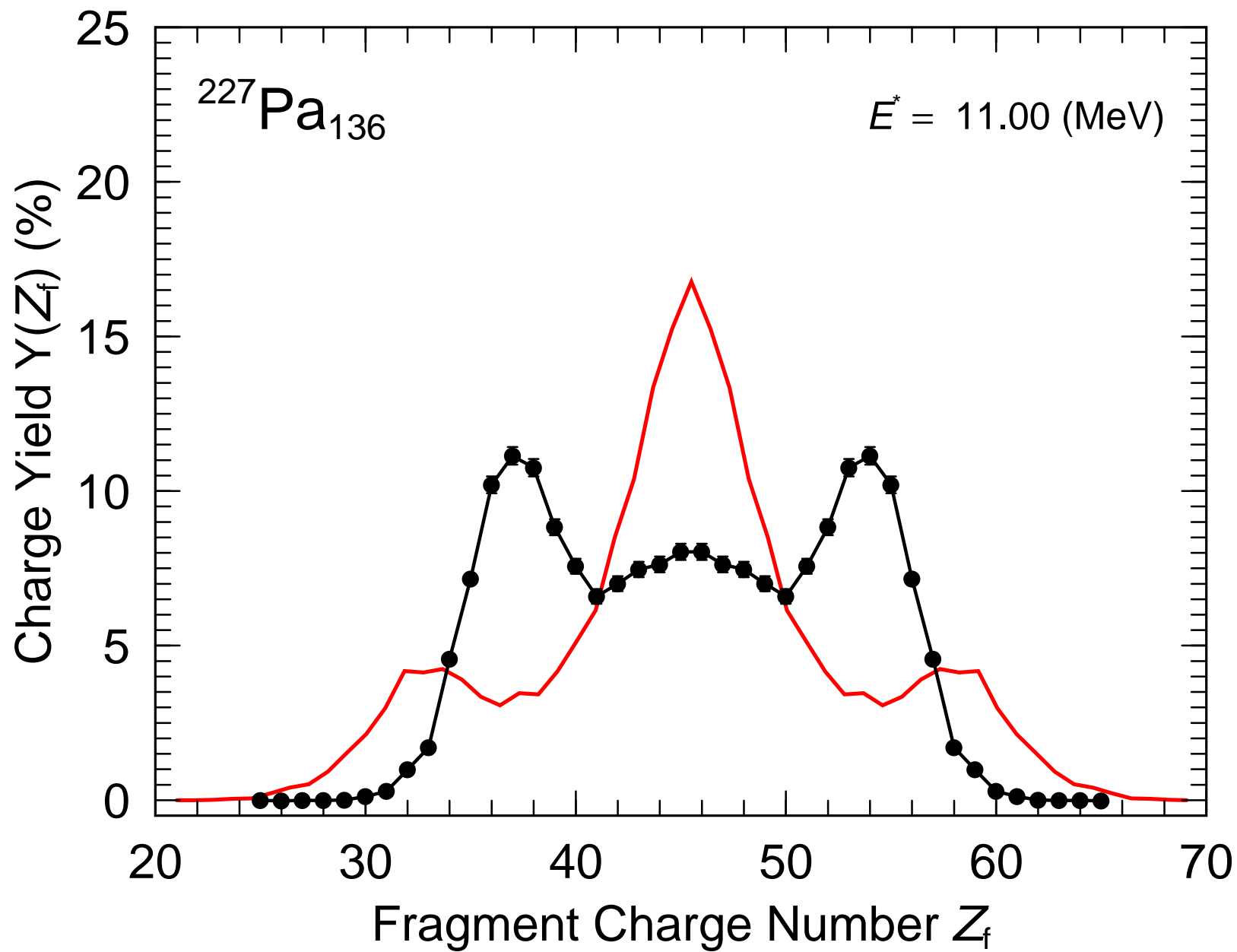


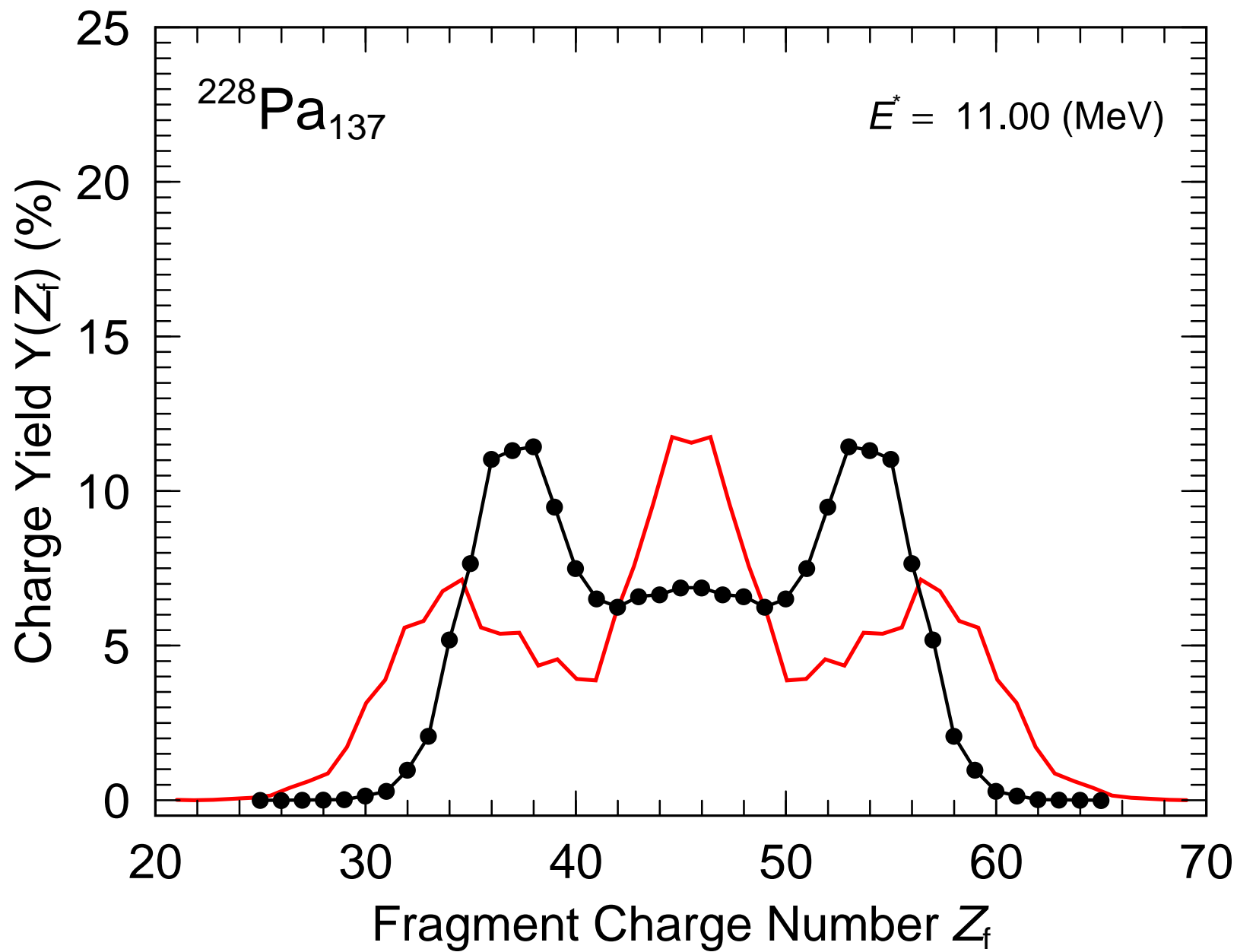


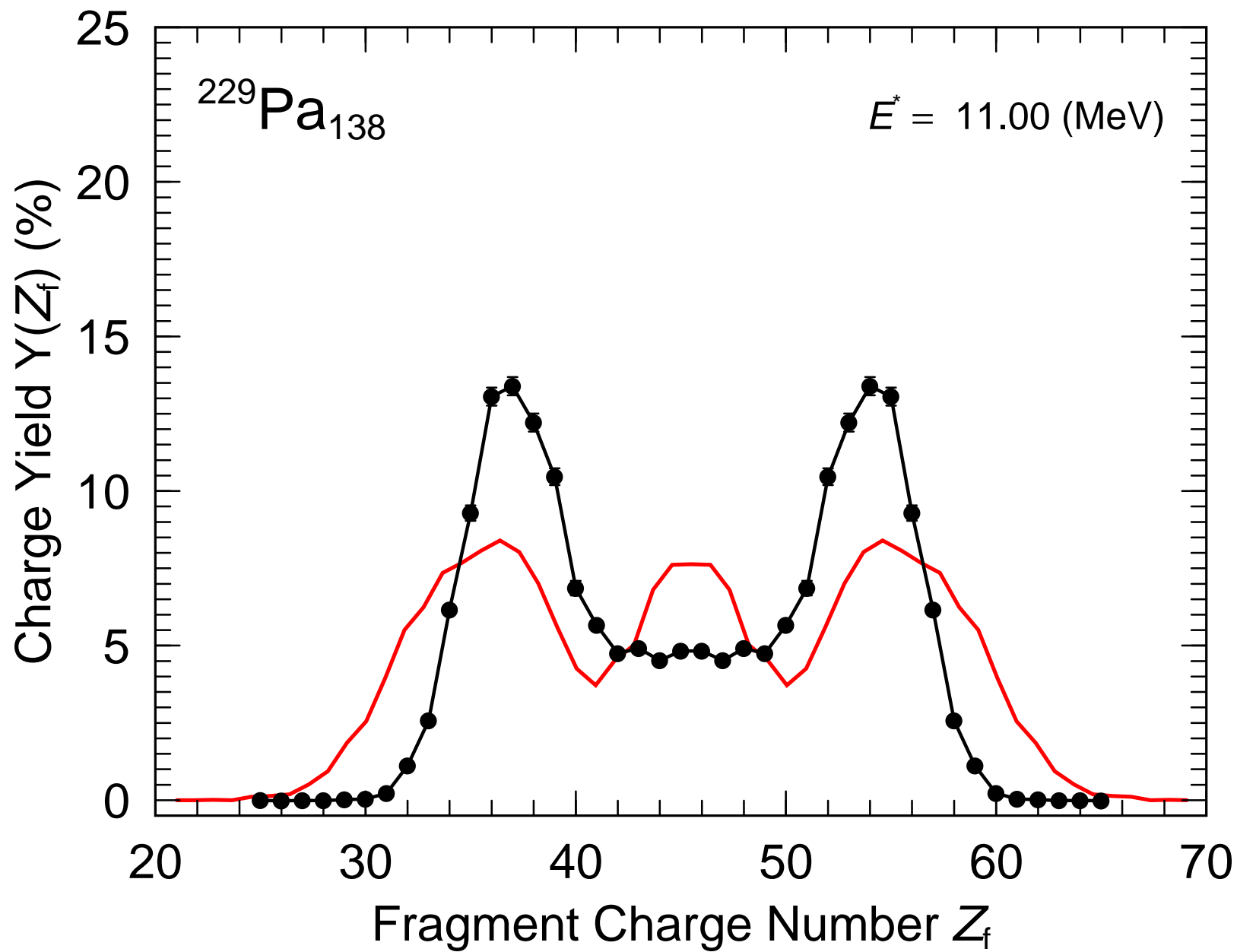




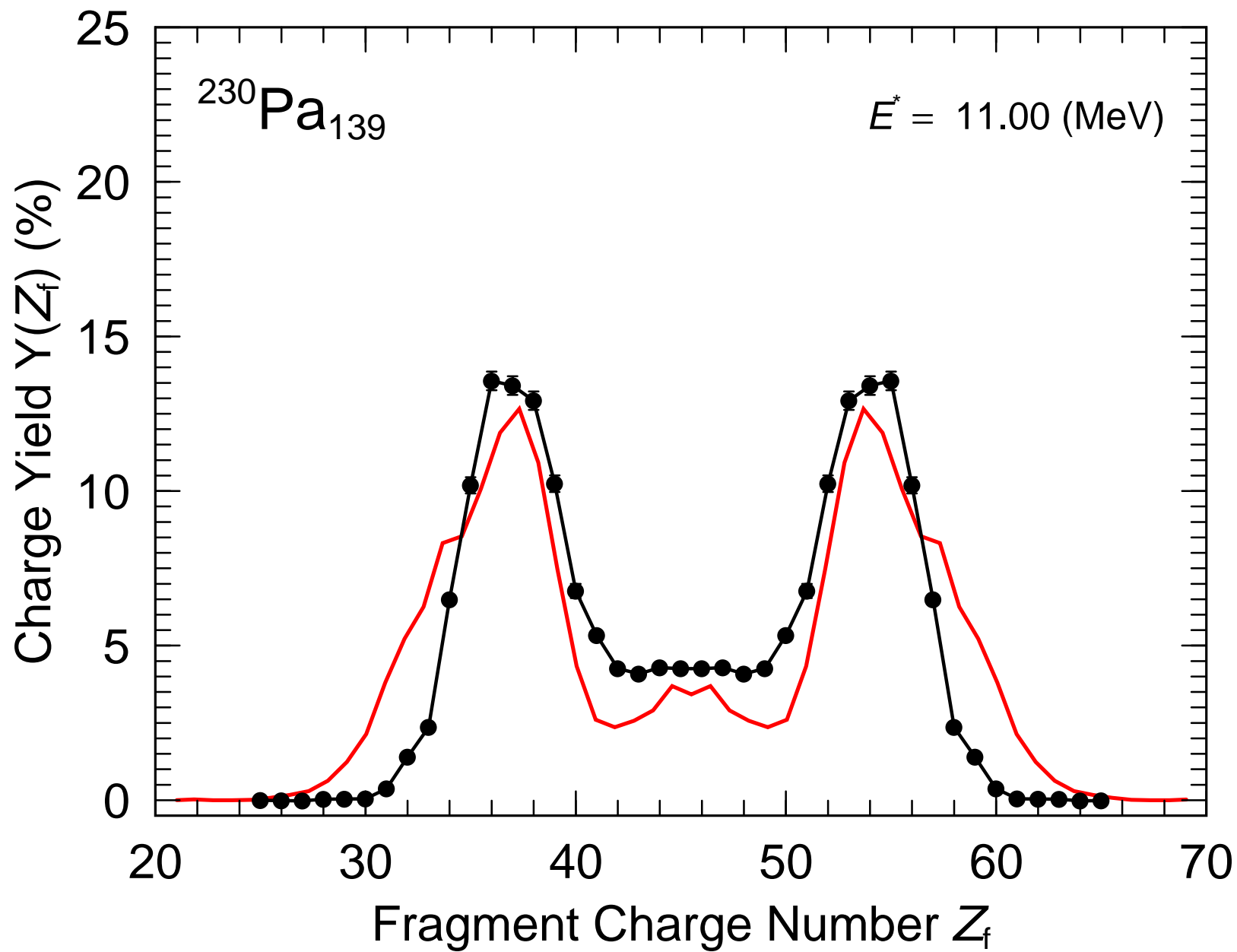


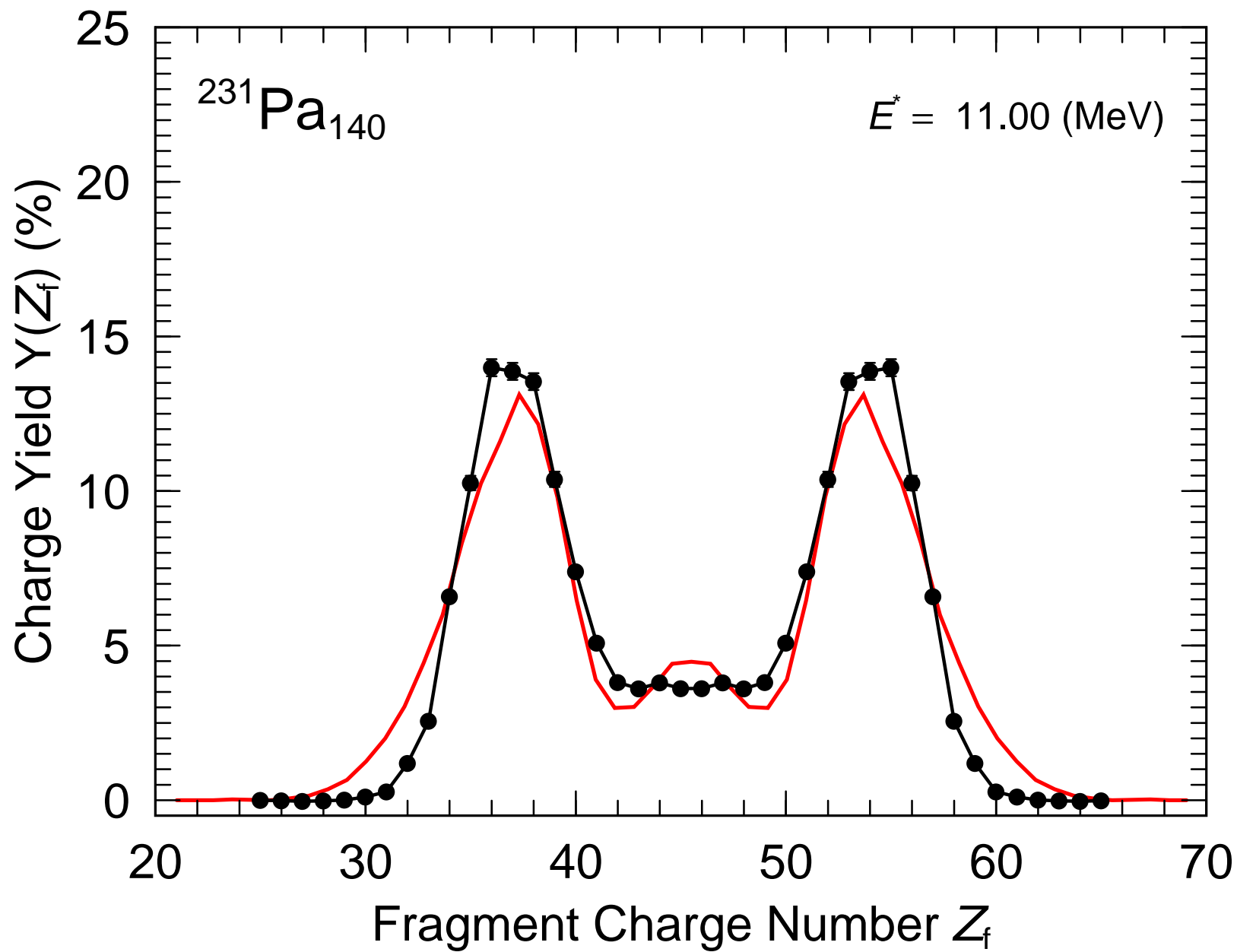


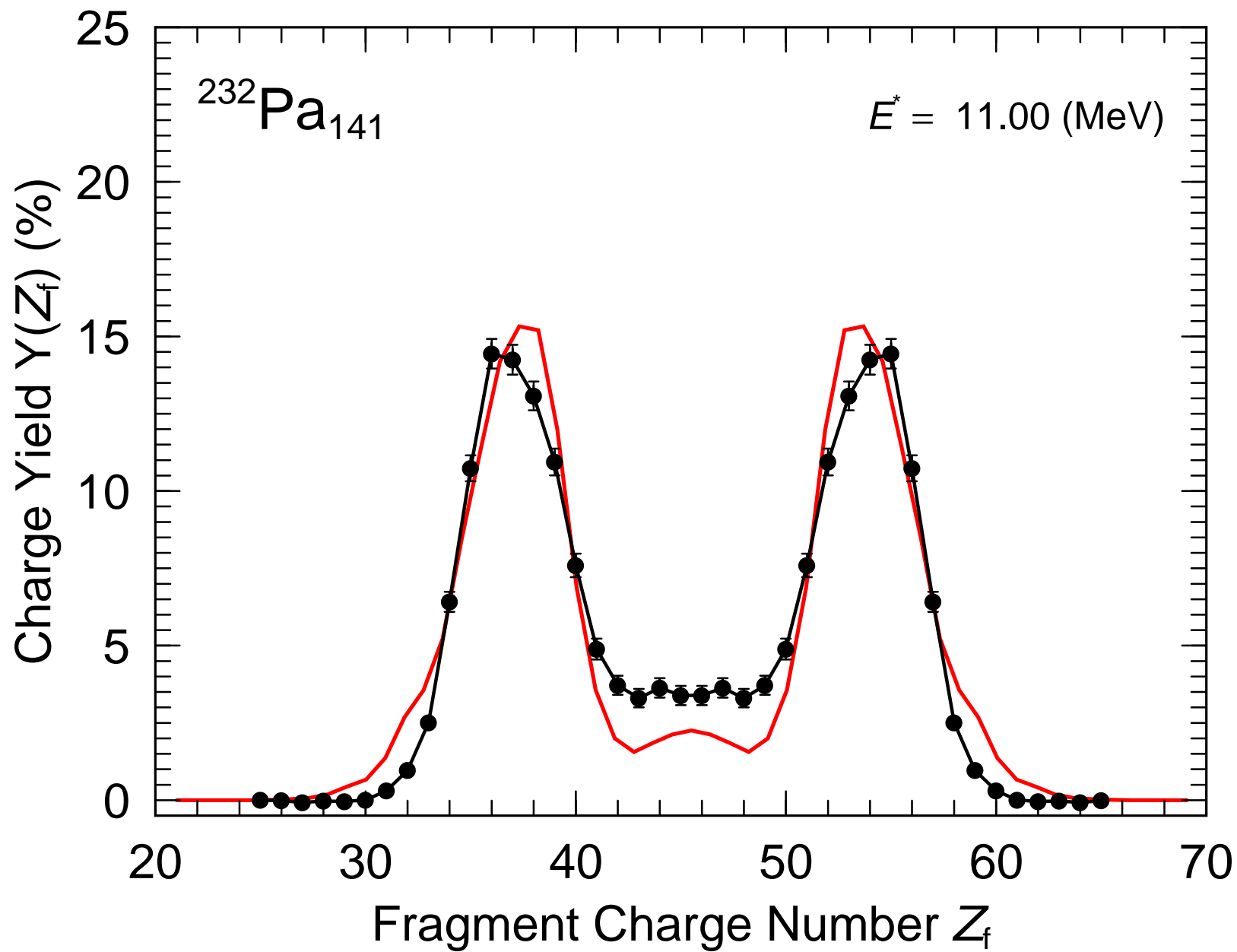


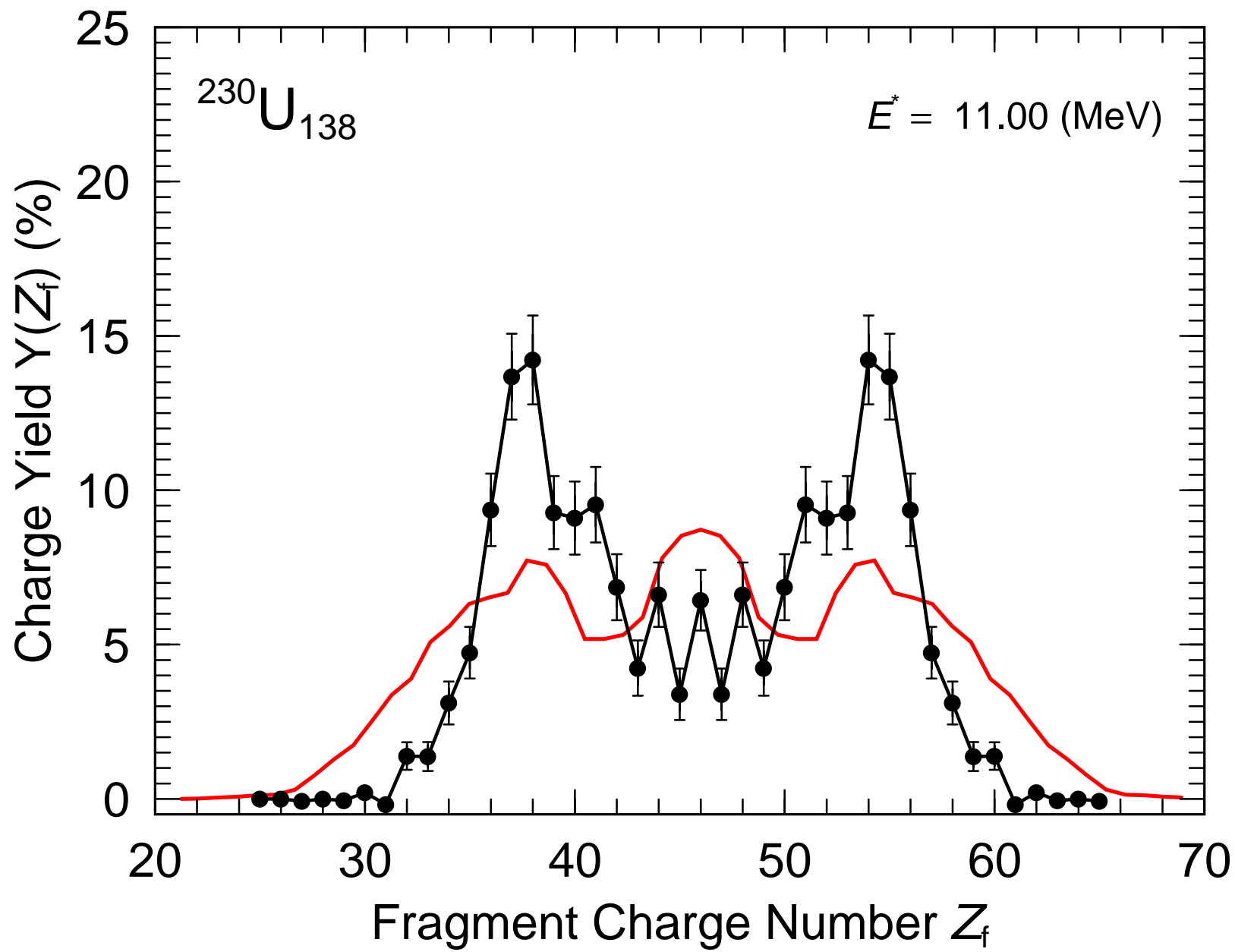


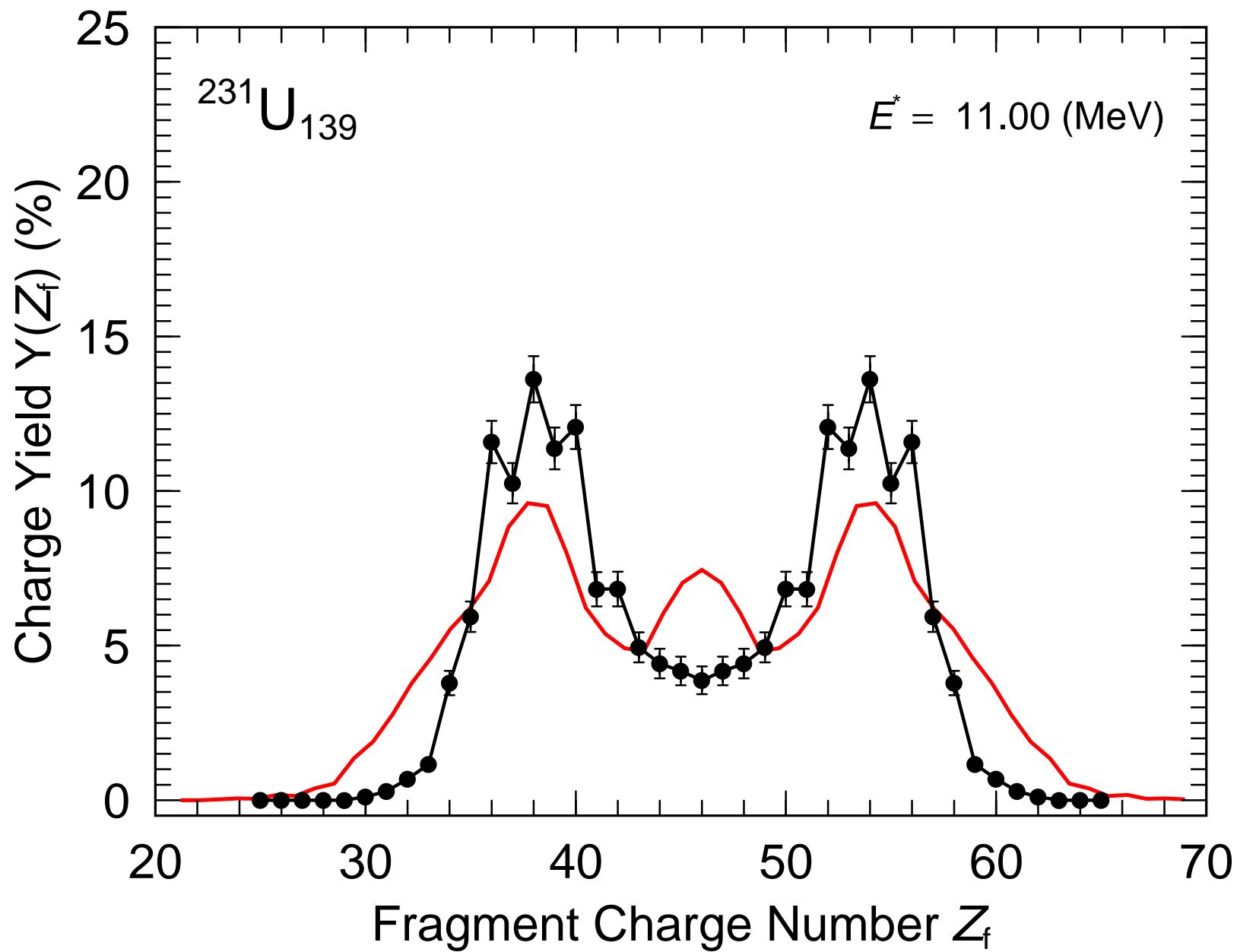


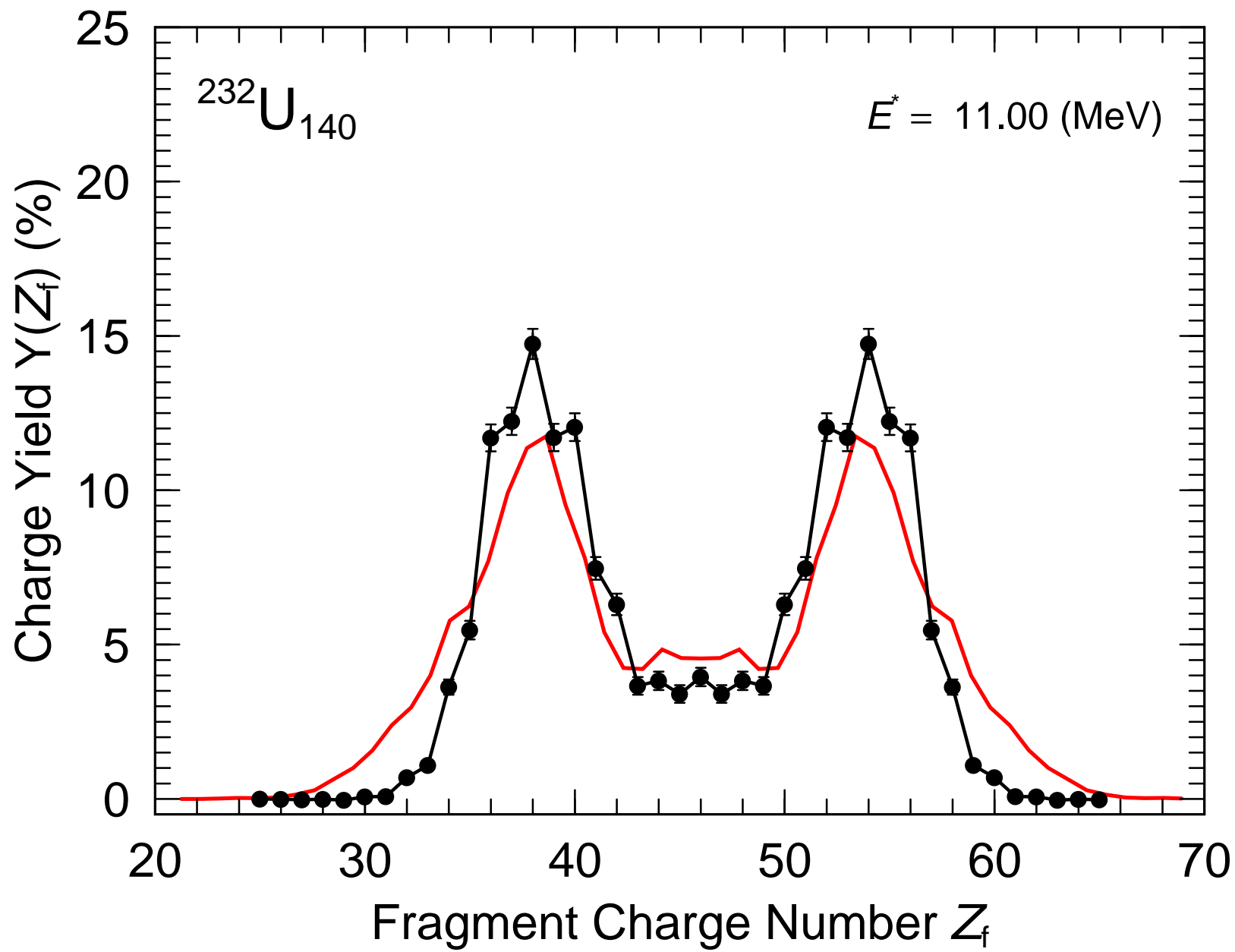


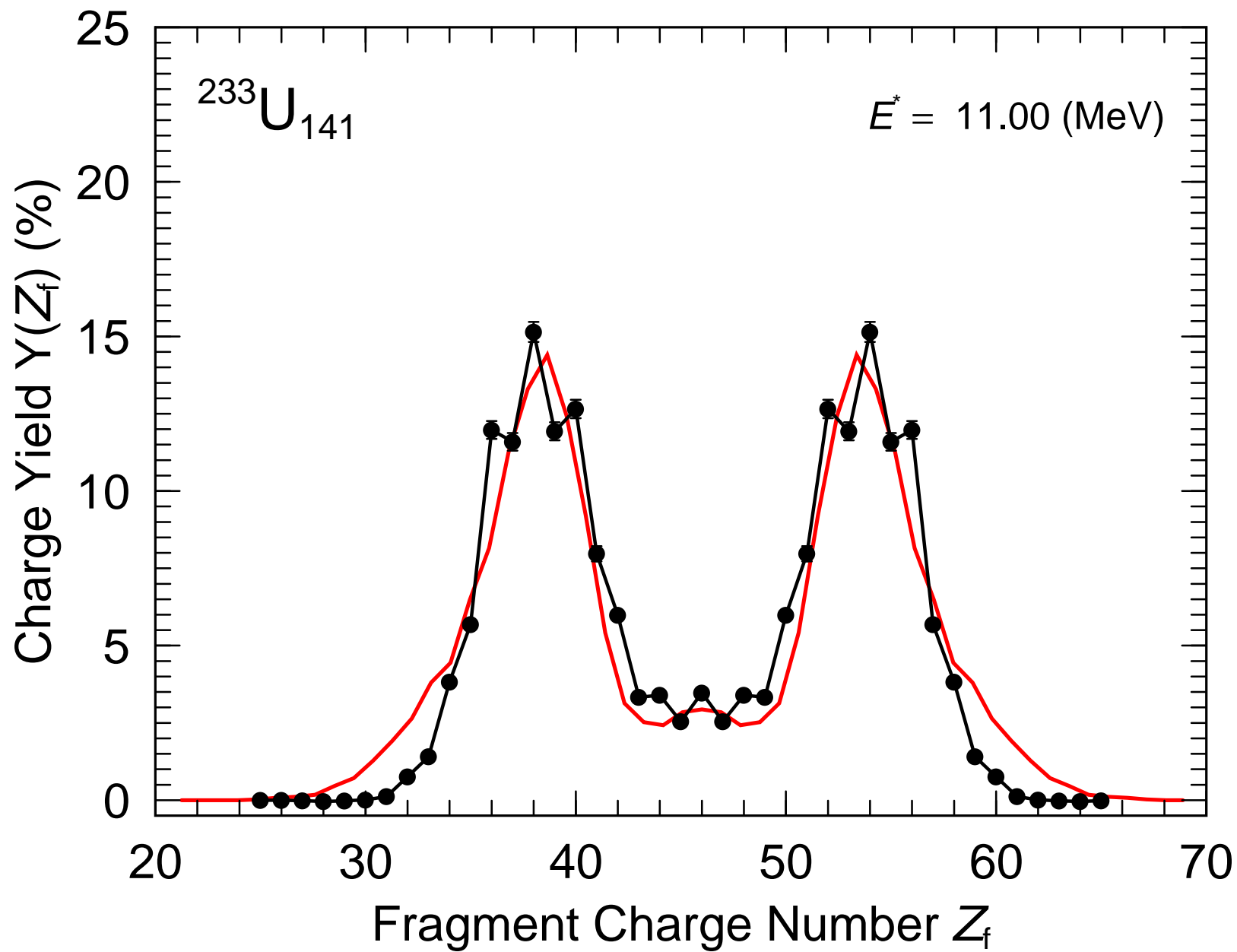


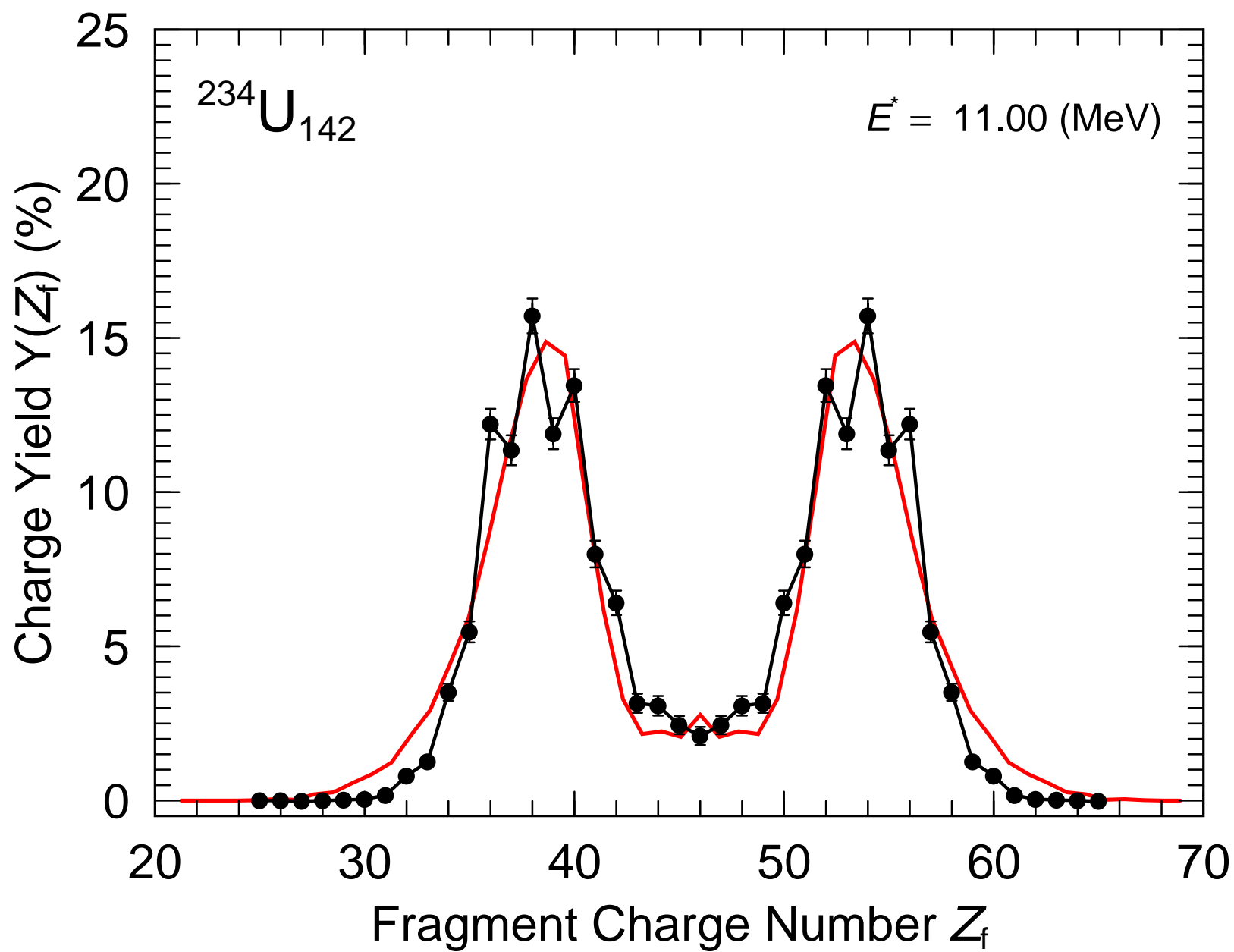




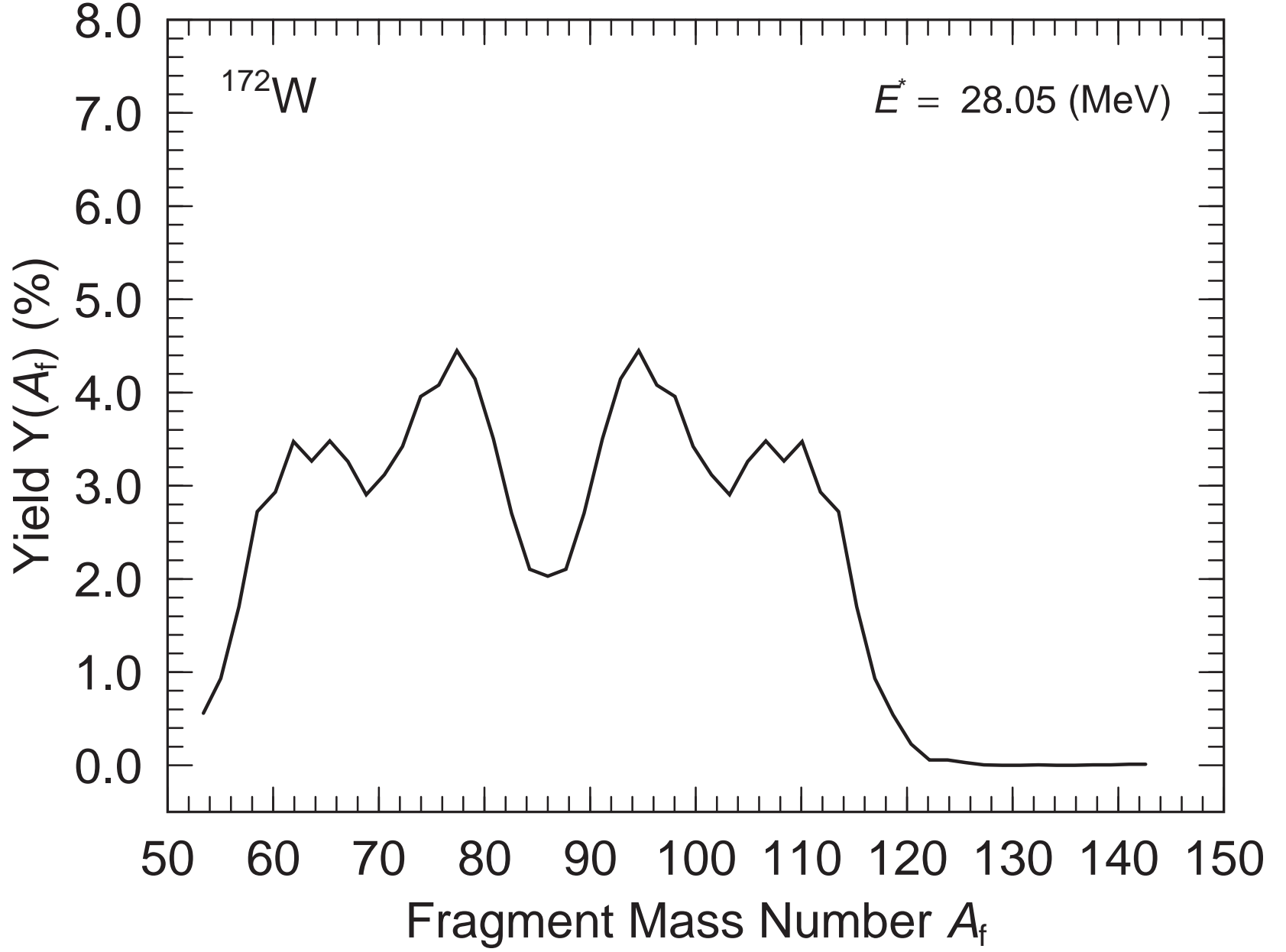


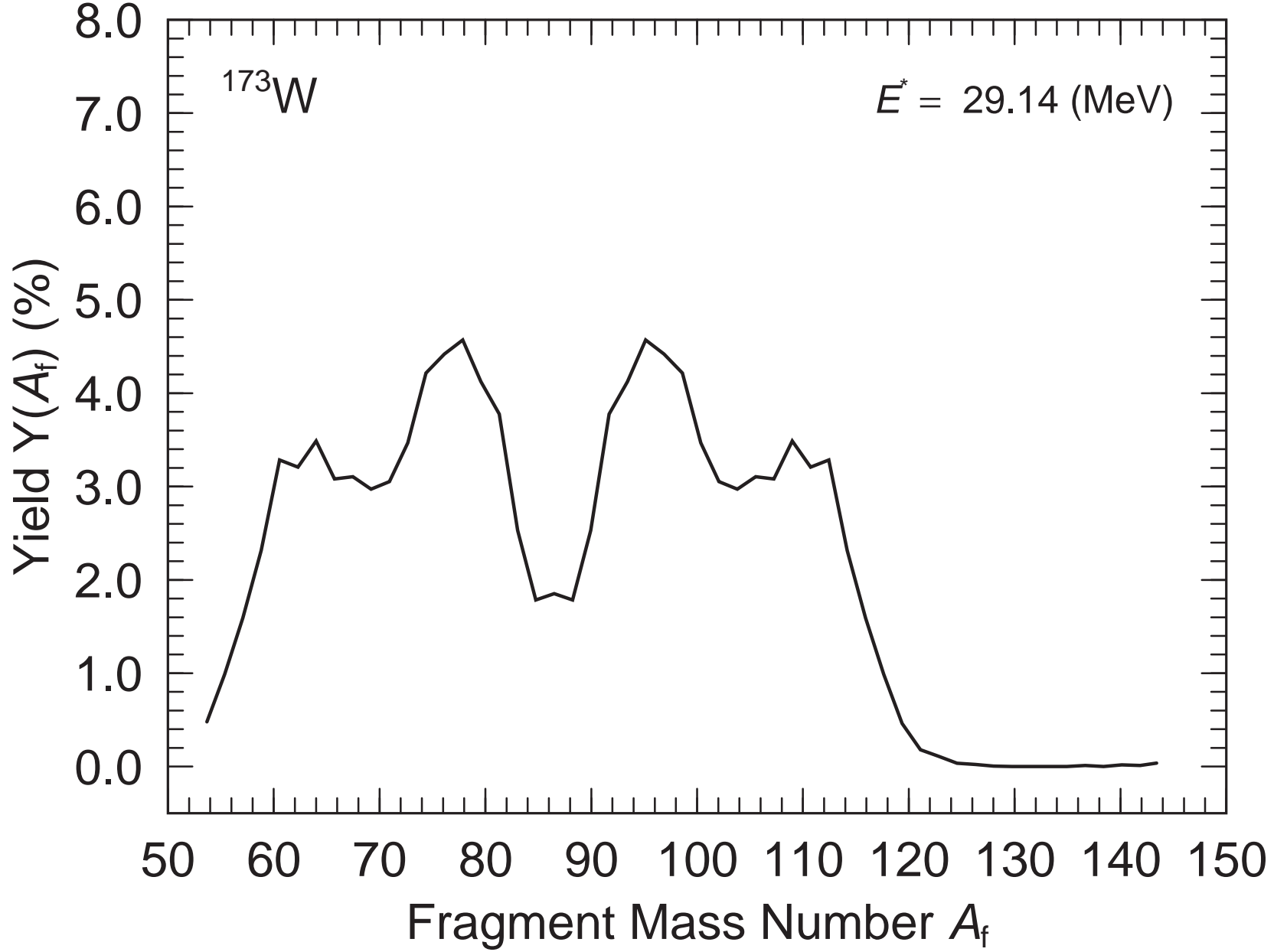


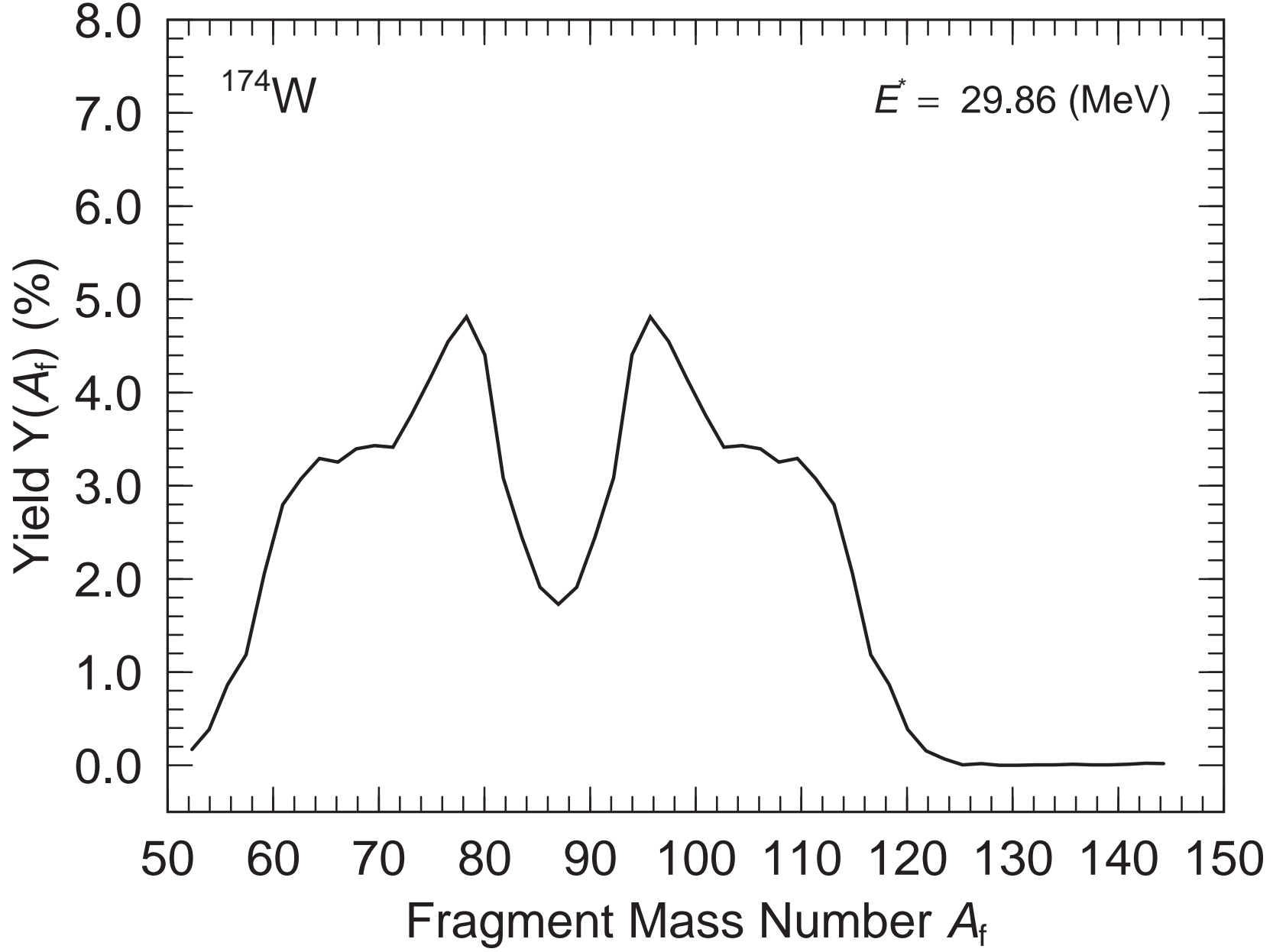


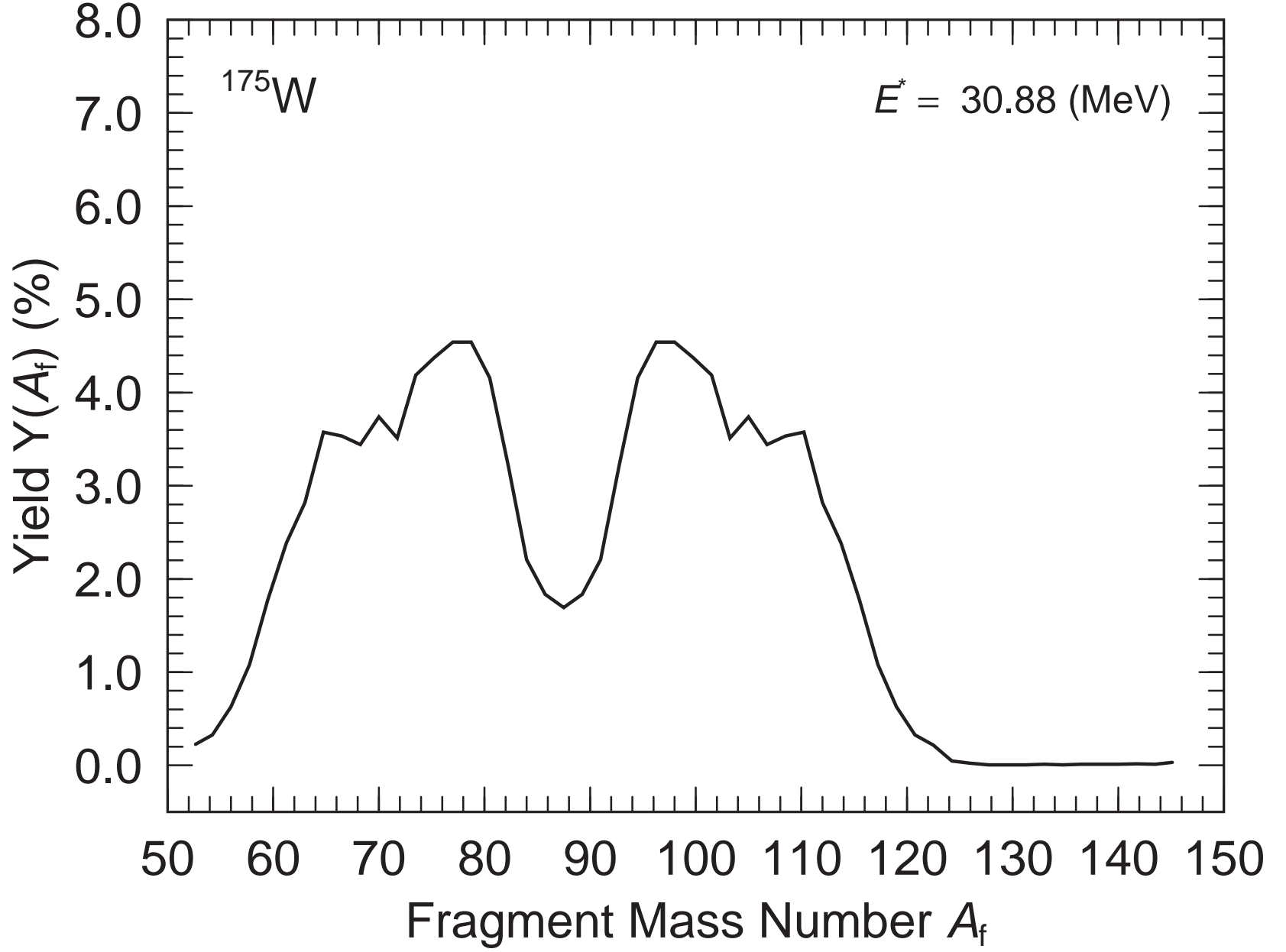


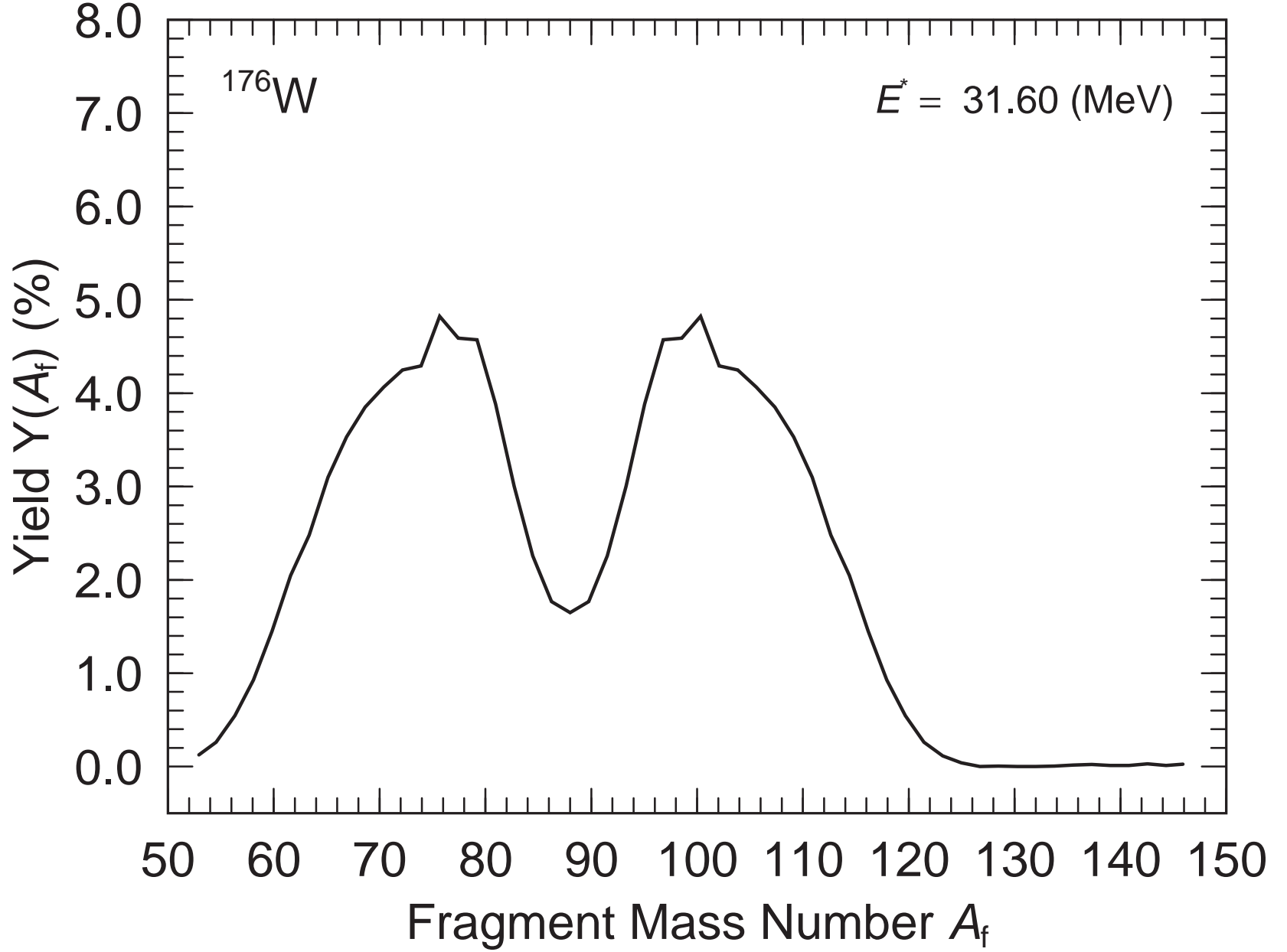


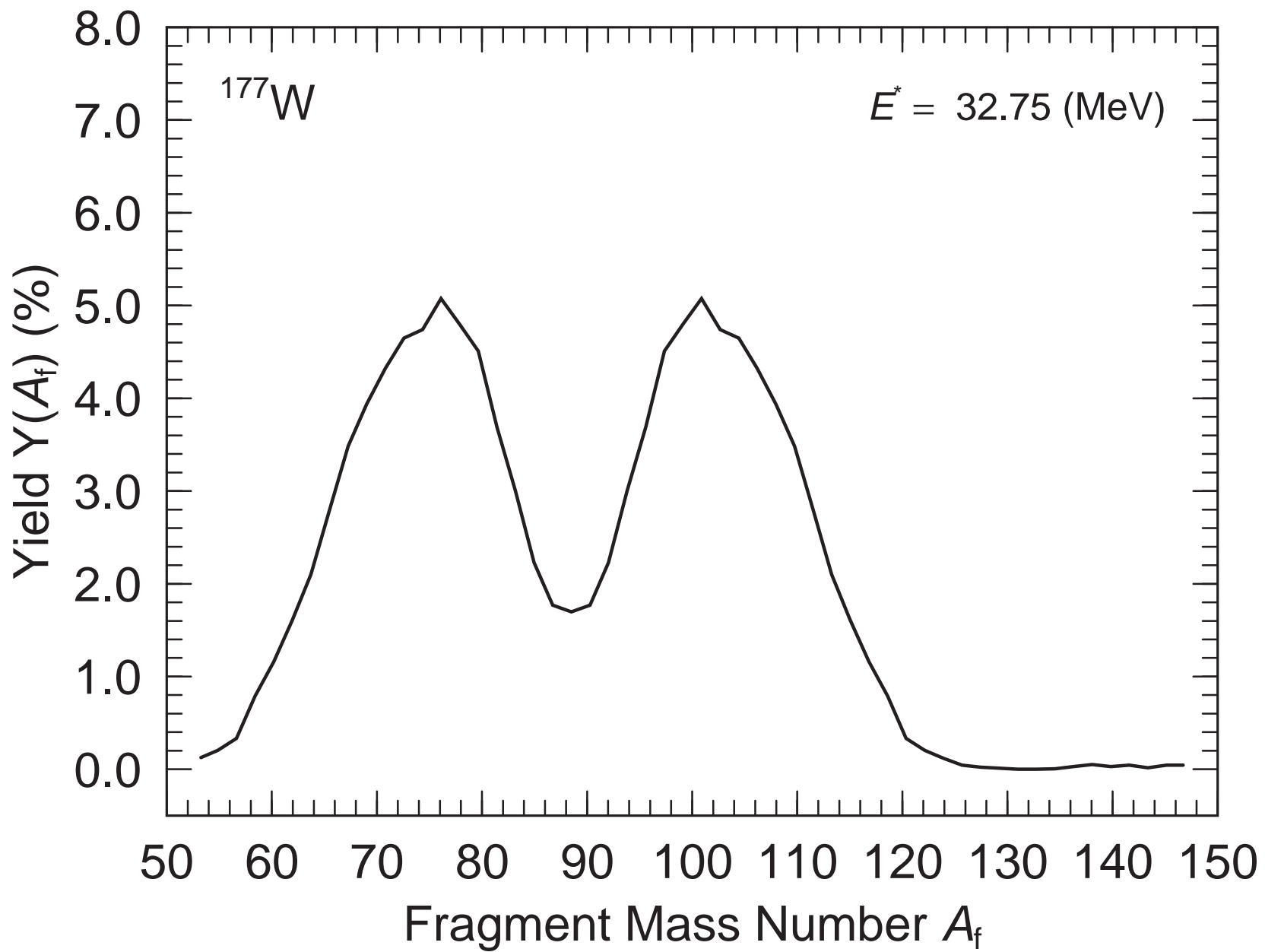


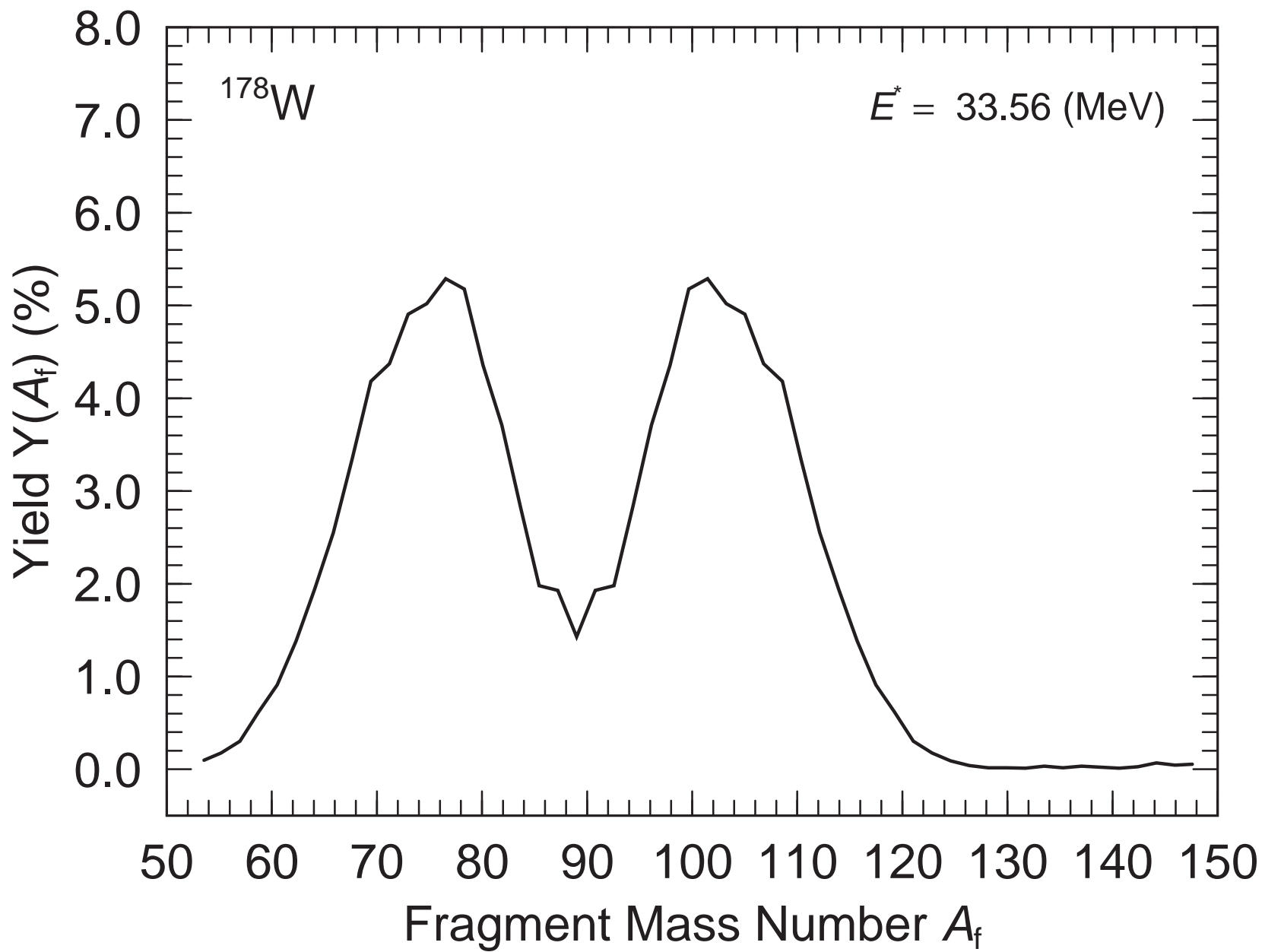


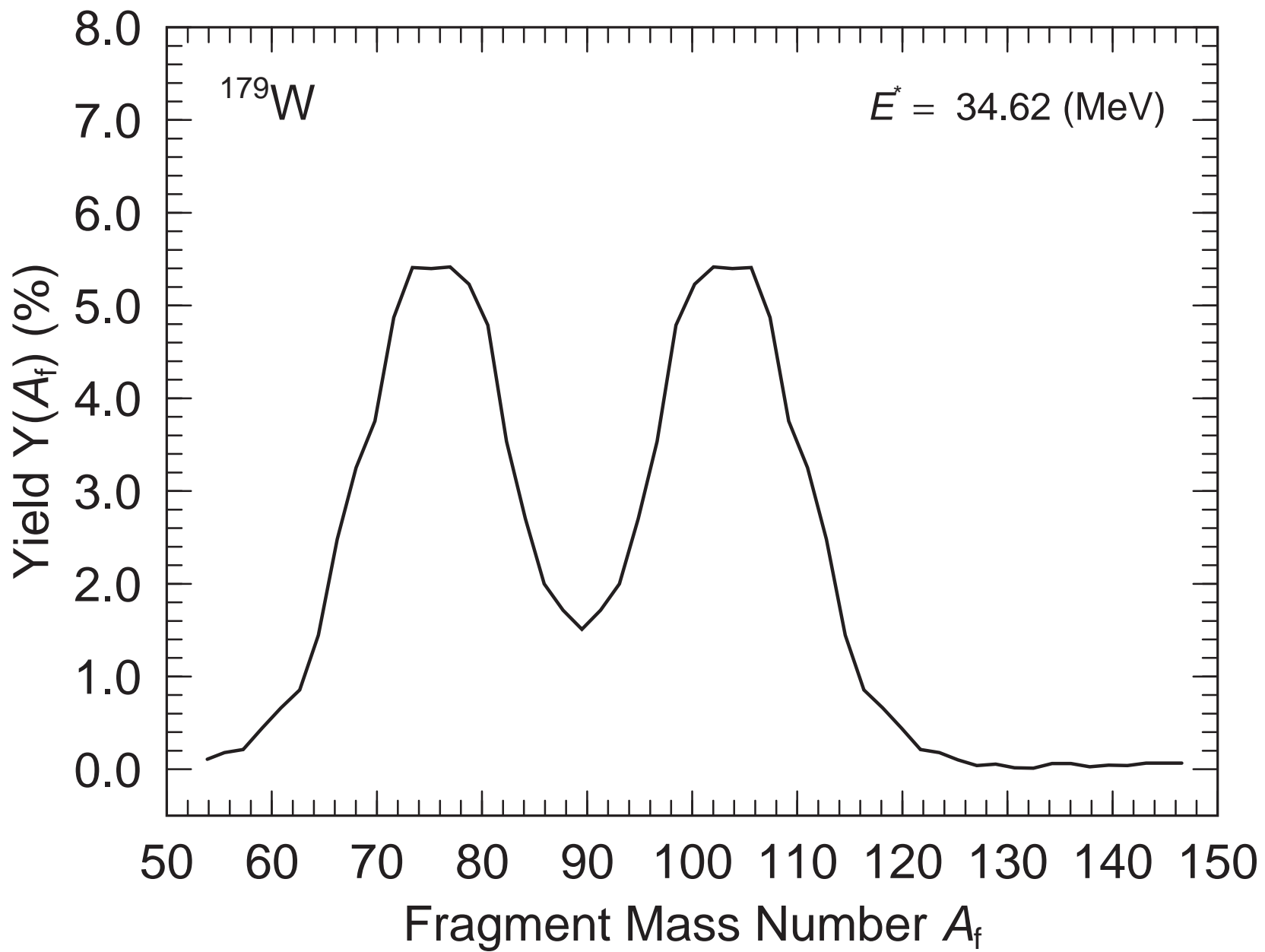




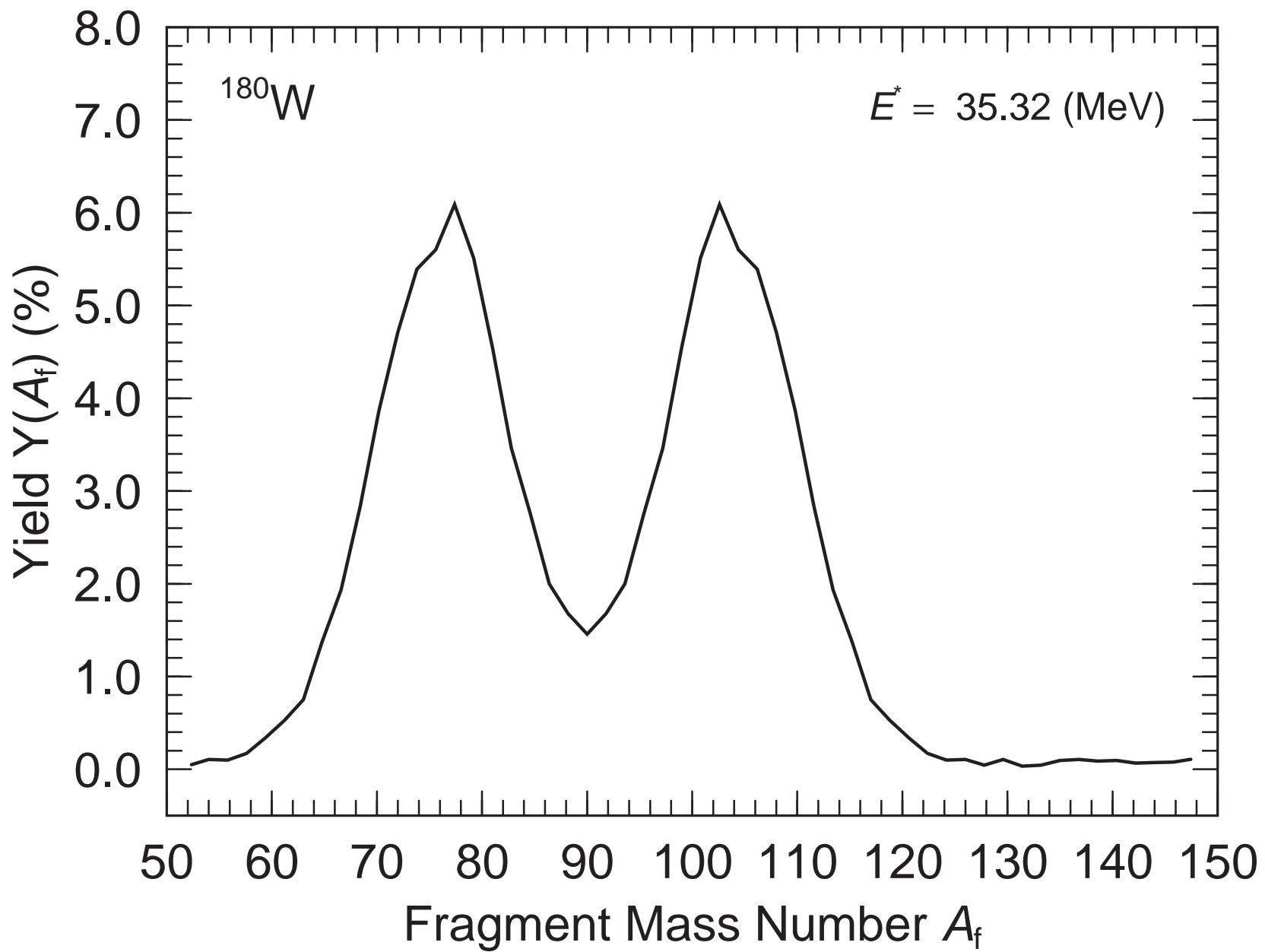


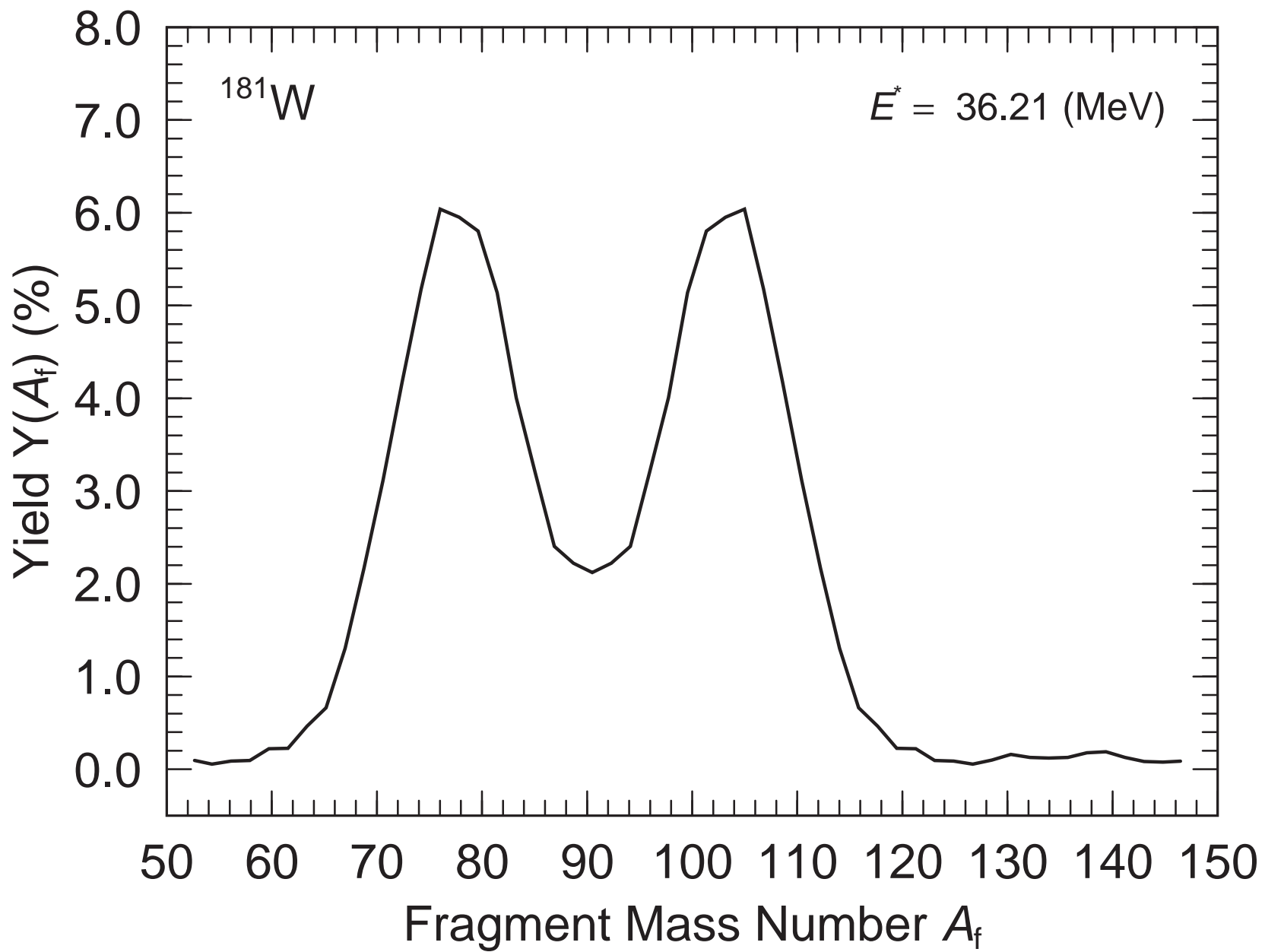


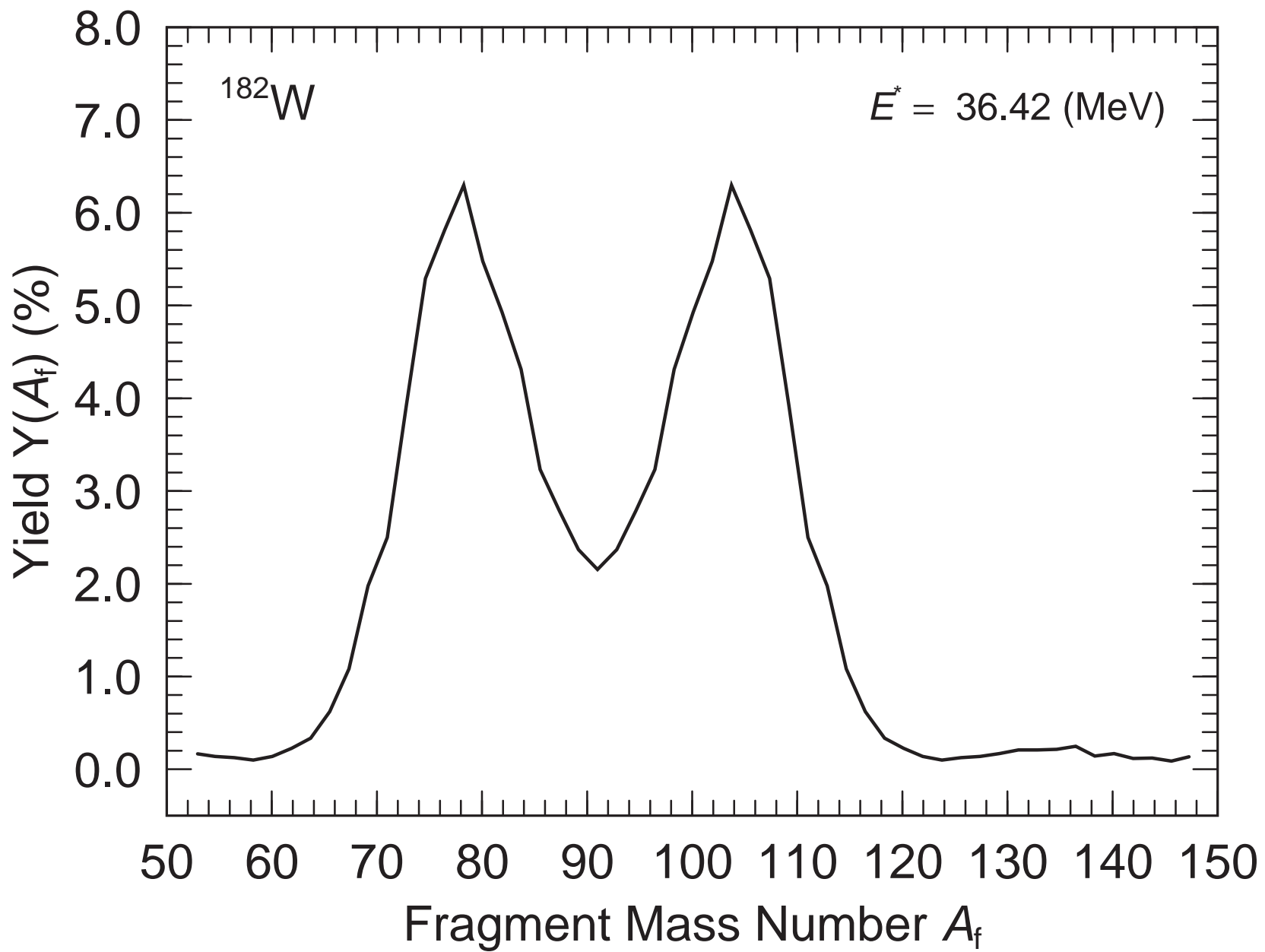


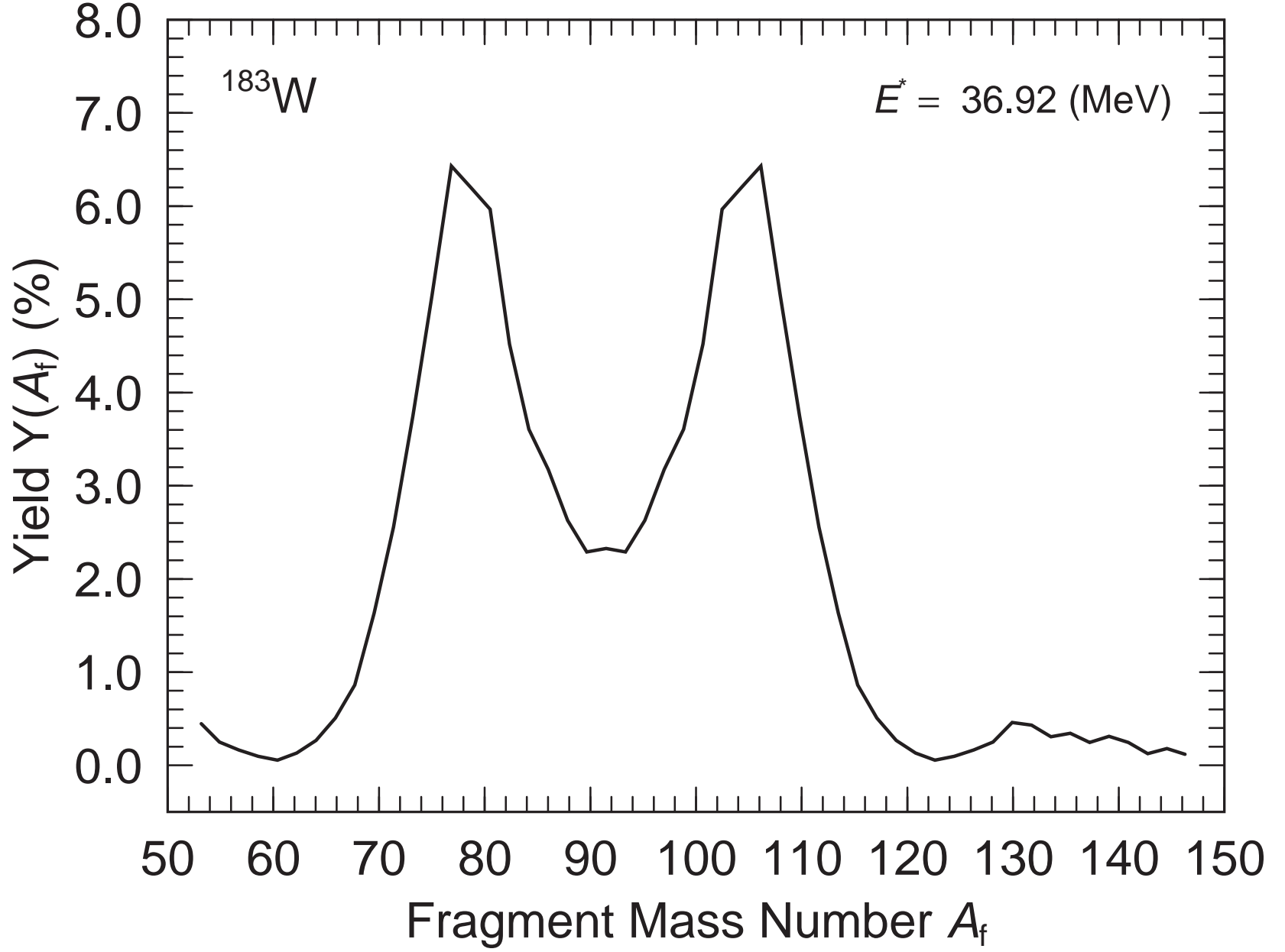


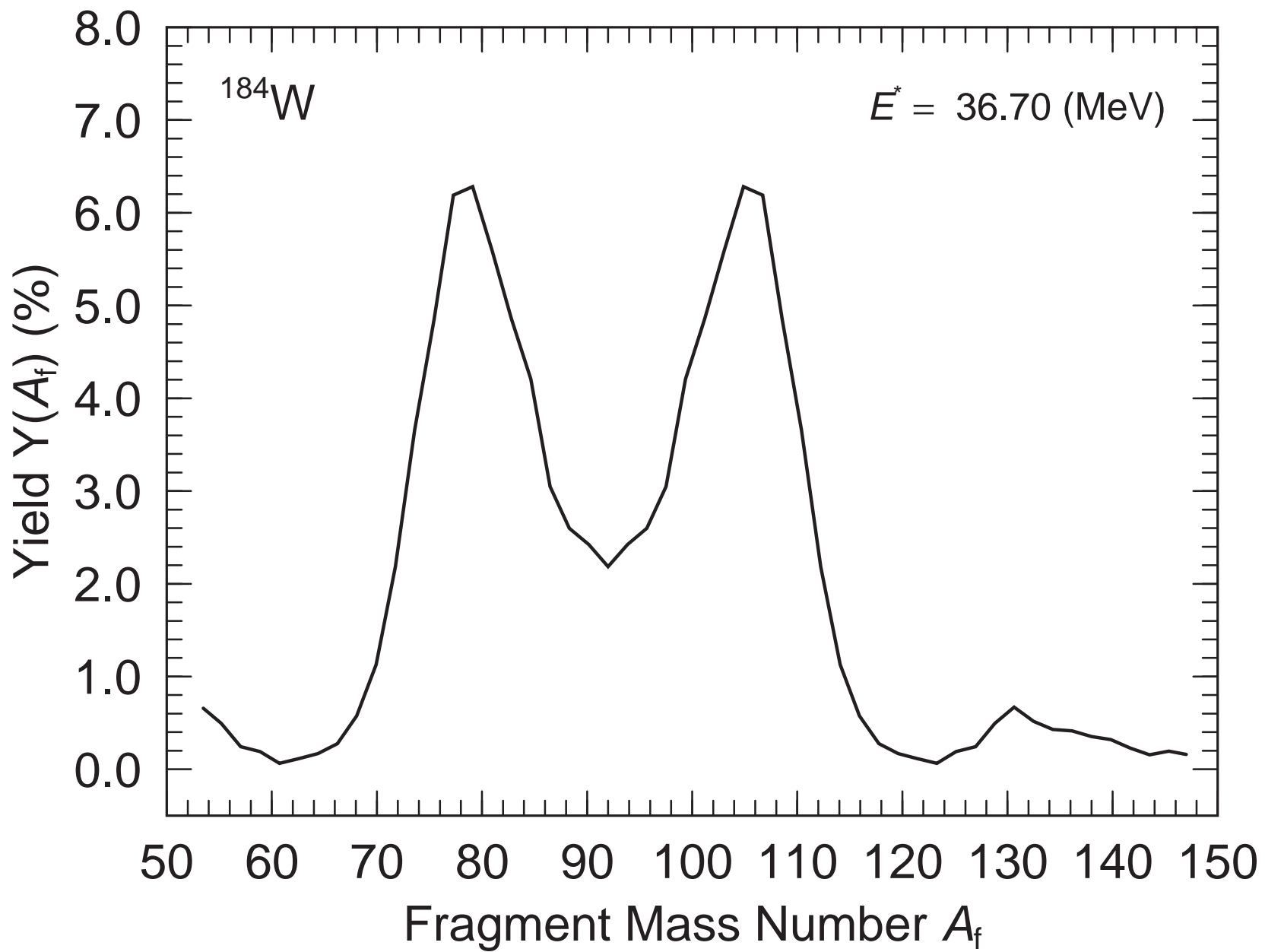


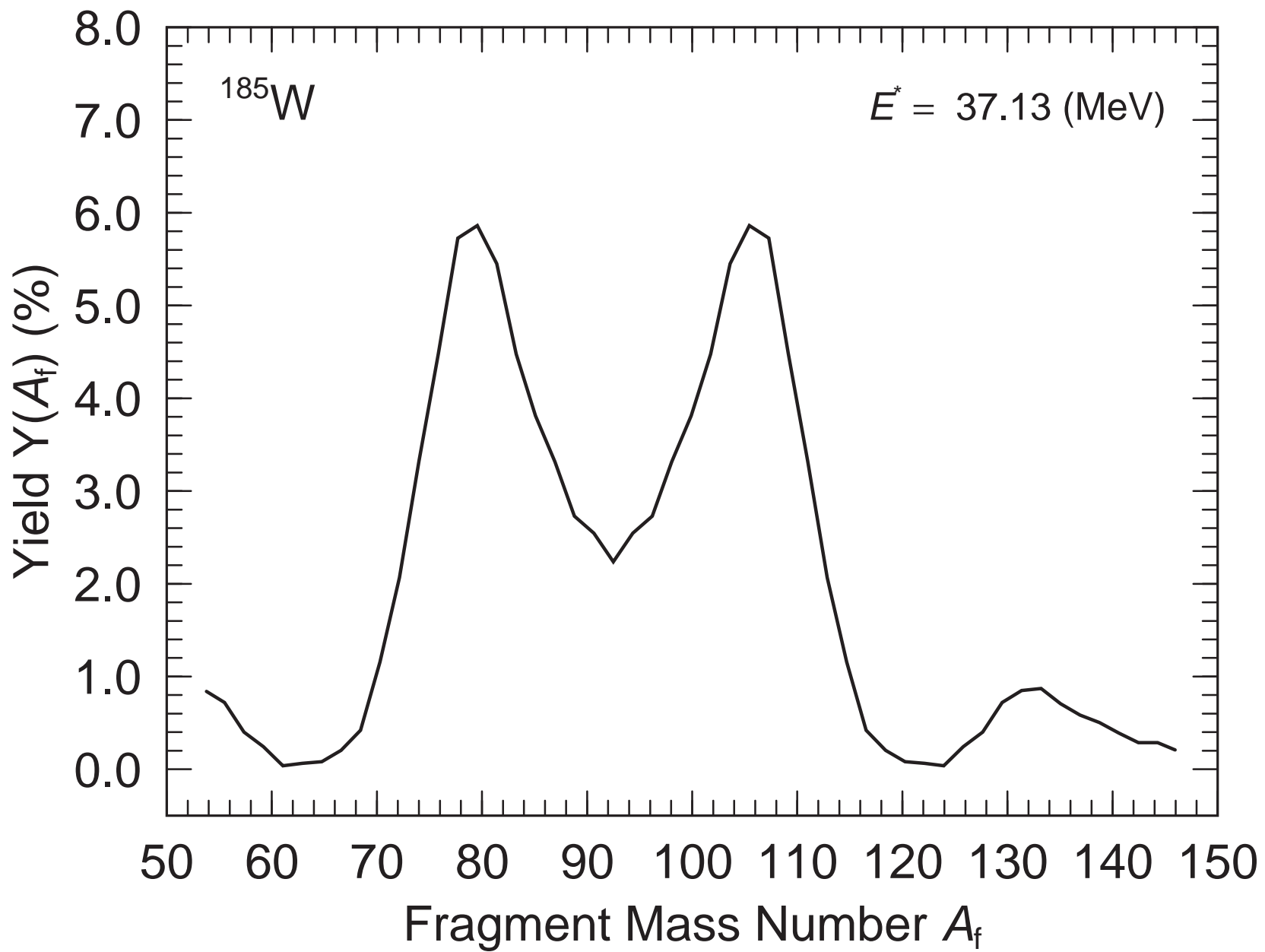


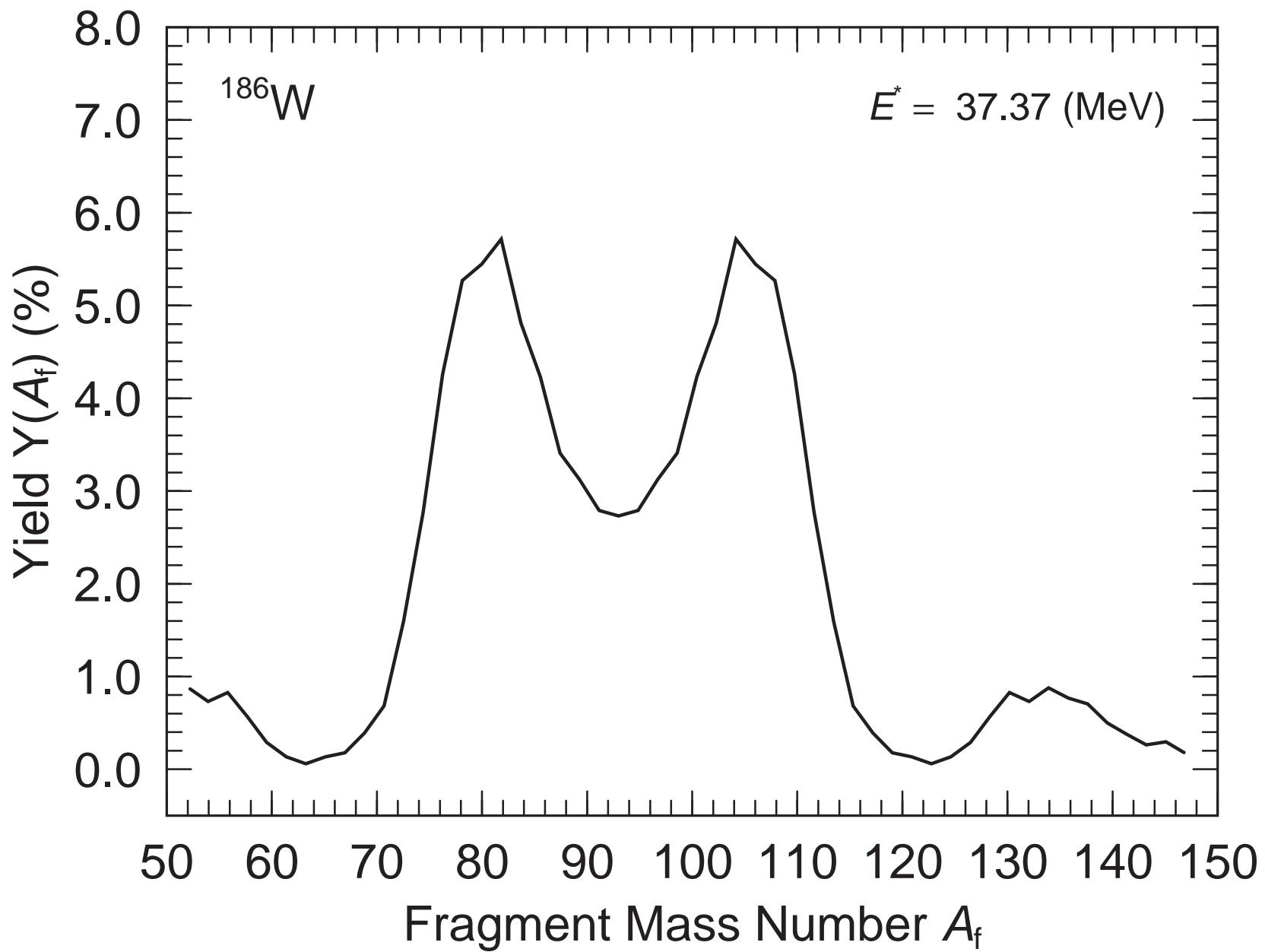


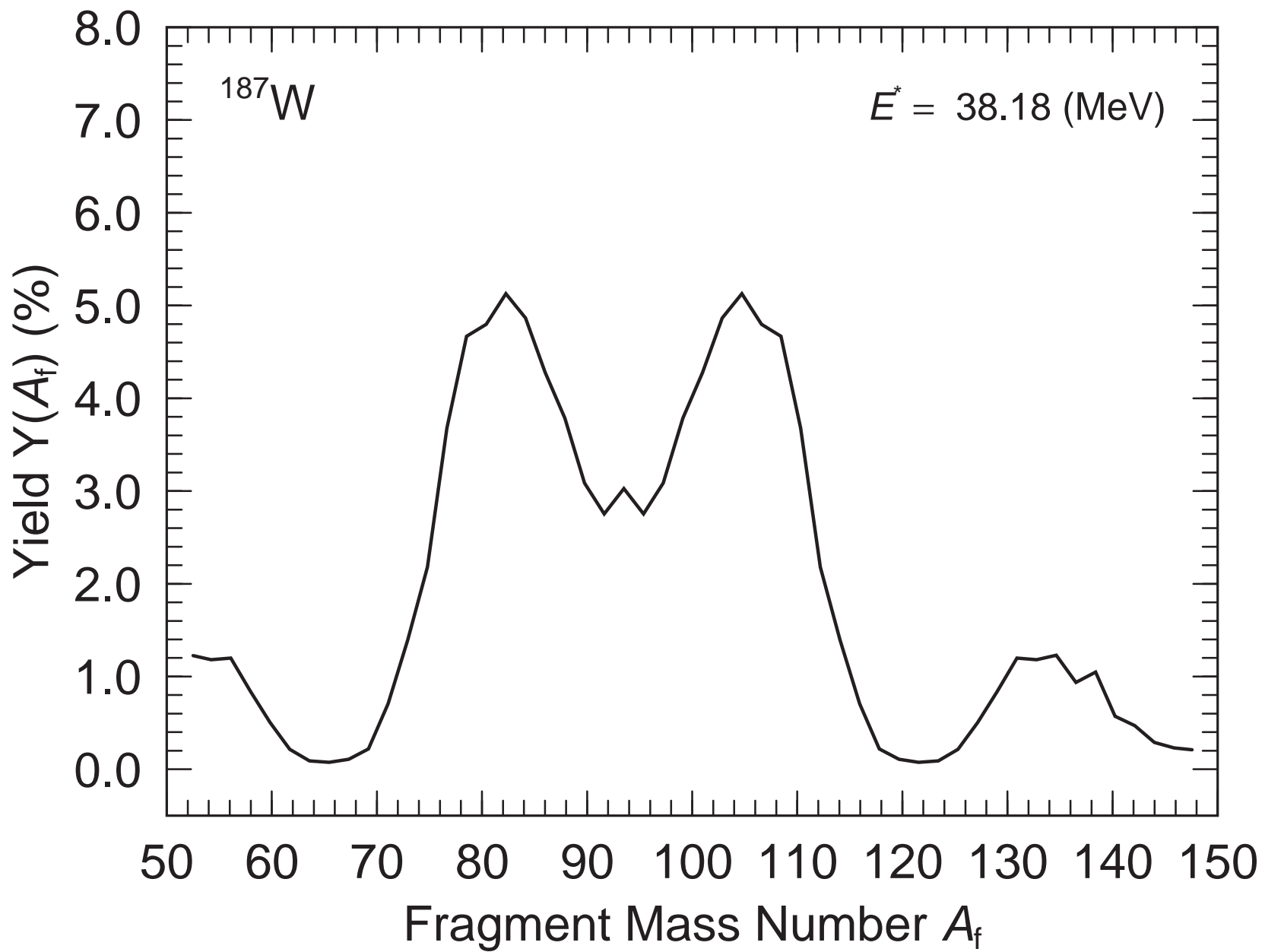




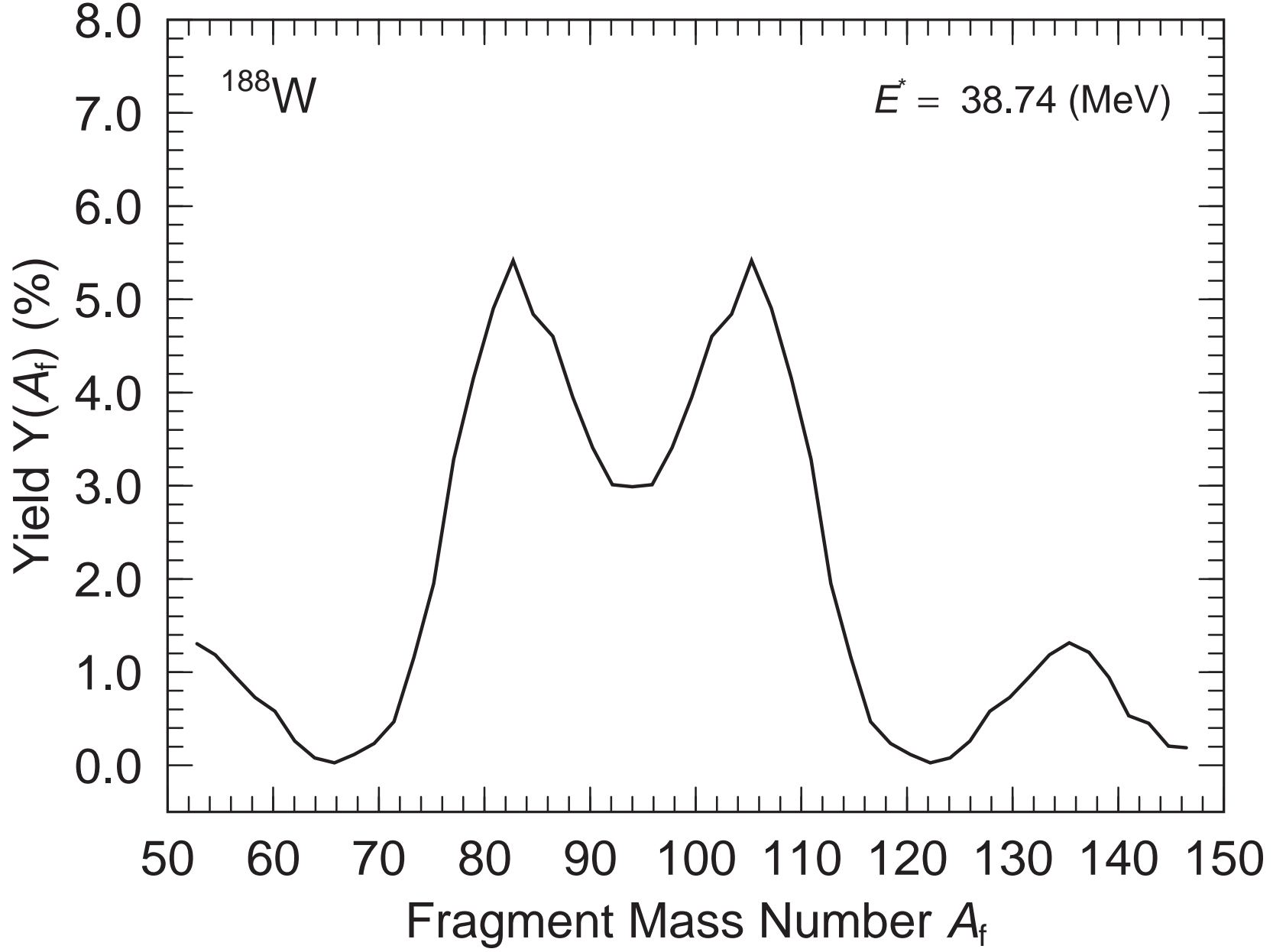


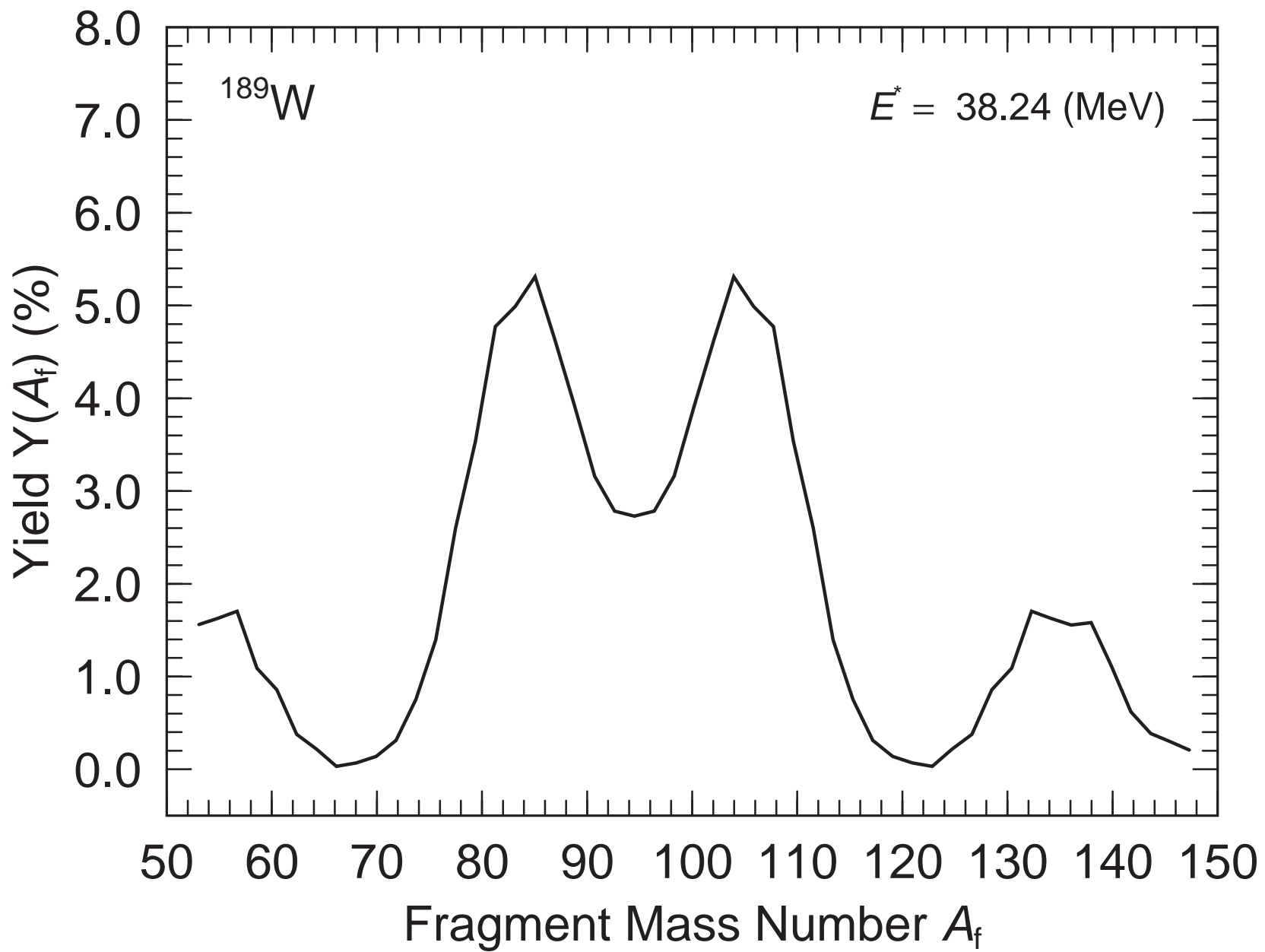


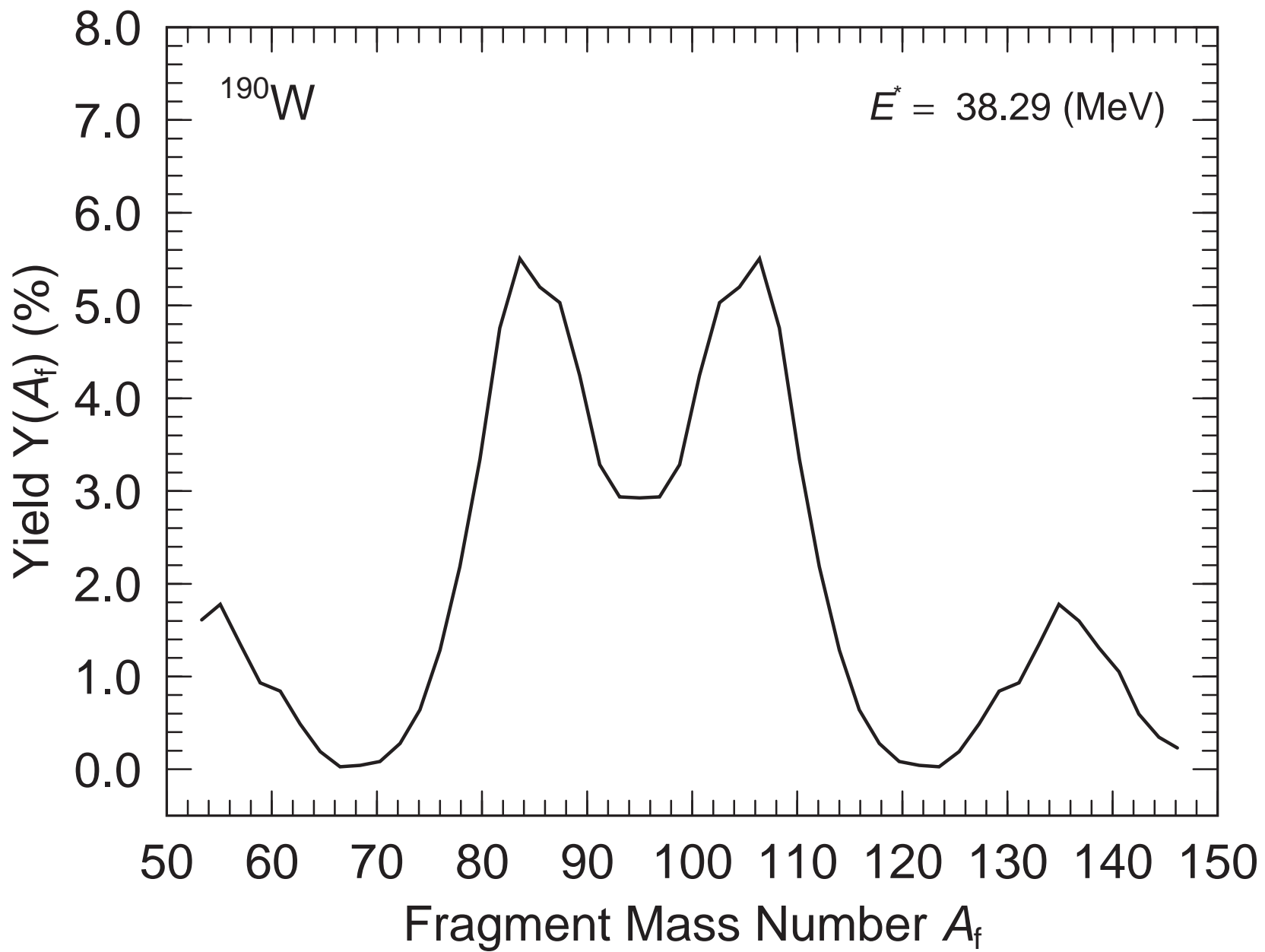


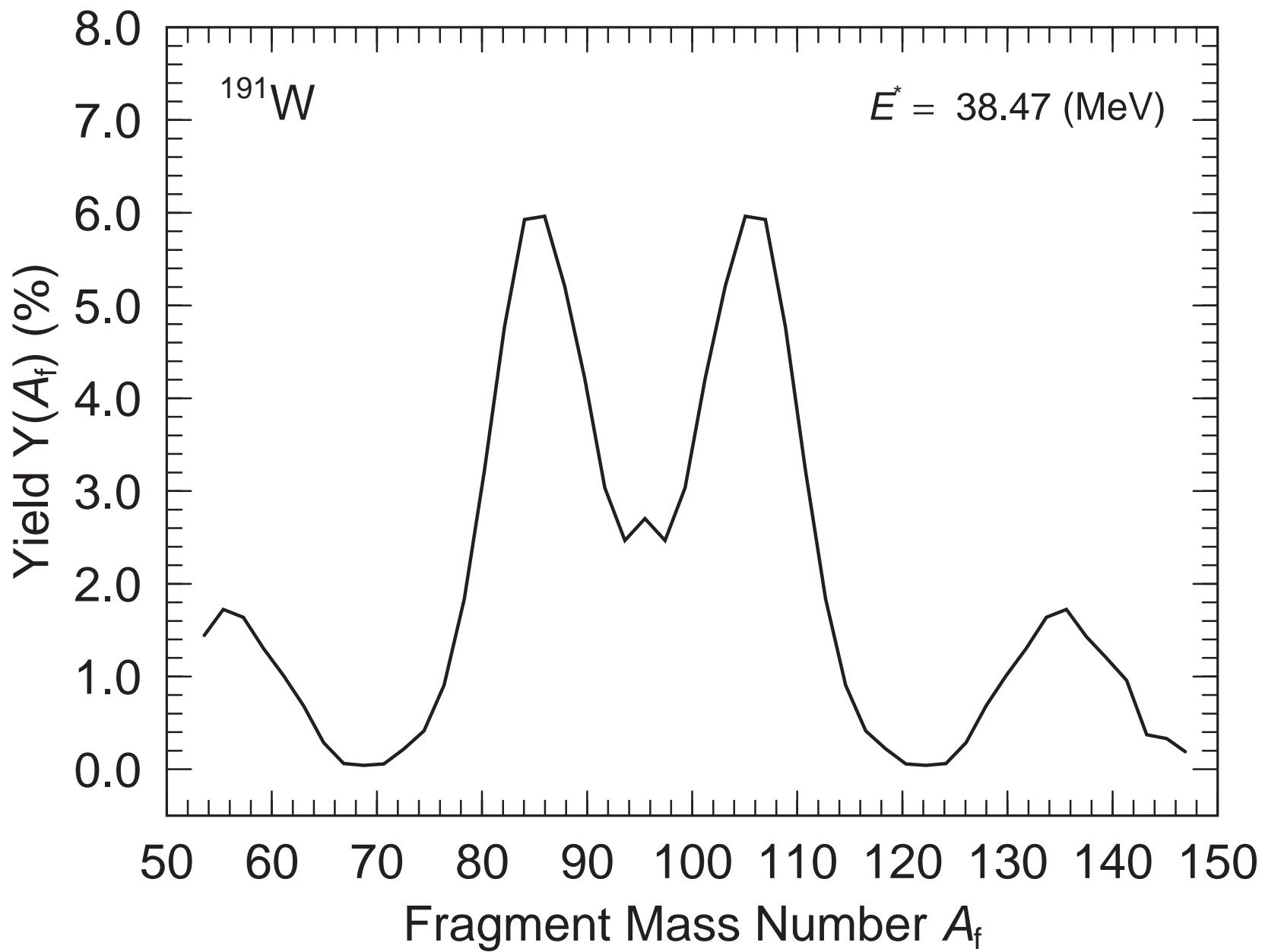


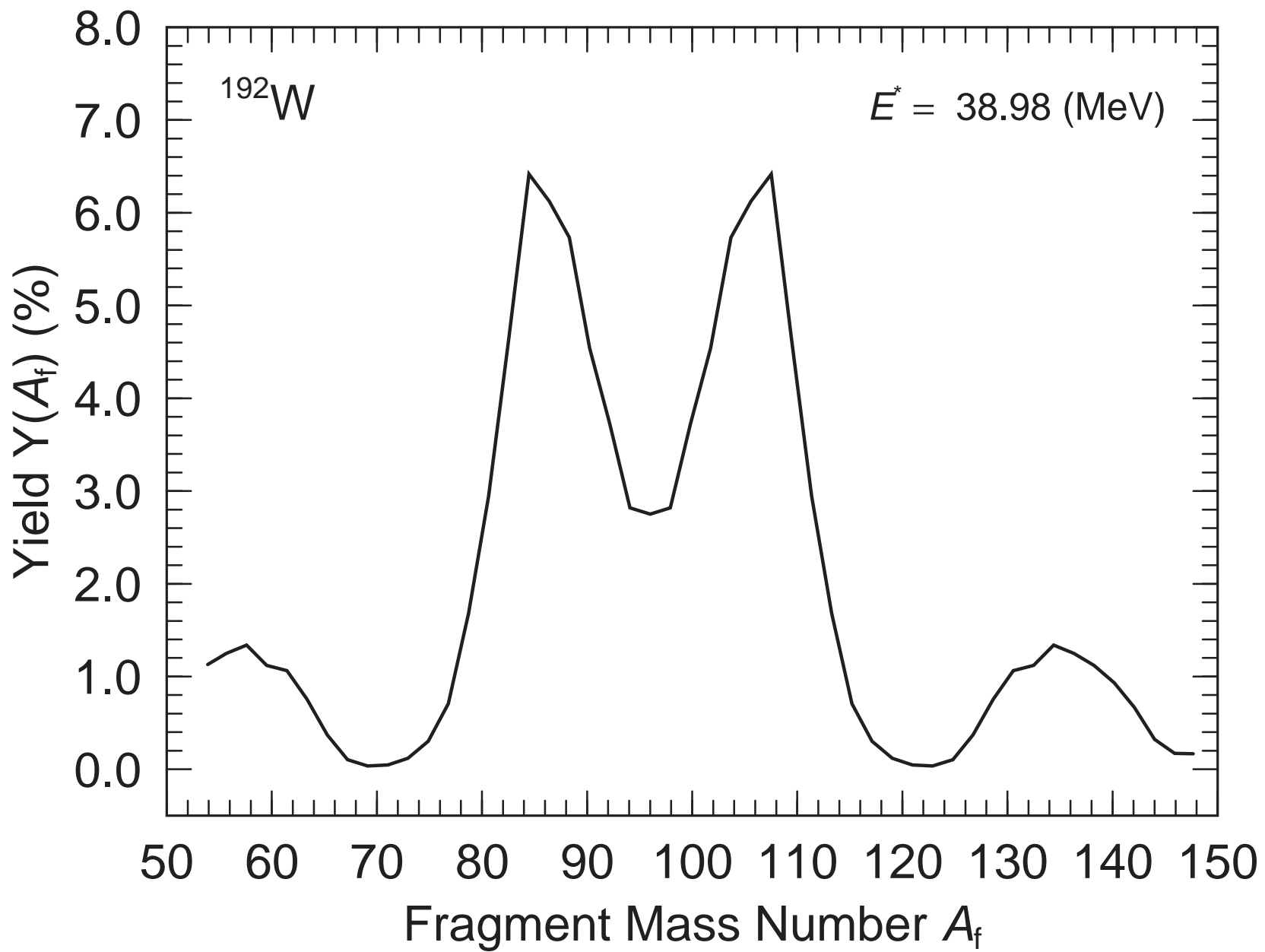


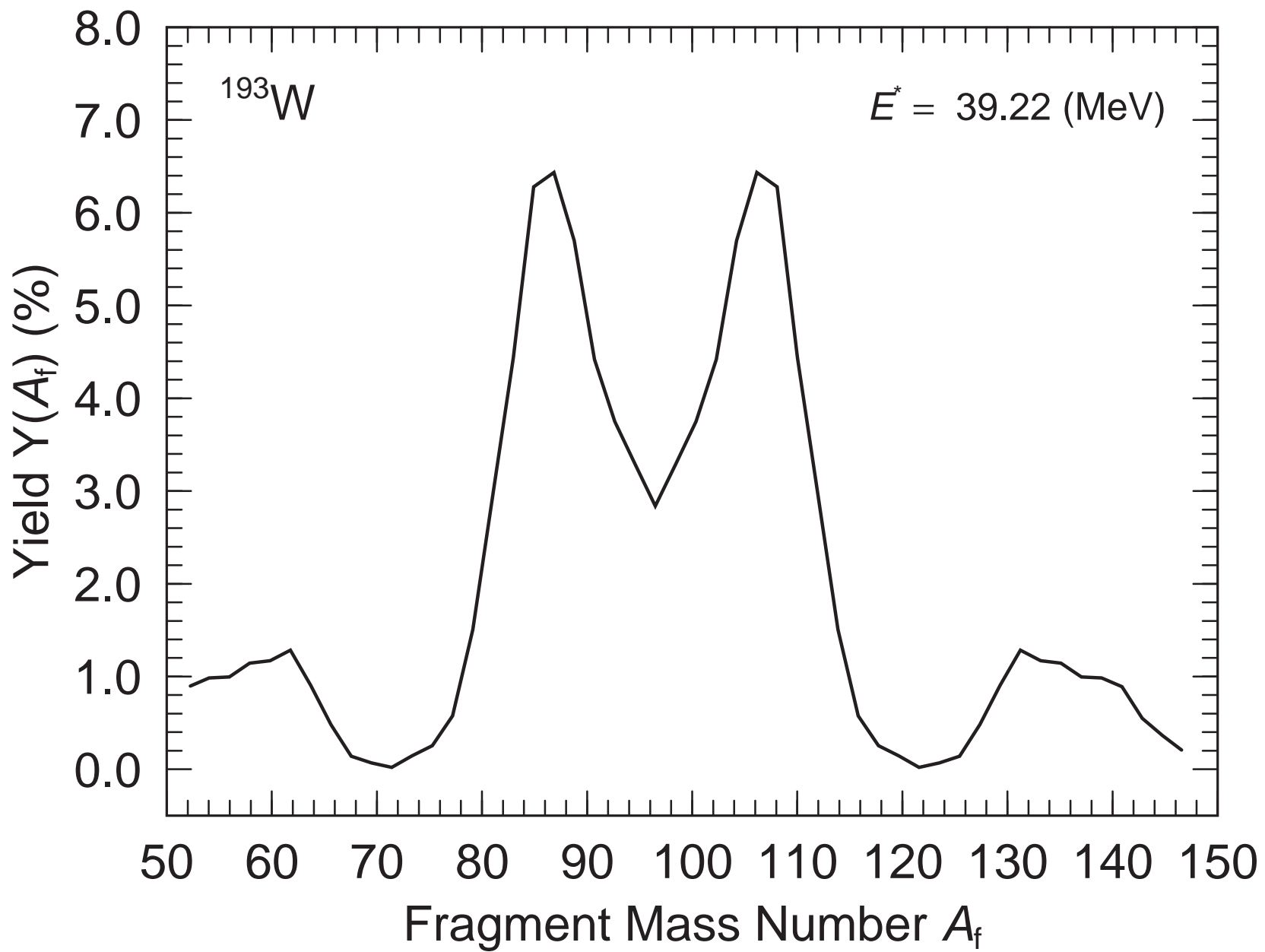


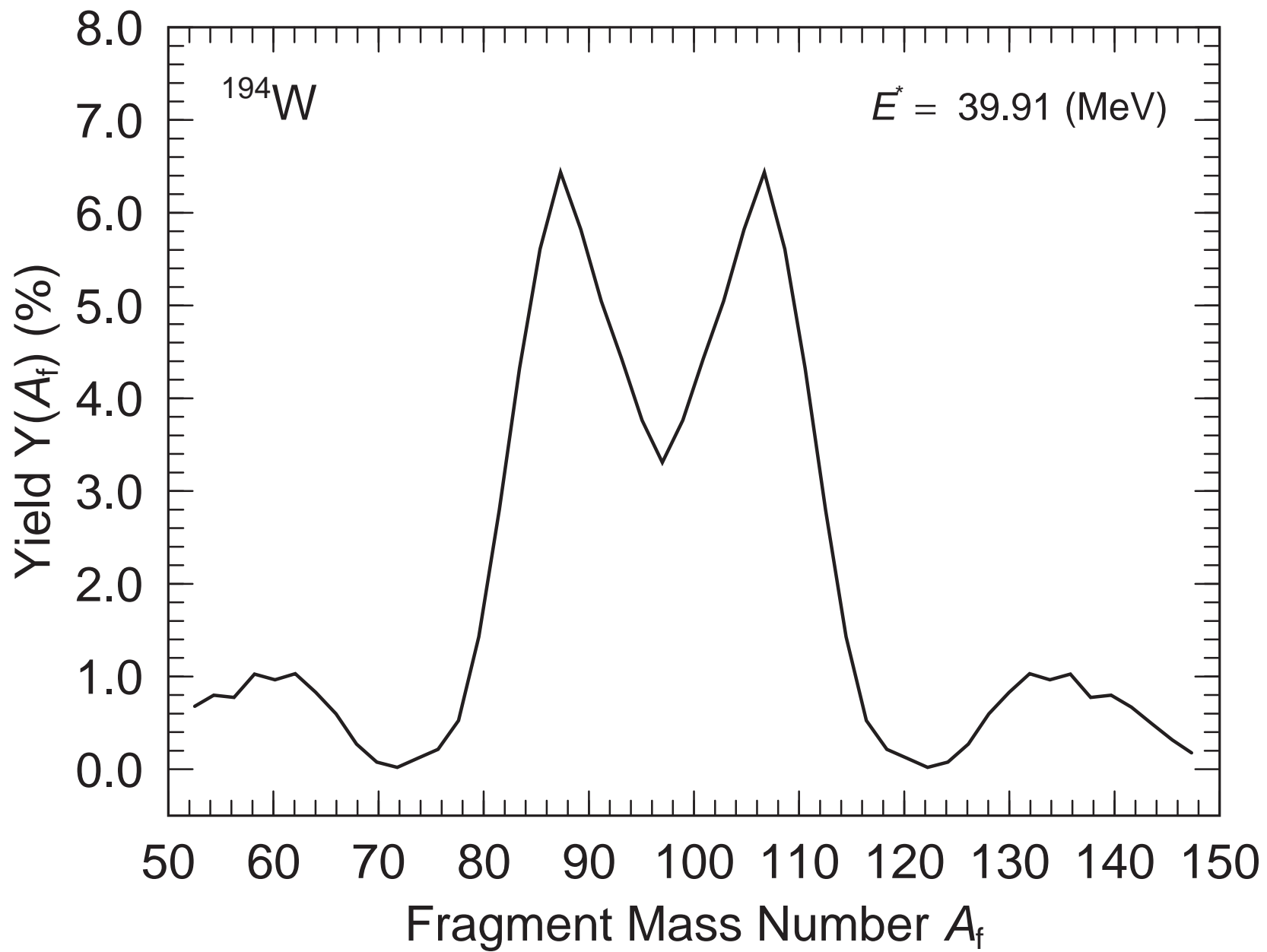


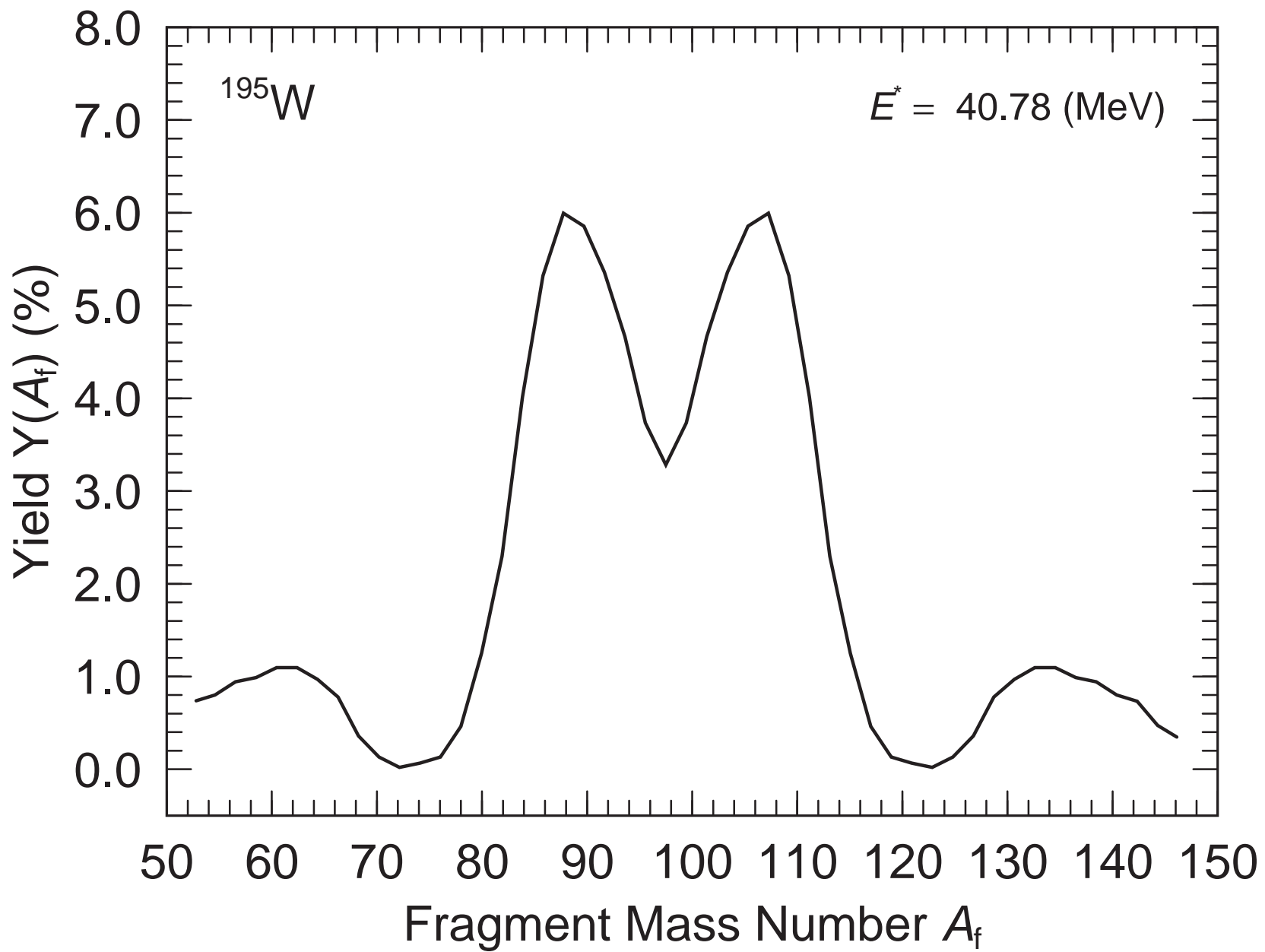




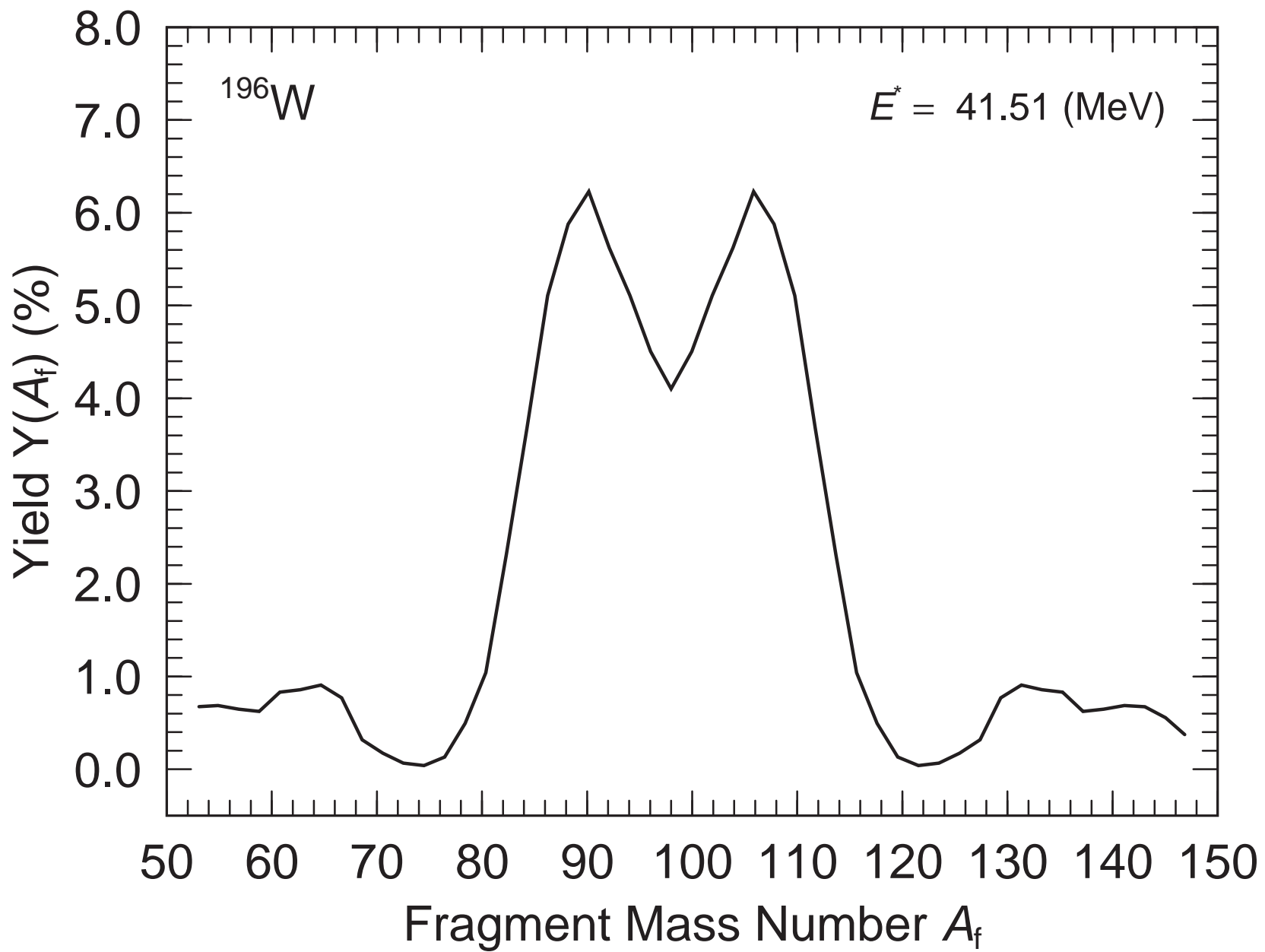


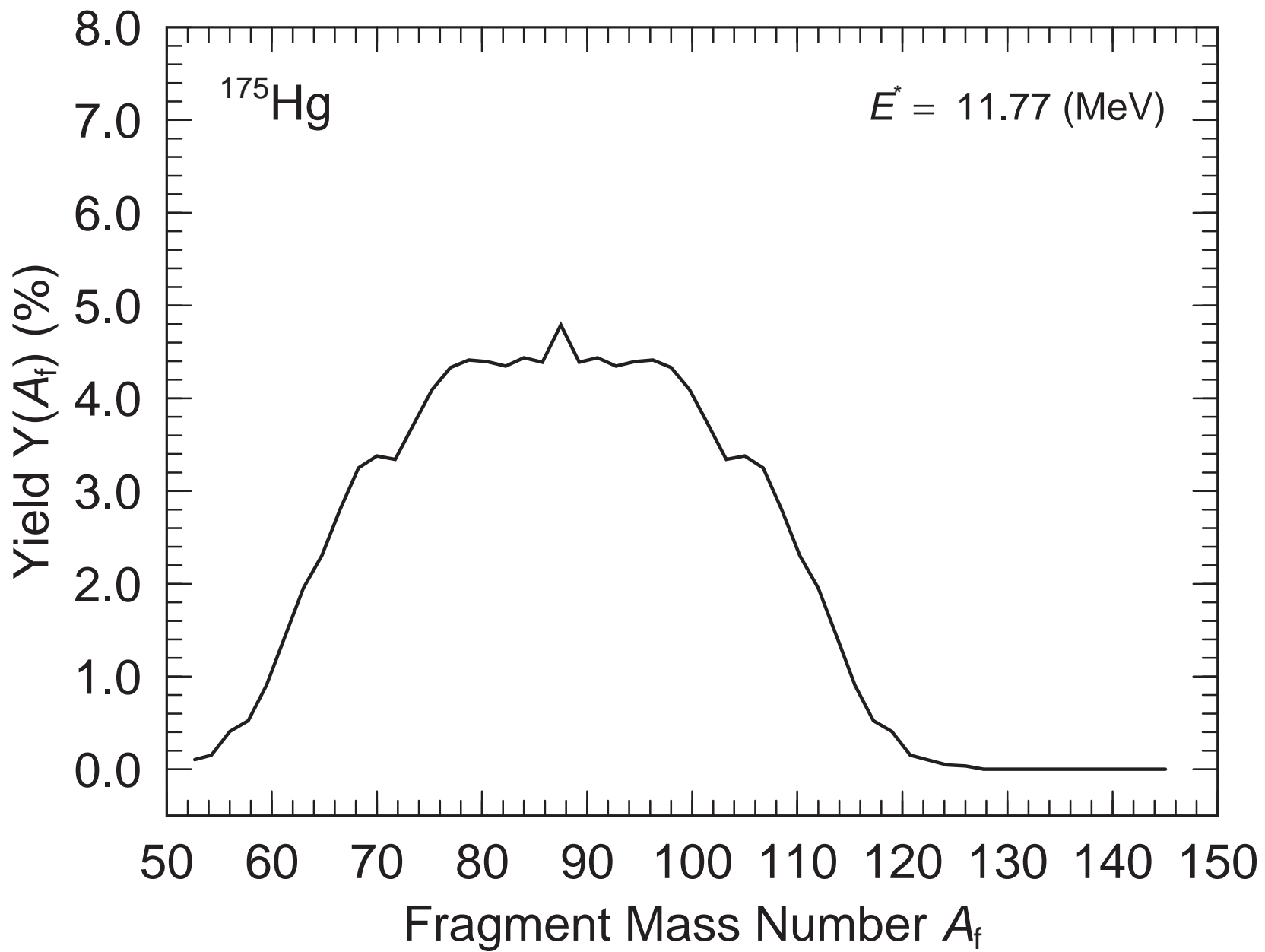


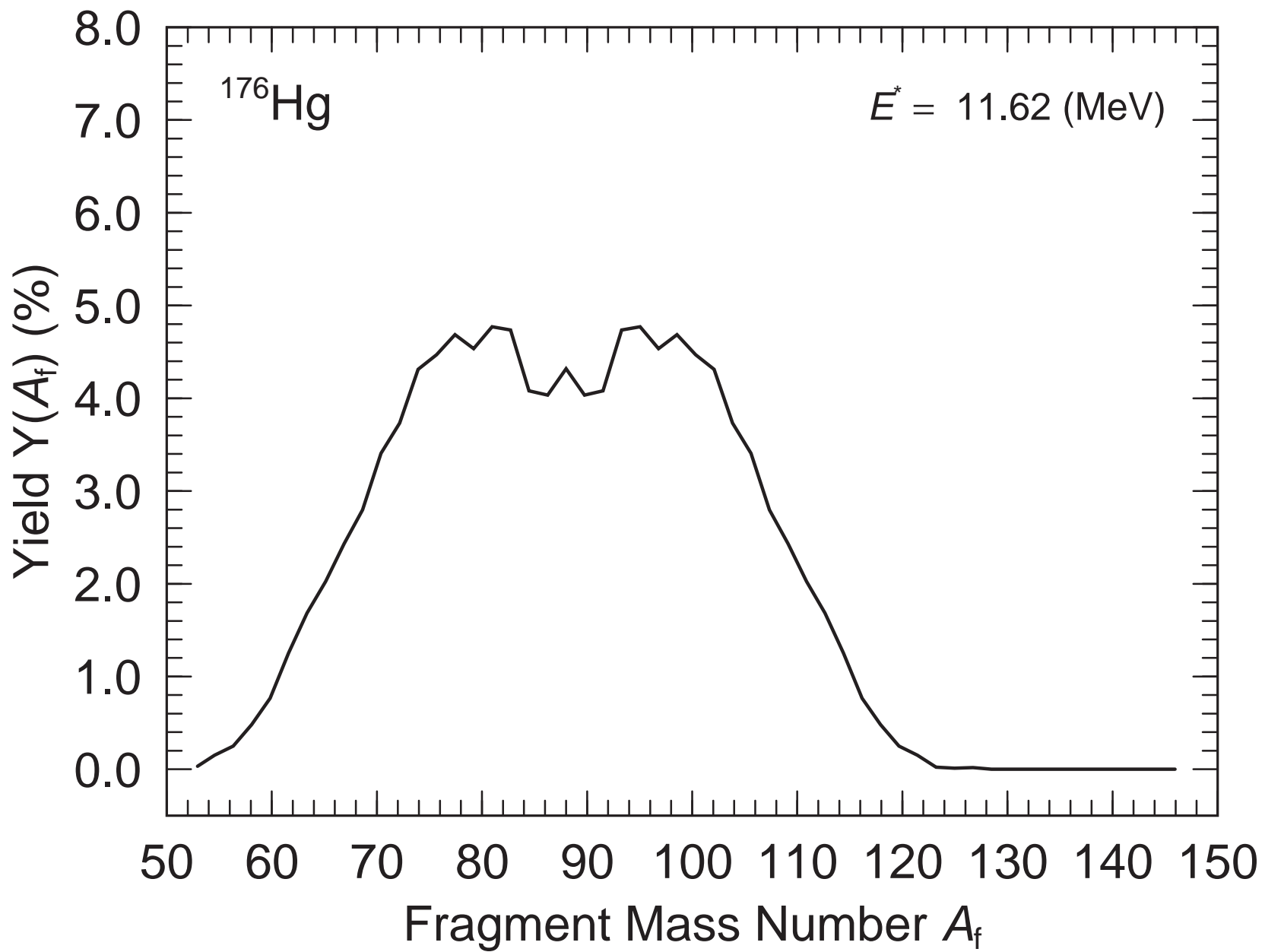


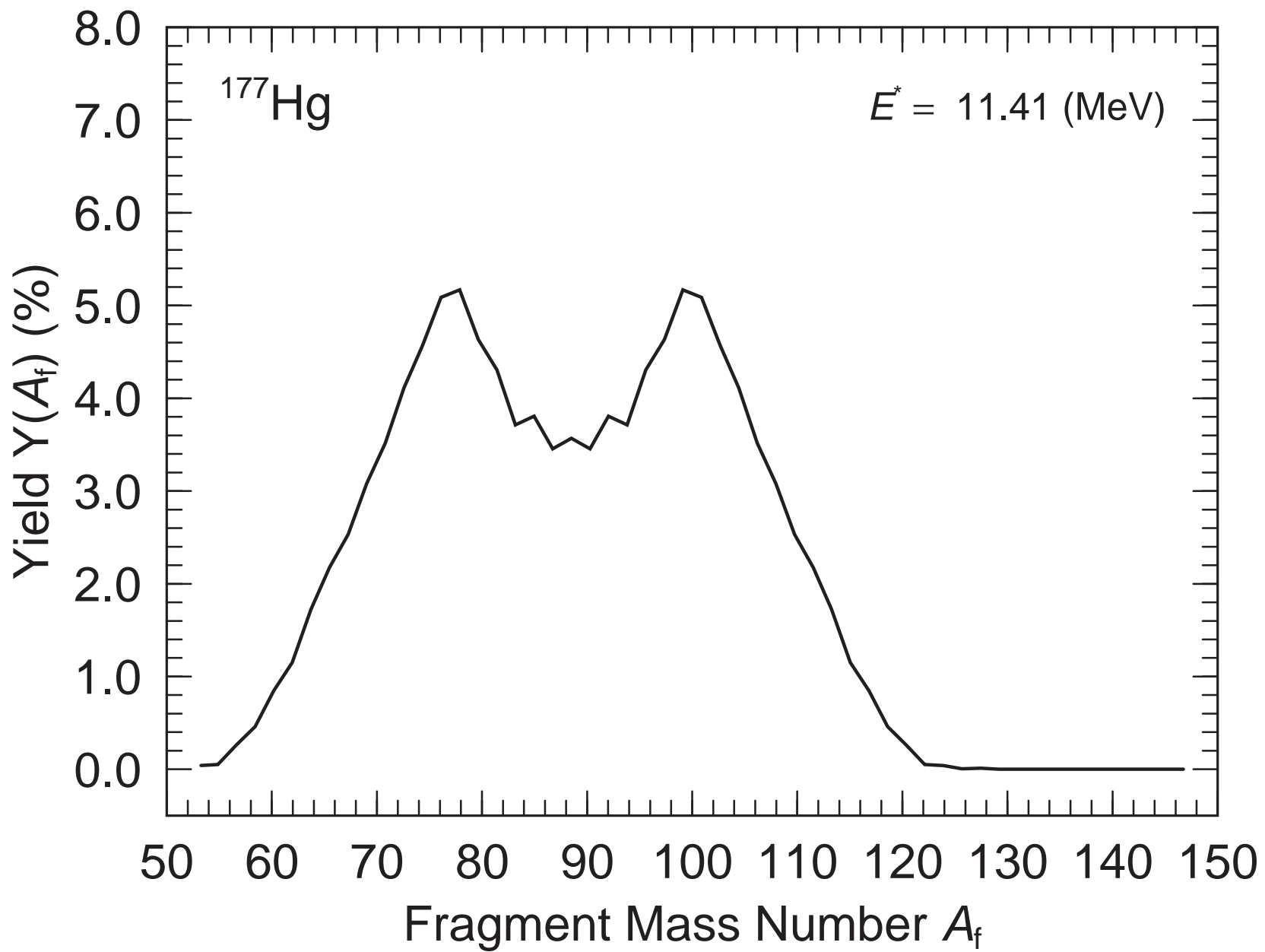


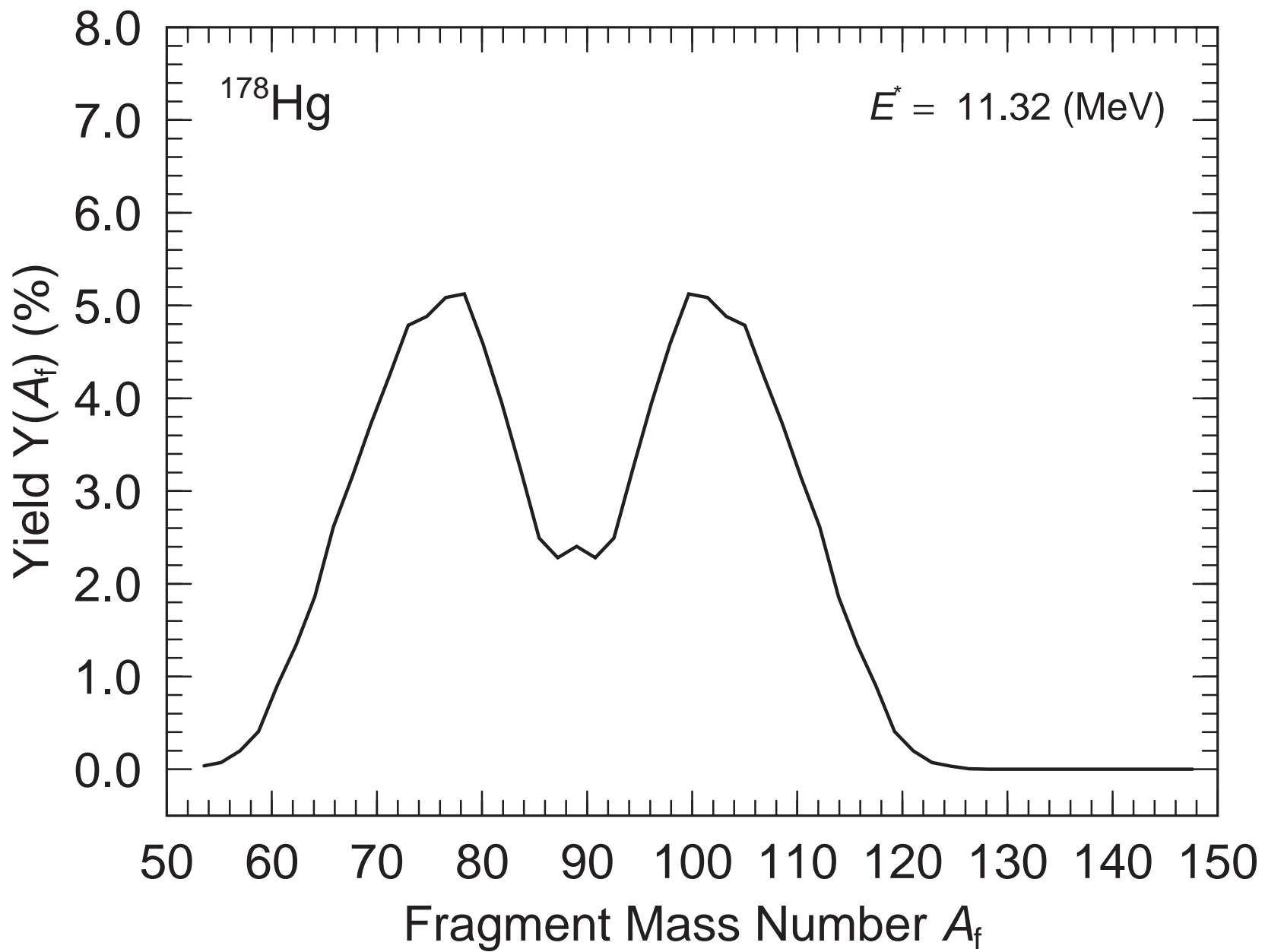


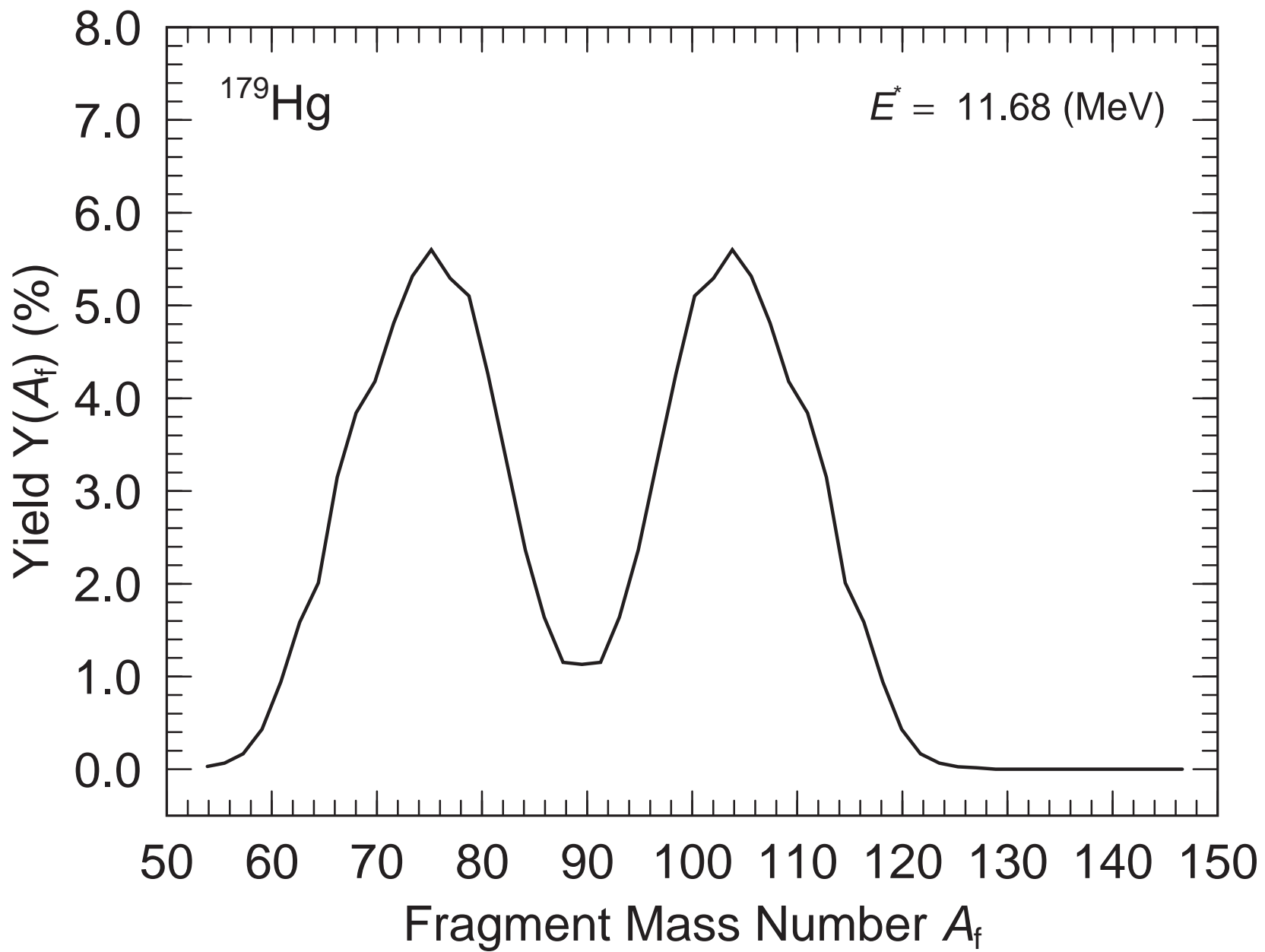


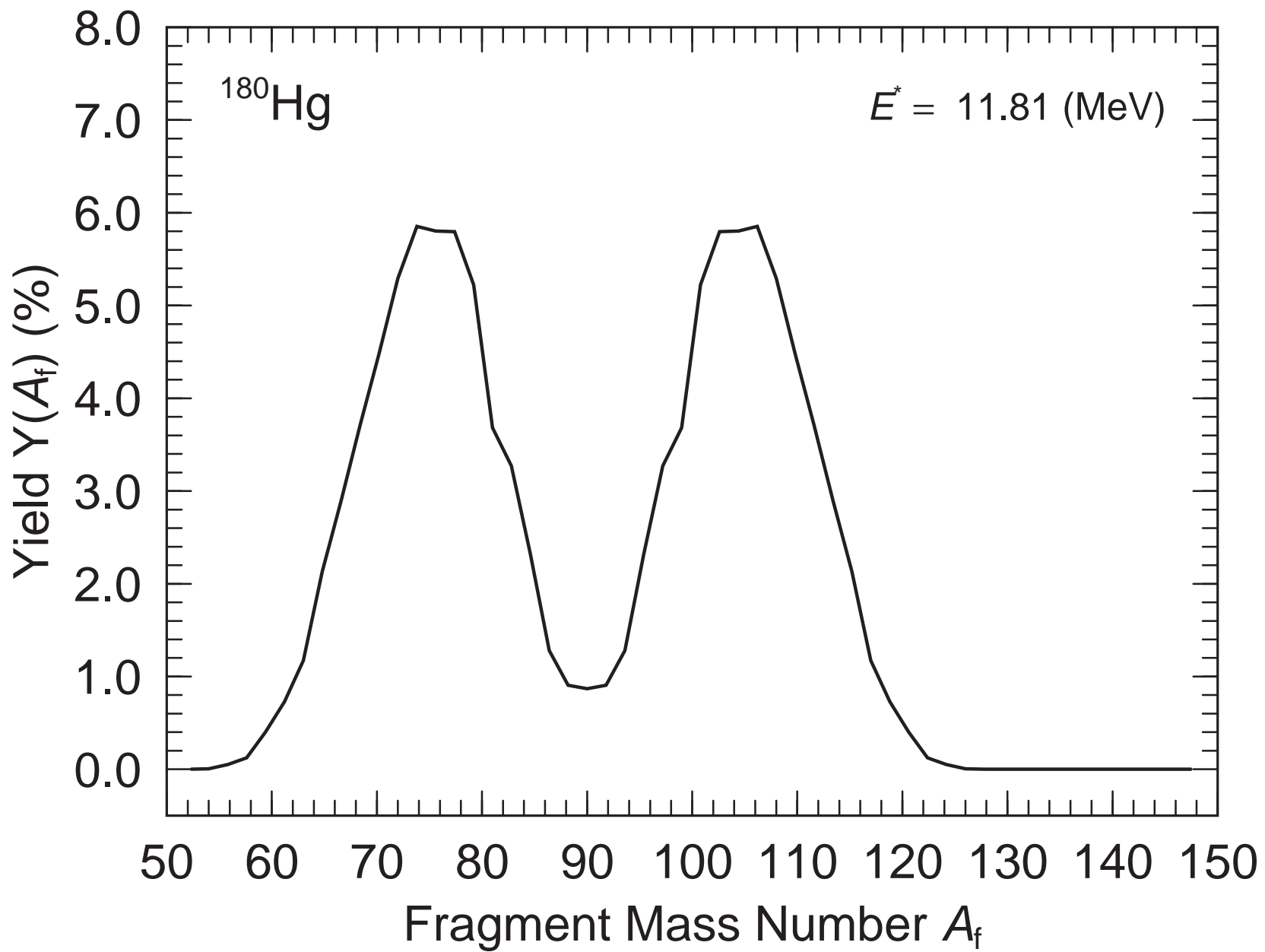




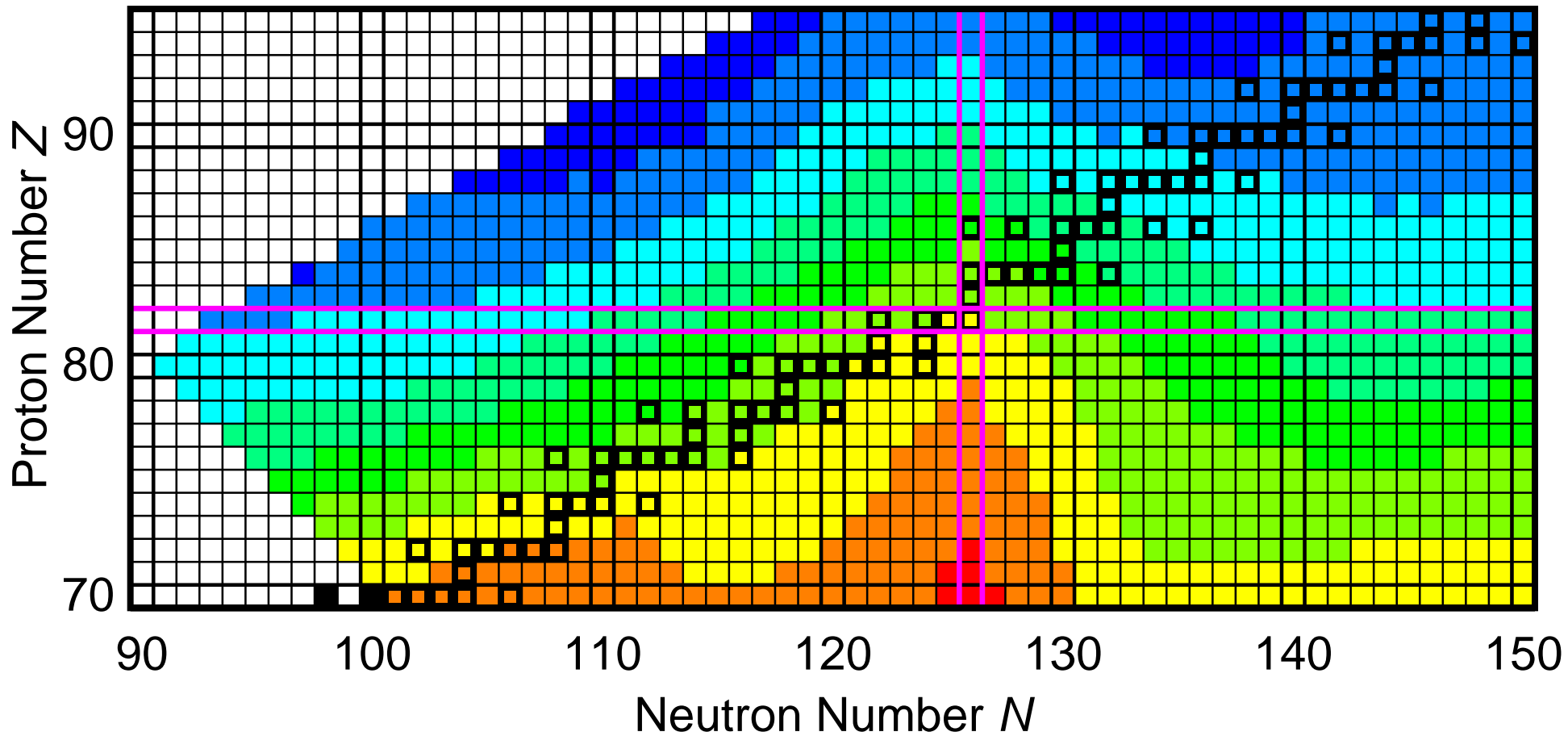
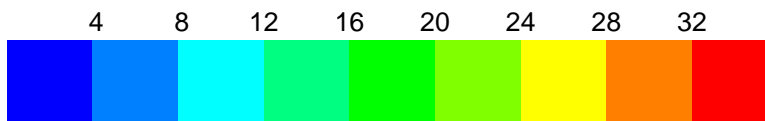








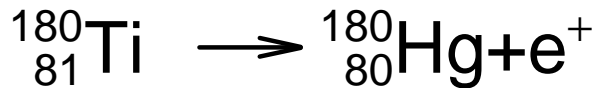
# Fission-Barrier Height (MeV)





Folded-Yukawa potential

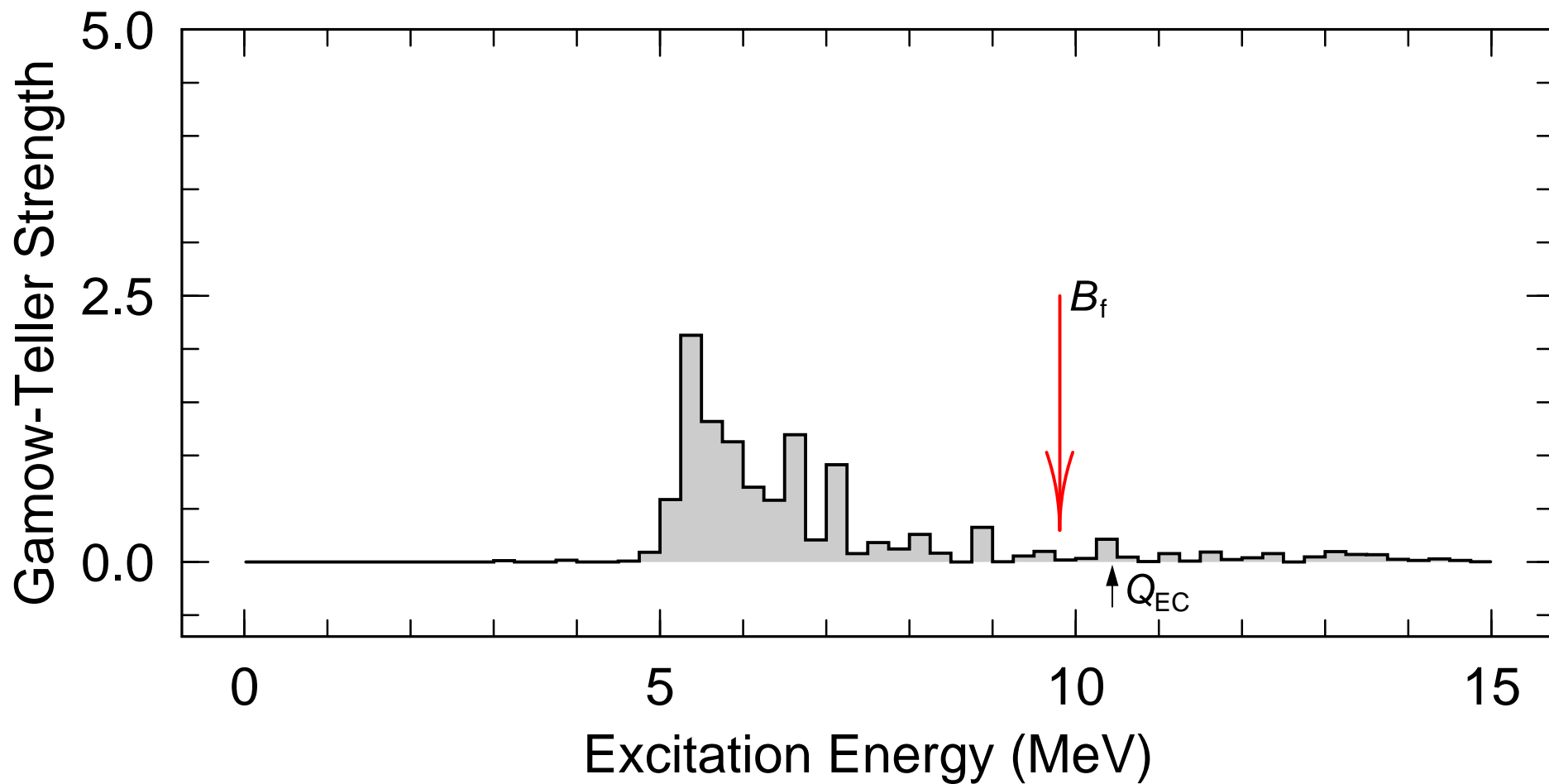
$T_{1/2} = 1.74$  (s)



$\varepsilon_2 = -0.130$     $\Delta_n = 0.99$  MeV    $\lambda_n = 34.88$  MeV

$\varepsilon_4 = 0.010$     $\Delta_p = 0.51$  MeV    $\lambda_p = 32.50$  MeV

$\varepsilon_6 = 0.010$    (L-N)    $a = 0.80$  fm



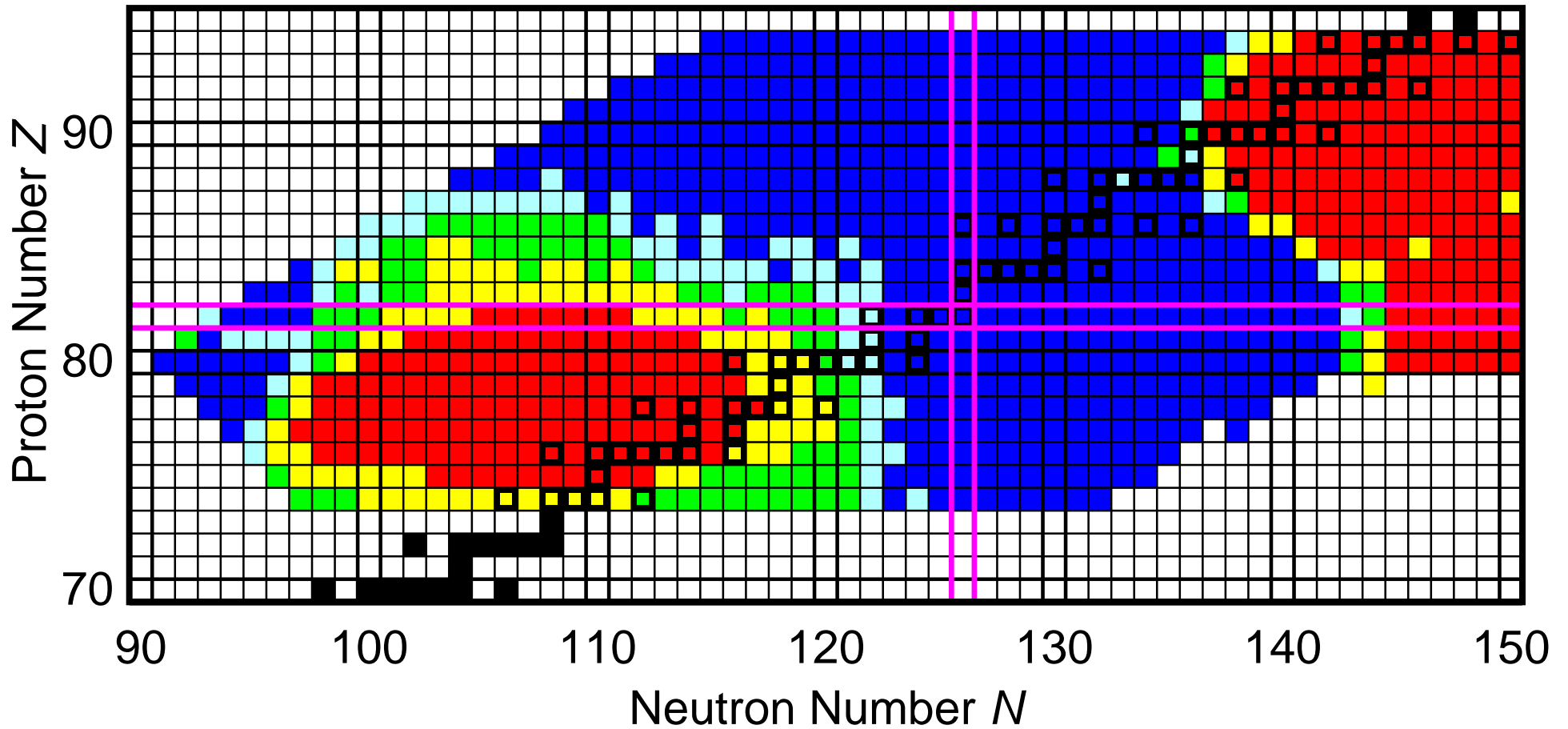
# Fission-Yield Valley-to-Peak Ratio

0.2 0.4 0.6 0.8

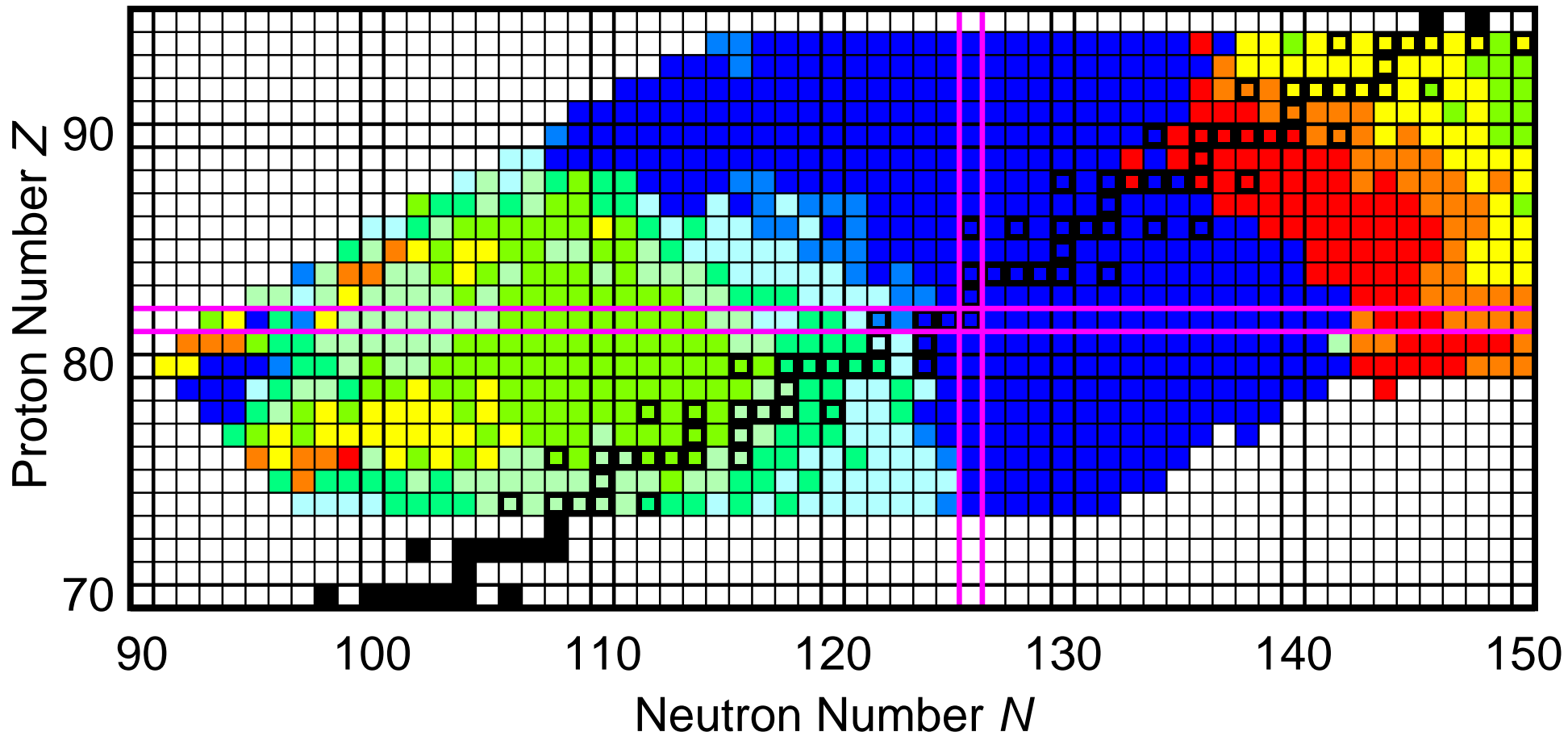
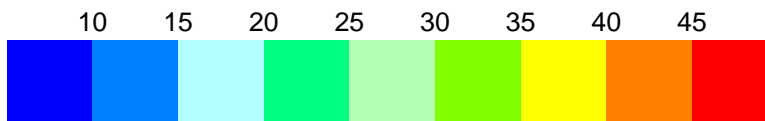
Asymmetric



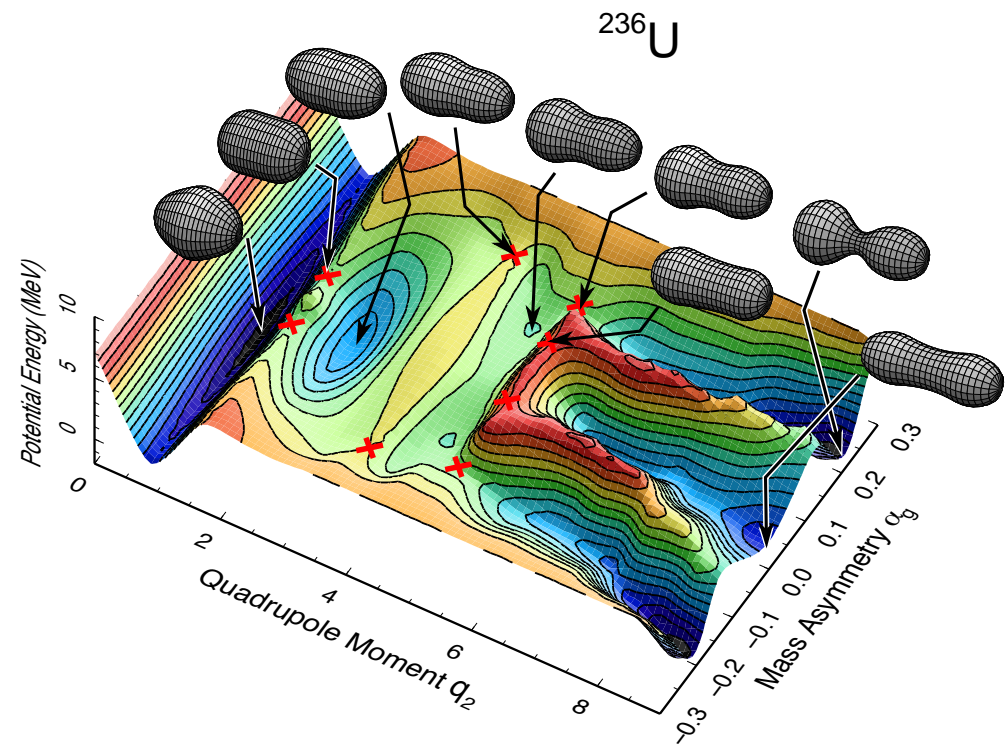
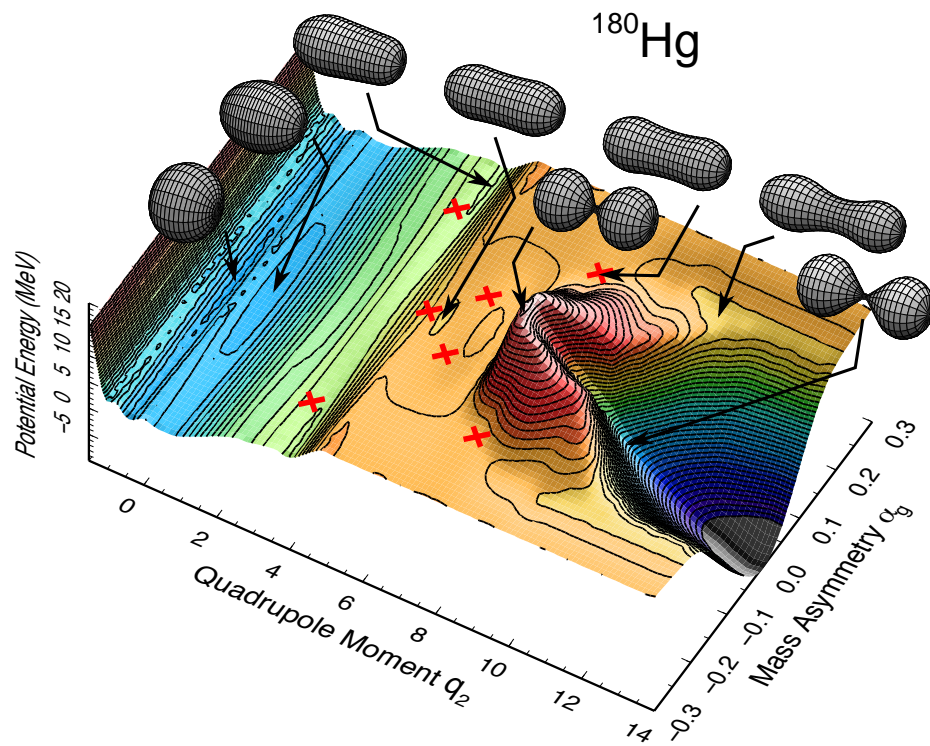
Symmetric



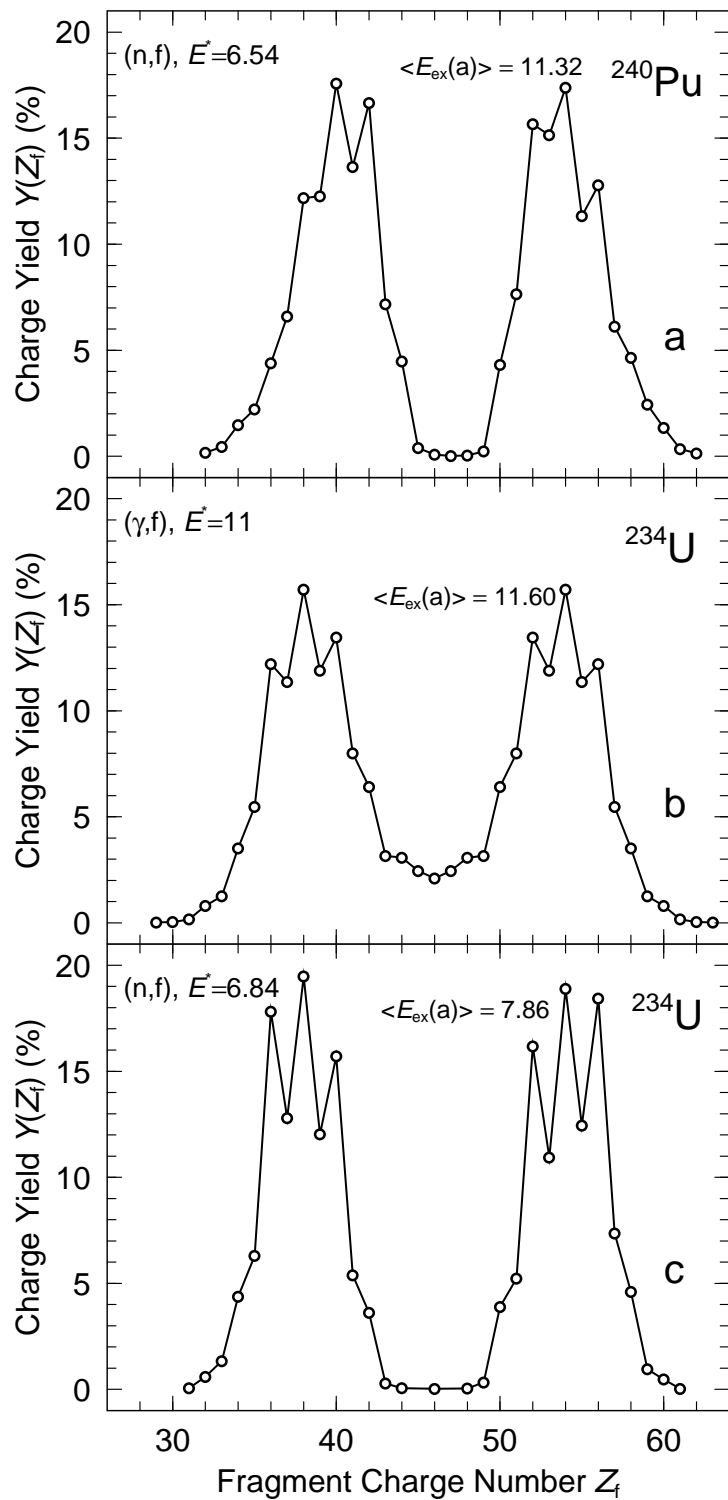
# Fission-Fragment Mass Division (MH-ML)

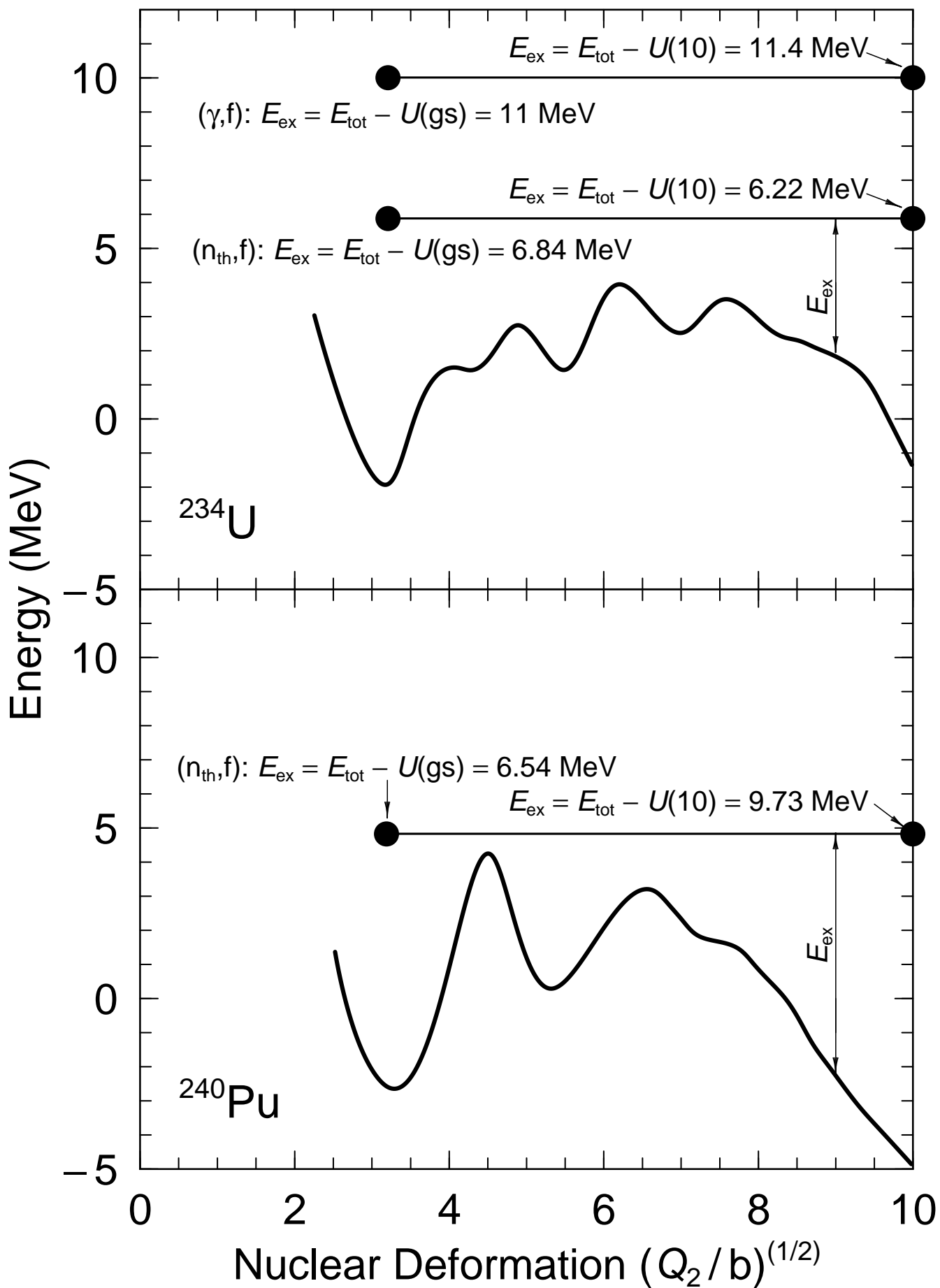


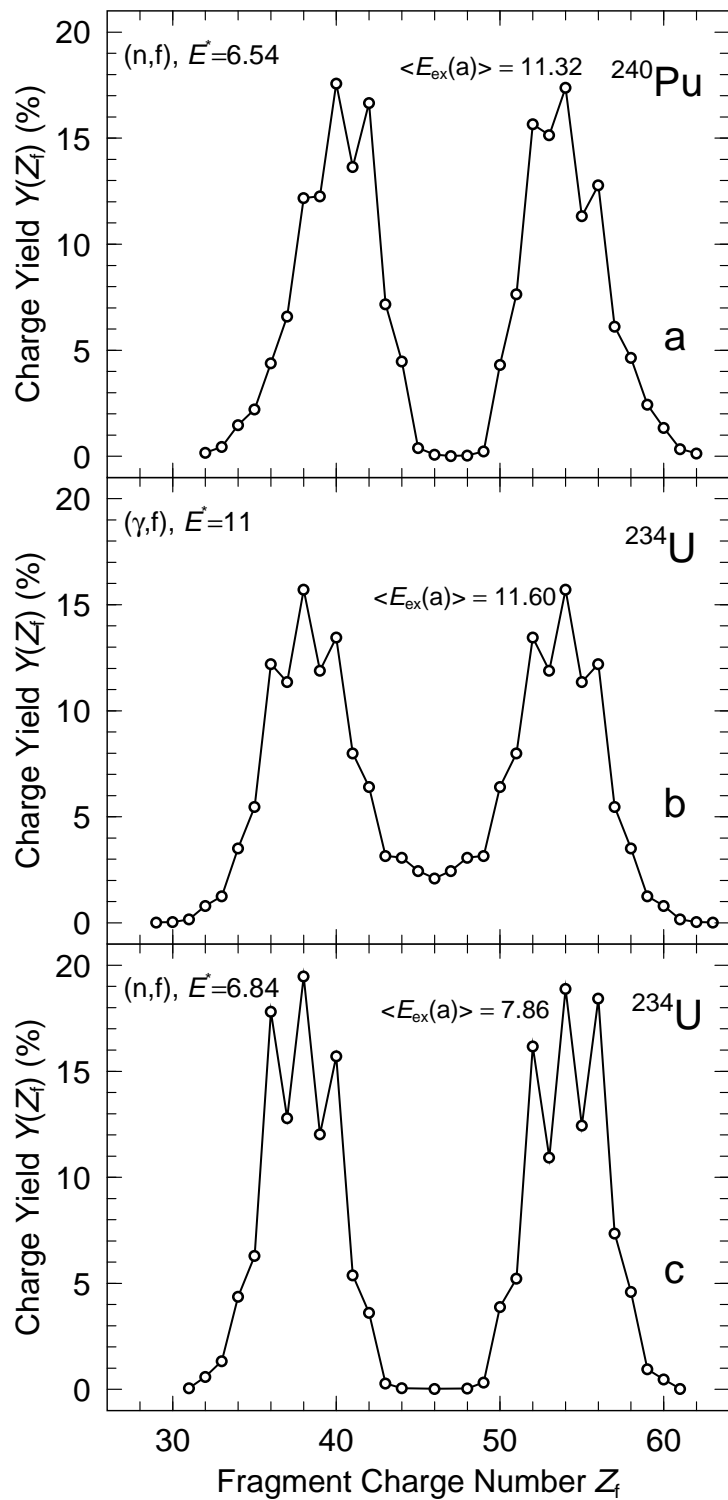
# Contrasting Fission Potential-Energy Surfaces $\text{Hg} \leftrightarrow \text{U}$



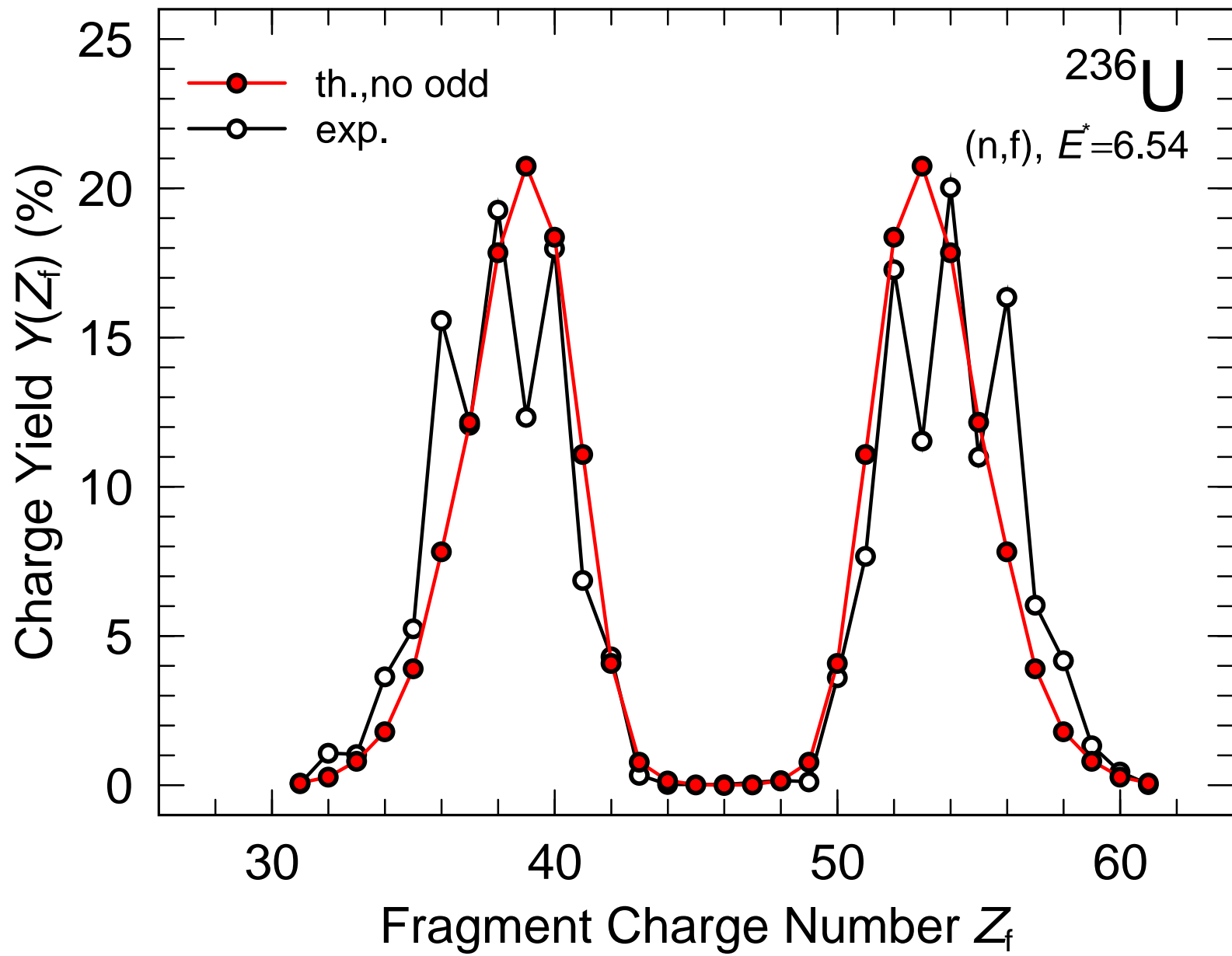
Compound		Calc.	Exp.	Calc	Exp.	Calc.
$Z$	$A$	$A_L/A_H$	$A_L/A_H$	$Z_L/Z_H$	$Z_L/Z_H$	$\epsilon_L/\epsilon_H$
80	180	80/100	80/100	36/44		0.60/0.50
90	222	108/114		44/46	44/46	0.55/0.55
90	228	<b>112/116</b>	89/139	<b>44/46</b>	36/54	0.55/0.55
92	234	<b>116/118</b>	95/139	<b>46/46</b>	38/54	0.55/0.55
94	240	<b>110/130</b>	102/140	<b>44/50</b>	41/53	0.55/0.65
98	252	112/140	108/144	44/54		0.55/0.75
100	252	110/142	110/142	44/56		0.55/0.75
100	258	<b>118/140</b>	129/129	<b>46/54</b>		0.55/0.75
100	260	<b>118/142</b>	130/130	<b>46/54</b>		0.55/0.65
100	264	132/132	132/132	50/50	50/50	0.65/0.65











## Modeling in BSM of

$$Y(Z_1, N_1, Z - Z_1, N - N_1)$$

We need total potential energy versus fragment proton and neutron numbers. Shell correction is actually straightforward.

**Total shell correction:**

$$ESH_{Z+N}(Z_1, N_1, Z - Z_1, N - N_1)$$

“Field” asymmetry  $\alpha_g \rightarrow$  Asymmetry in  $N$  and  $Z$ ! This means 2 asymmetry coordinates rather than a single “field” asymmetry. How?

Calculate neutron shell correction for grid of  $\alpha_g$  corresponding to integer  $N$  values. Save the *neutron* shell corrections  $ESH_N(N_1, N - N_1)$ .

Calculate proton shell correction for grid of  $\alpha_g$  corresponding to integer  $Z$  values. Save the *proton* shell corrections  $ESH_Z(Z_1, Z - Z_1)$ .

$$ESH_{Z+N}(Z_1, N_1, Z - Z_1, N - N_1) = \\ ESH_Z(Z_1, Z - Z_1) + ESH_N(N_1, N - N_1)$$

## Modeling in BSM of

$$Y(Z_1, N_1, Z - Z_1, N - N_1)$$

We need total potential energy versus fragment proton and neutron numbers. Now what about the

### Macroscopic energy:

$$EMAC_{Z+N}(Z_1, N_1, Z - Z_1, N - N_1)$$

Start by calculating  $EMAC_{\text{comp}}$  for the compound nucleus for a grid in  $\alpha_g$  corresponding to integer  $Z_1$  and  $Z - Z_1$ .

The neutron numbers in the fragments corresponding to the  $\alpha_g$  yielding these integer  $Z_1$  are not integers.

Now fix  $Z_1$  and calculate the macroscopic energy for this (fixed)  $Z_1$  but for different integer  $N_\nu$  as the sum

$$EMAC_{Z+N}(Z_1, N_\nu, Z - Z_1, N - N_\nu) =$$

$$EMAC_{\text{comp}} + \Delta EMAC$$

To obtain the second term calculate the sum of the macroscopic energies for the separated fragments:

$$EMAC(Z_1, N_\nu) + EMAC(Z - Z_1, N - N_\nu)$$

where  $Z_1$  is fixed,  $N_\nu$  varies.  $\Delta EMAC$  for various  $N_\nu$  ( $Z_1$  is still fixed) is the difference between this function at  $N_\nu$  and at the noninteger  $N$  corresponding to the chosen  $Z_1$ .

FRAGMENT MACROSCOPIC ENERGIES AND THE SUMS

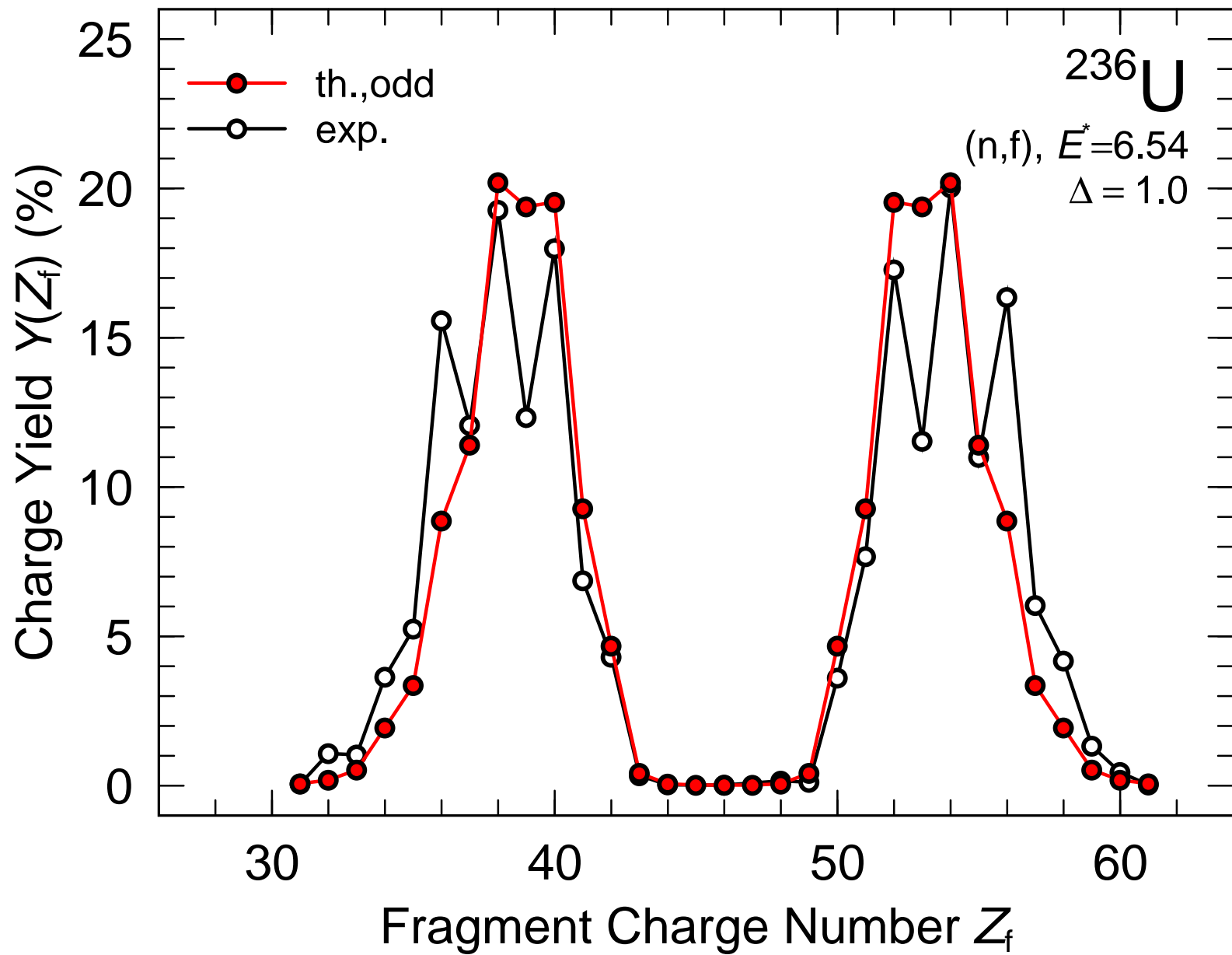
Z1	N1	Ef1	Z2	N2	Ef1	Ef1+Ef2
52	96	-15.90	40	48	-84.863	-100.759
52	94	-26.21	40	50	-87.564	-113.770
52	92	-35.87	40	52	-88.817	-124.691
52	90	-44.88	40	54	-88.701	-133.576
52	88	-53.18	40	56	-87.292	-140.473
52	86	-60.77	40	58	-84.659	-145.427
52	84	-67.60	40	60	-80.865	-148.469
52	82	-73.66	40	62	-75.973	-149.635C
52	80	-78.91	40	64	-70.036	-148.945
52	78	-83.31	40	66	-63.108	-146.419
52	76	-86.83	40	68	-55.237	-142.071
52	74	-89.44	40	70	-46.470	-135.910
52	72	-91.09	40	72	-36.849	-127.938
52	70	-91.74	40	74	-26.413	-118.154
52	68	-91.35	40	76	-15.202	-106.552
52	66	-89.87	40	78	-3.250	-93.122

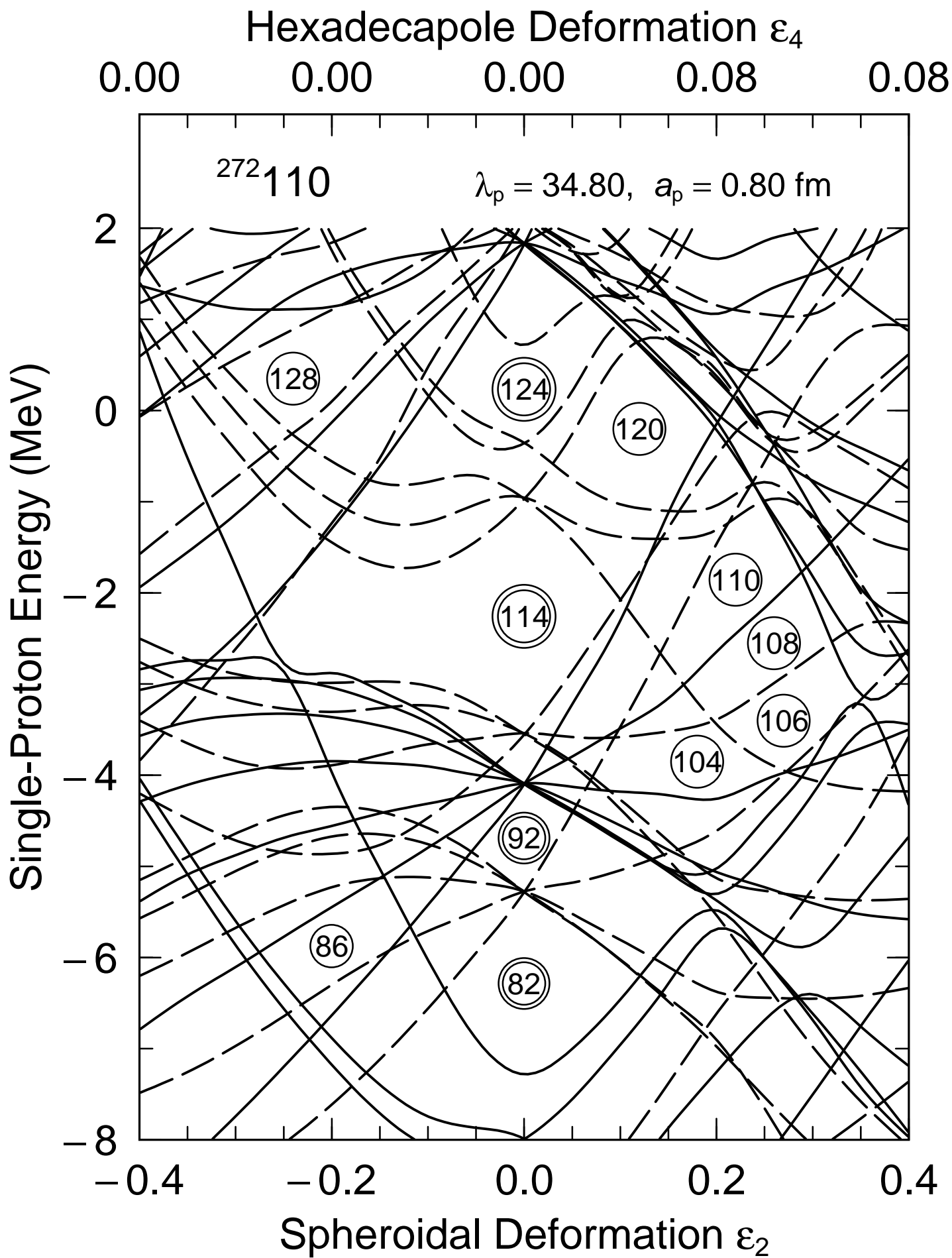
```
READ(LU,'(2f10.3)') r,rw
```

```
idiv =(N+1)/2
```

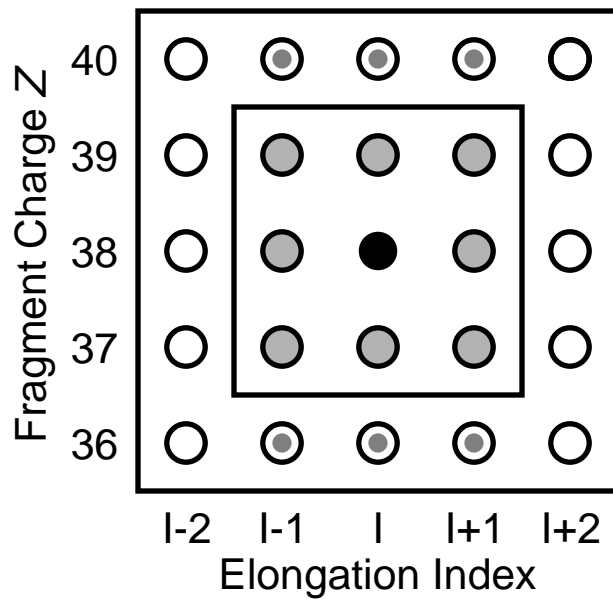
```
if(N+1 .eq. 2*idiv) r = r + (rw-1 +0.01)*2*1.0
```

```
E(I,J,K,L,N) = r
```

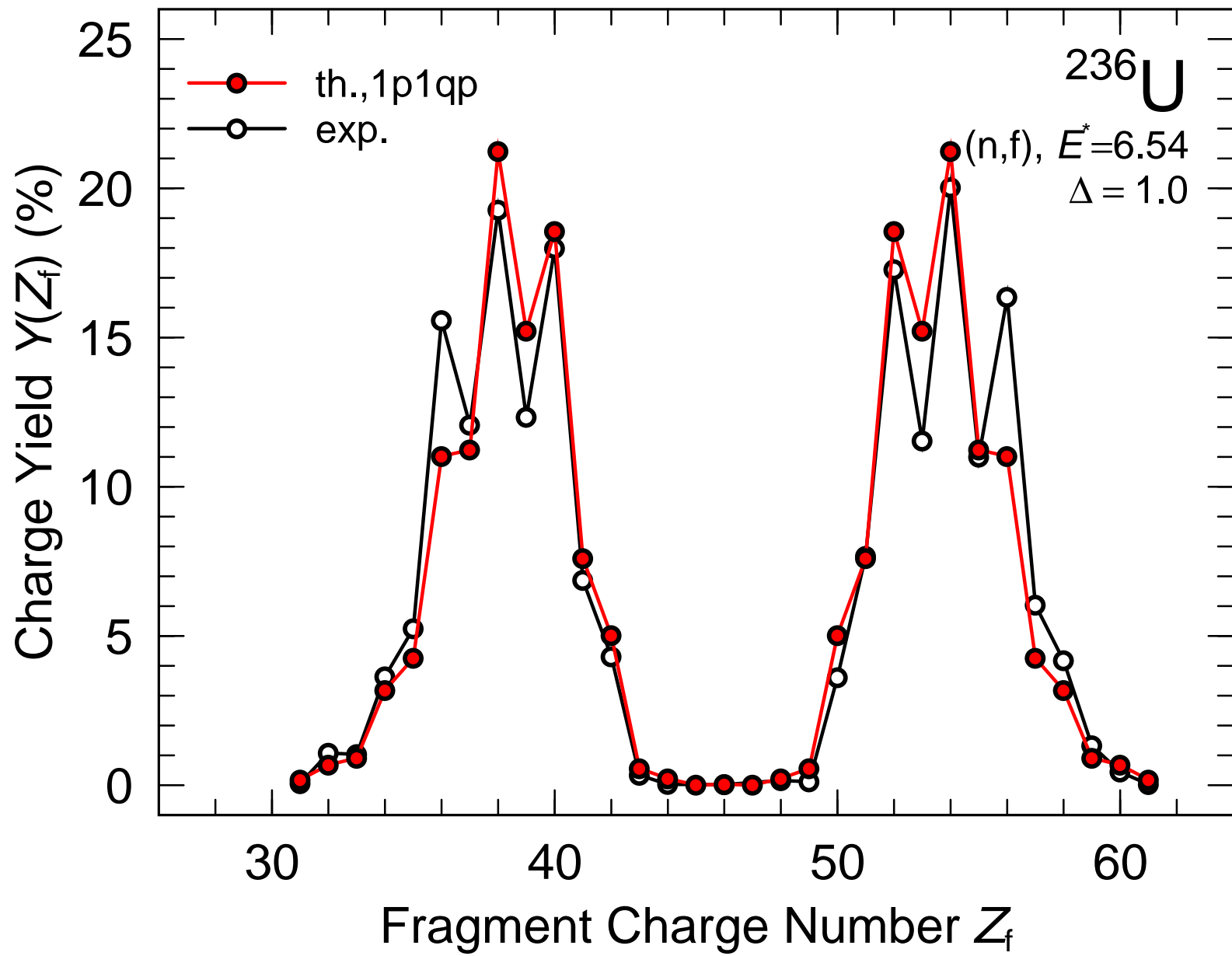


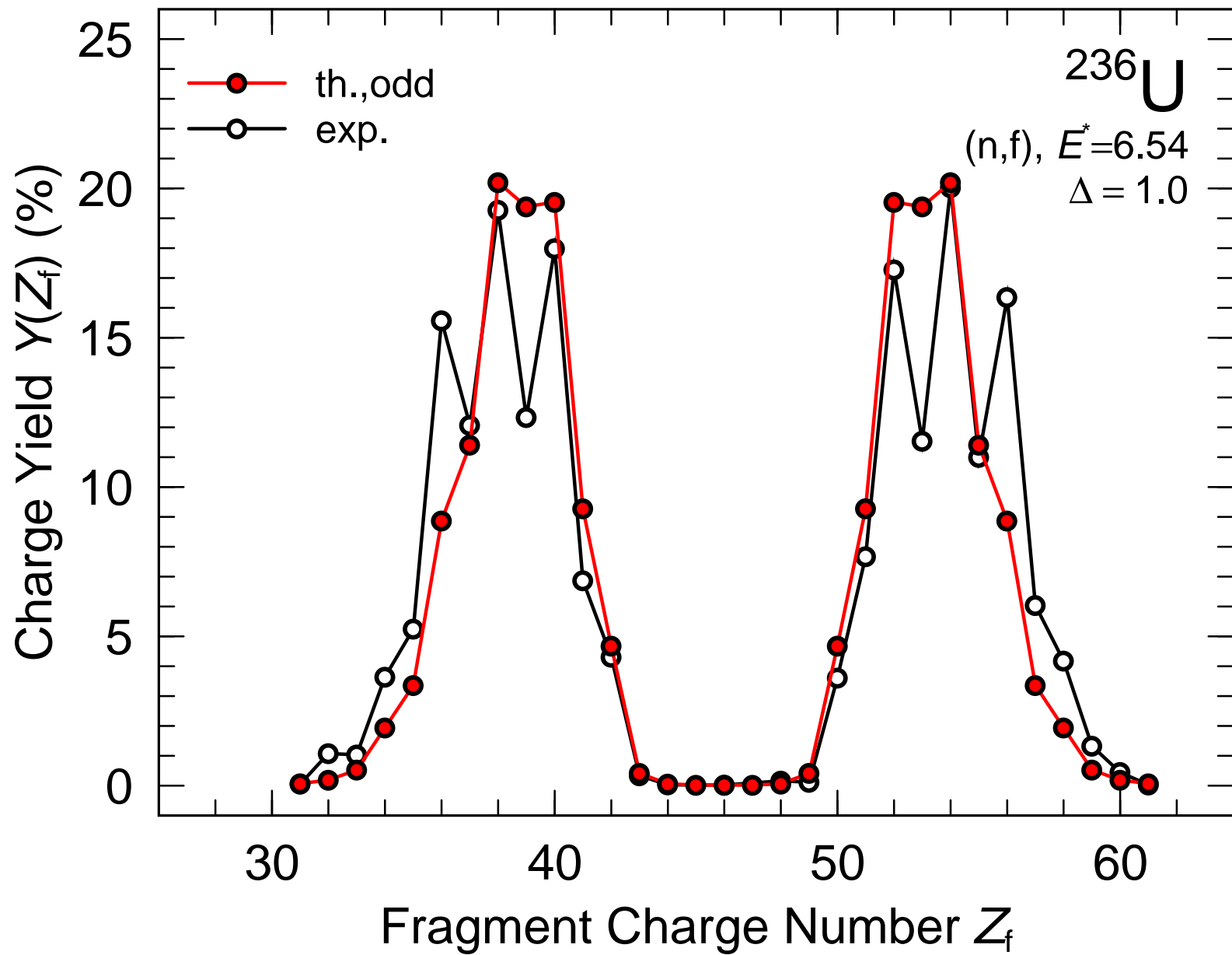


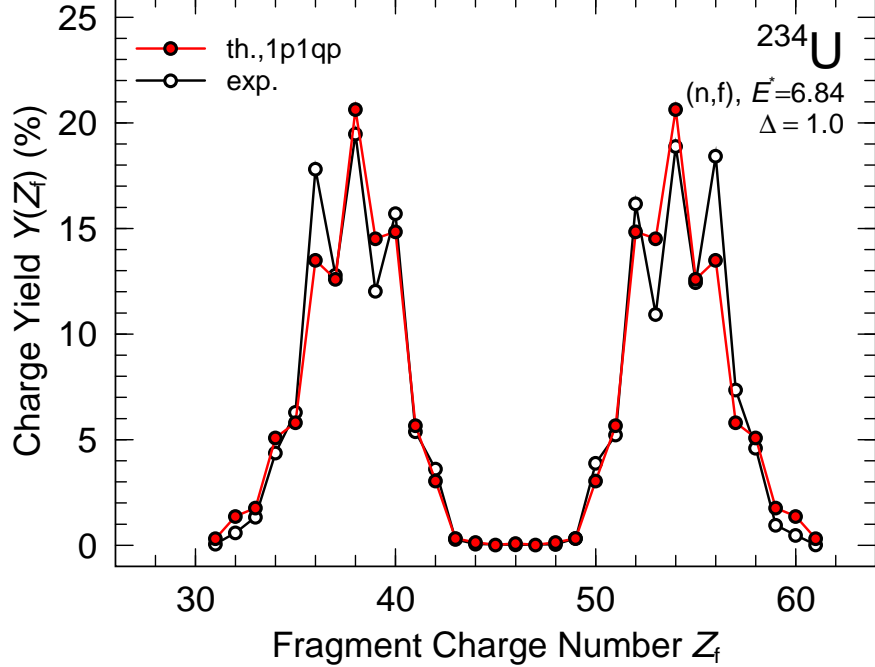
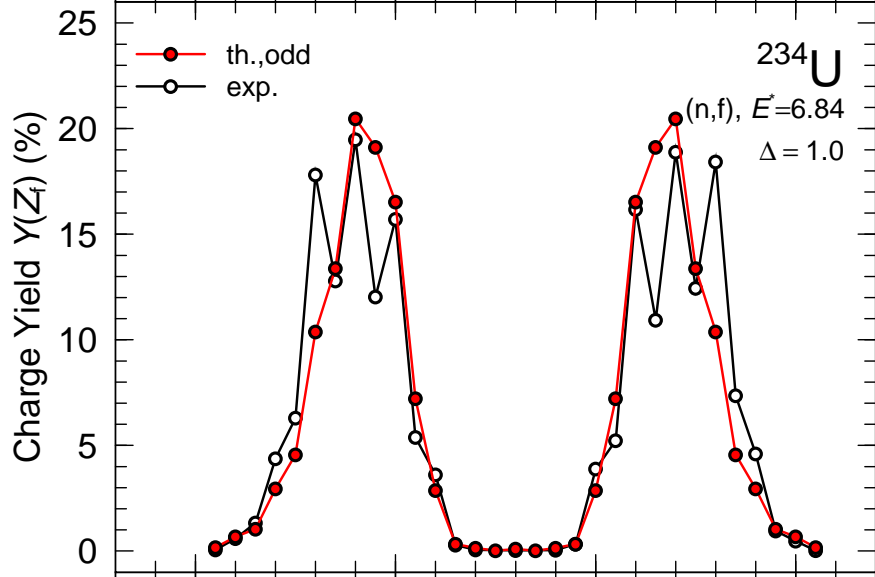
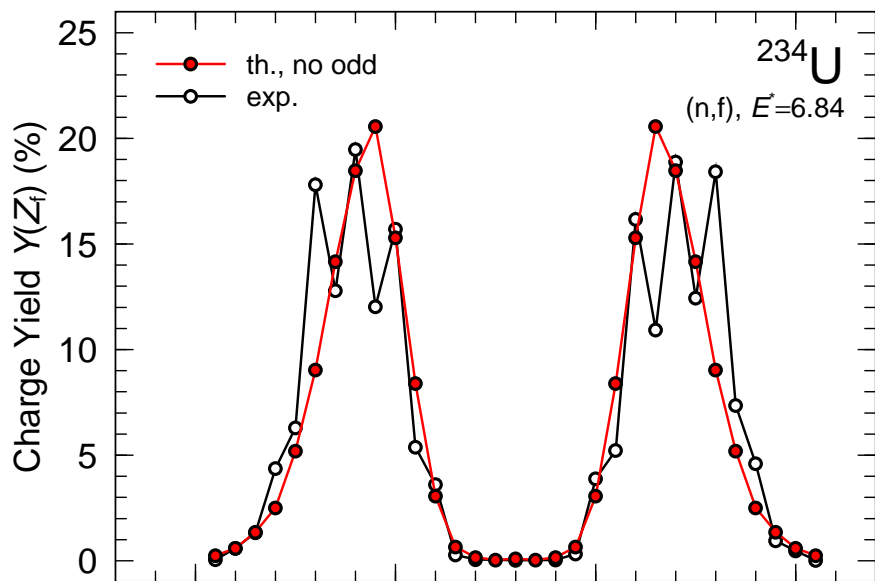
### Next Track-Point Candidates

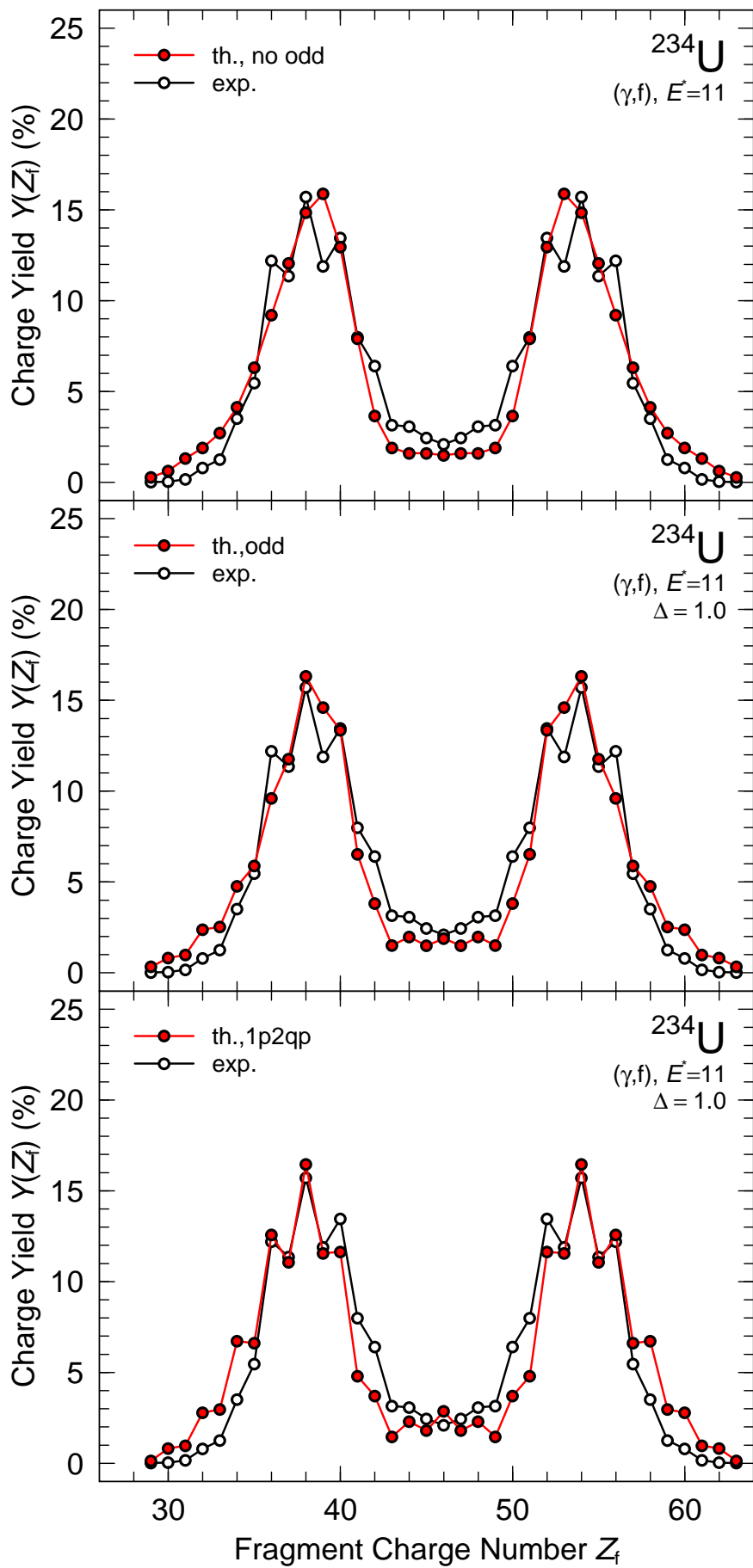


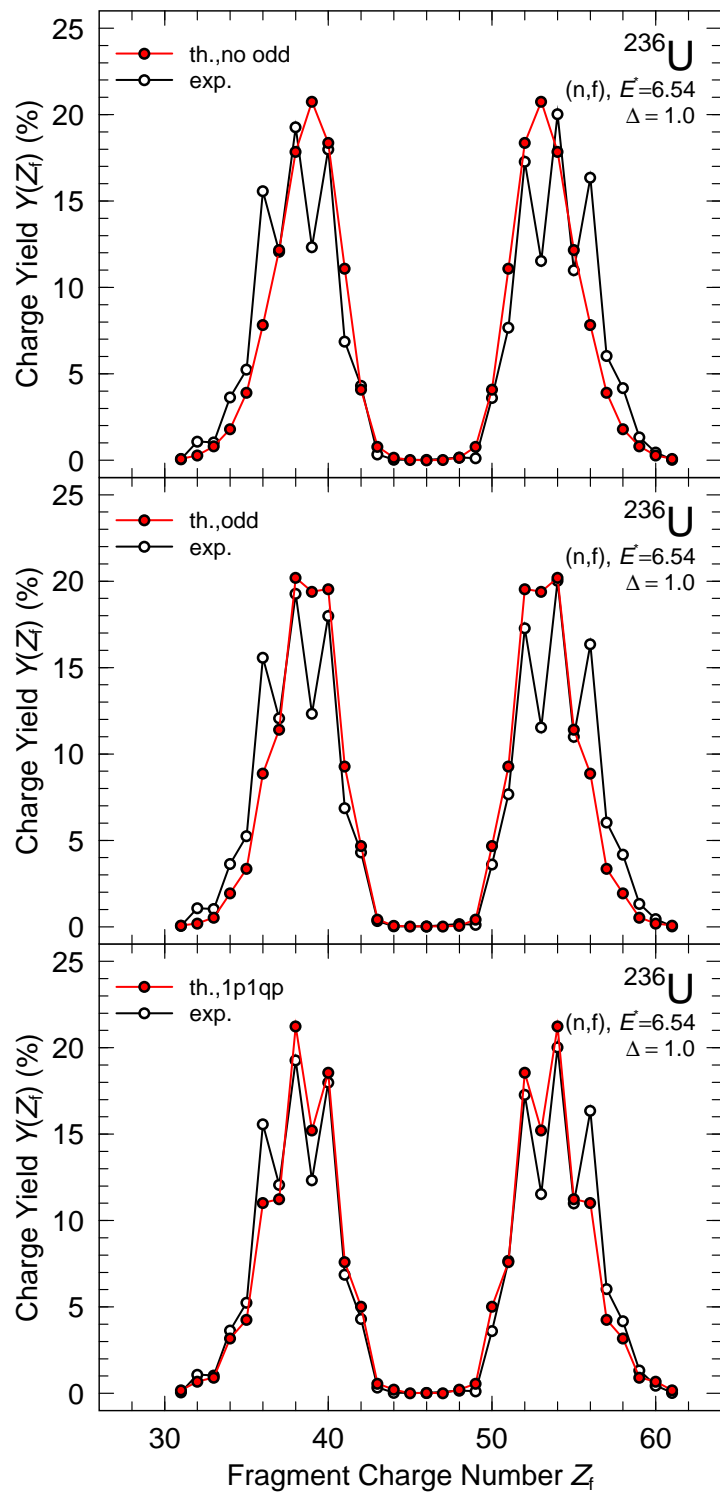


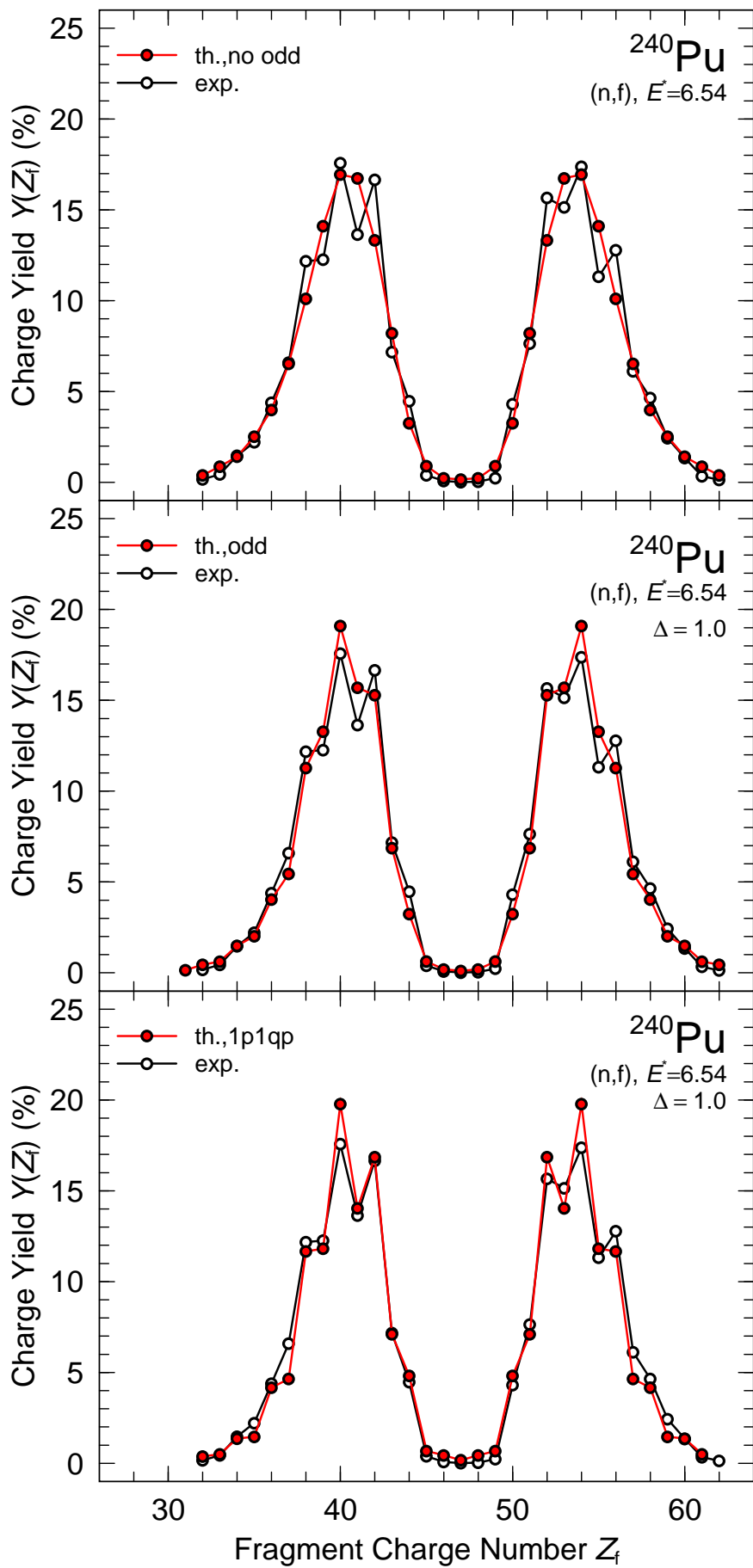


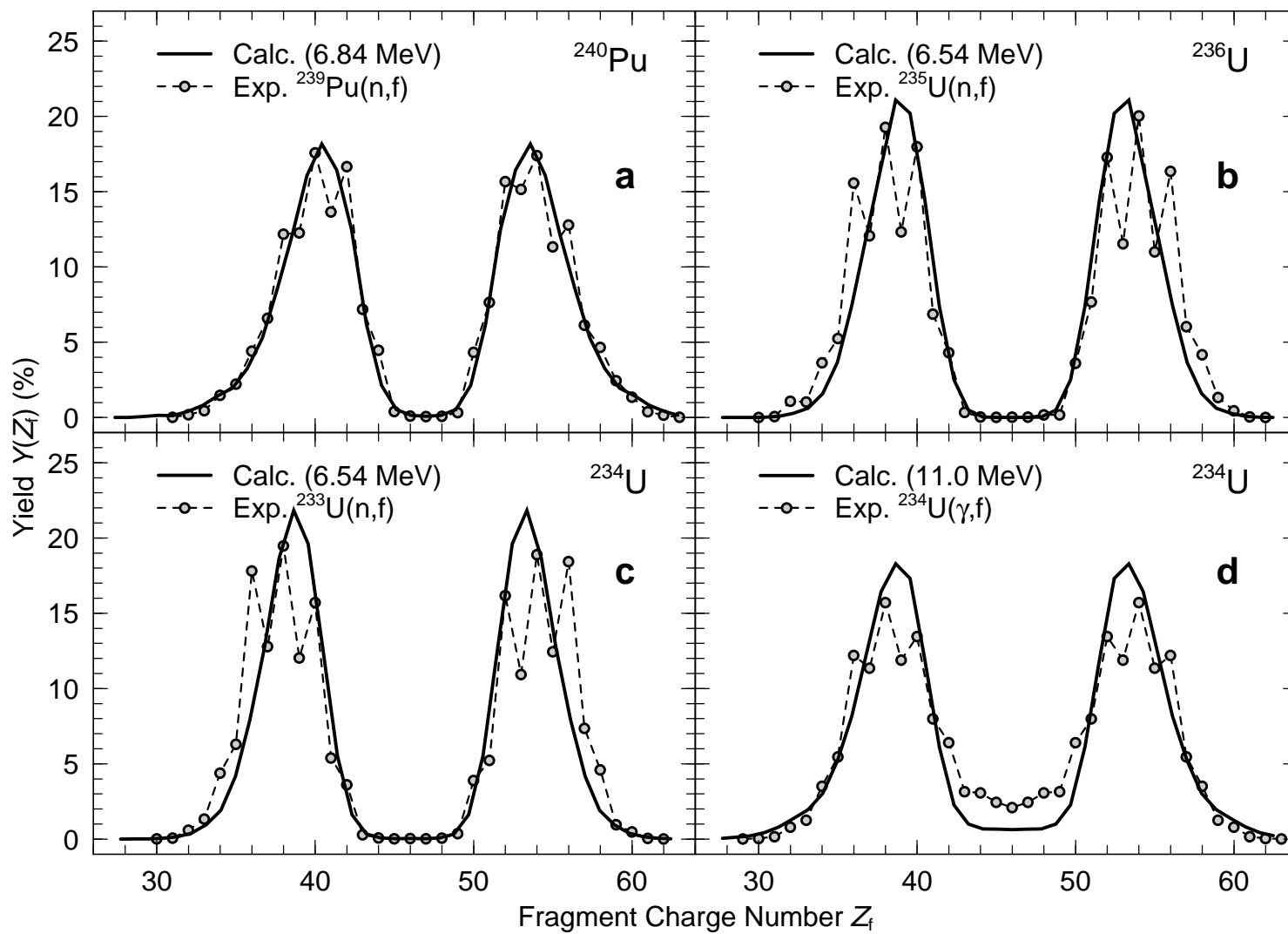


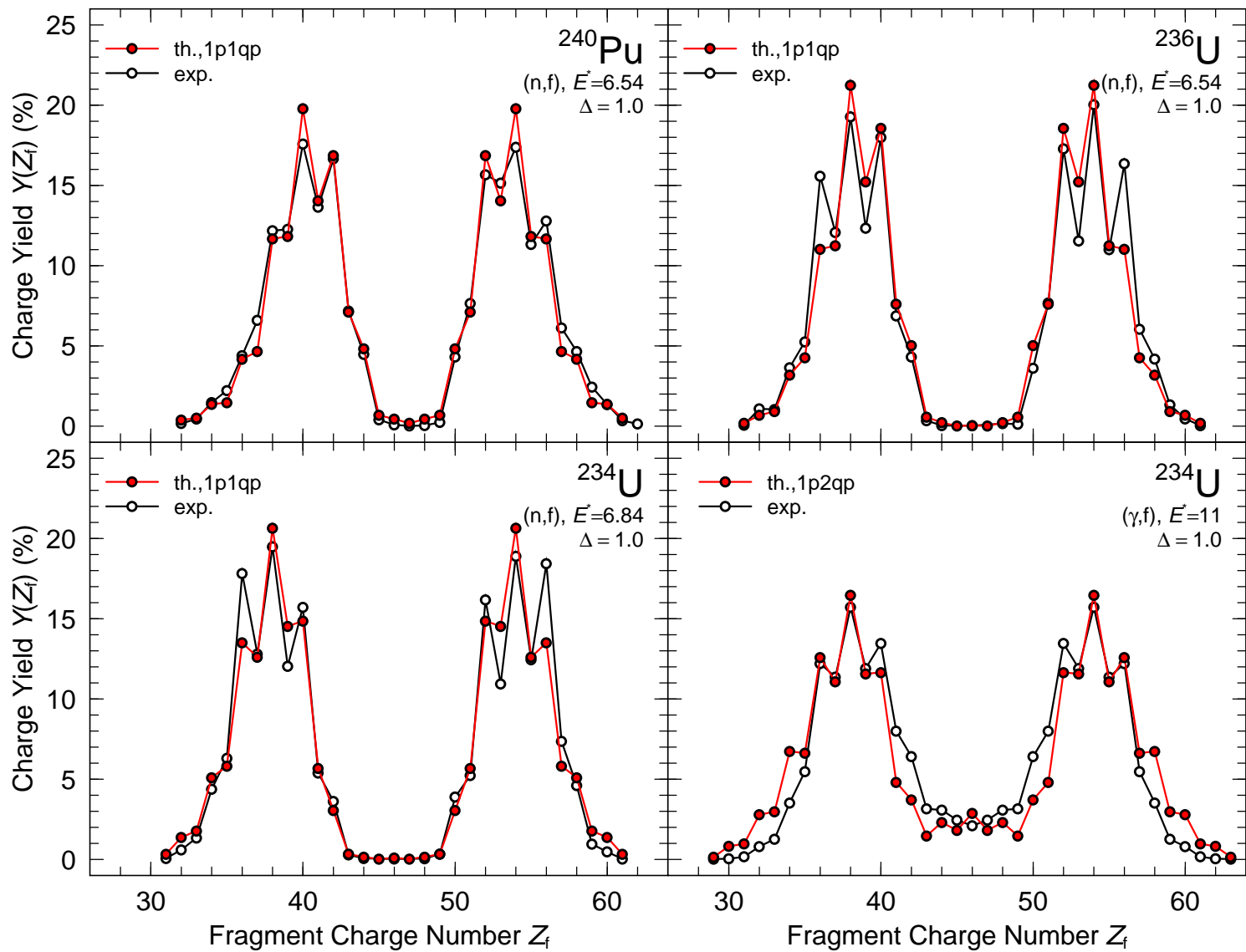












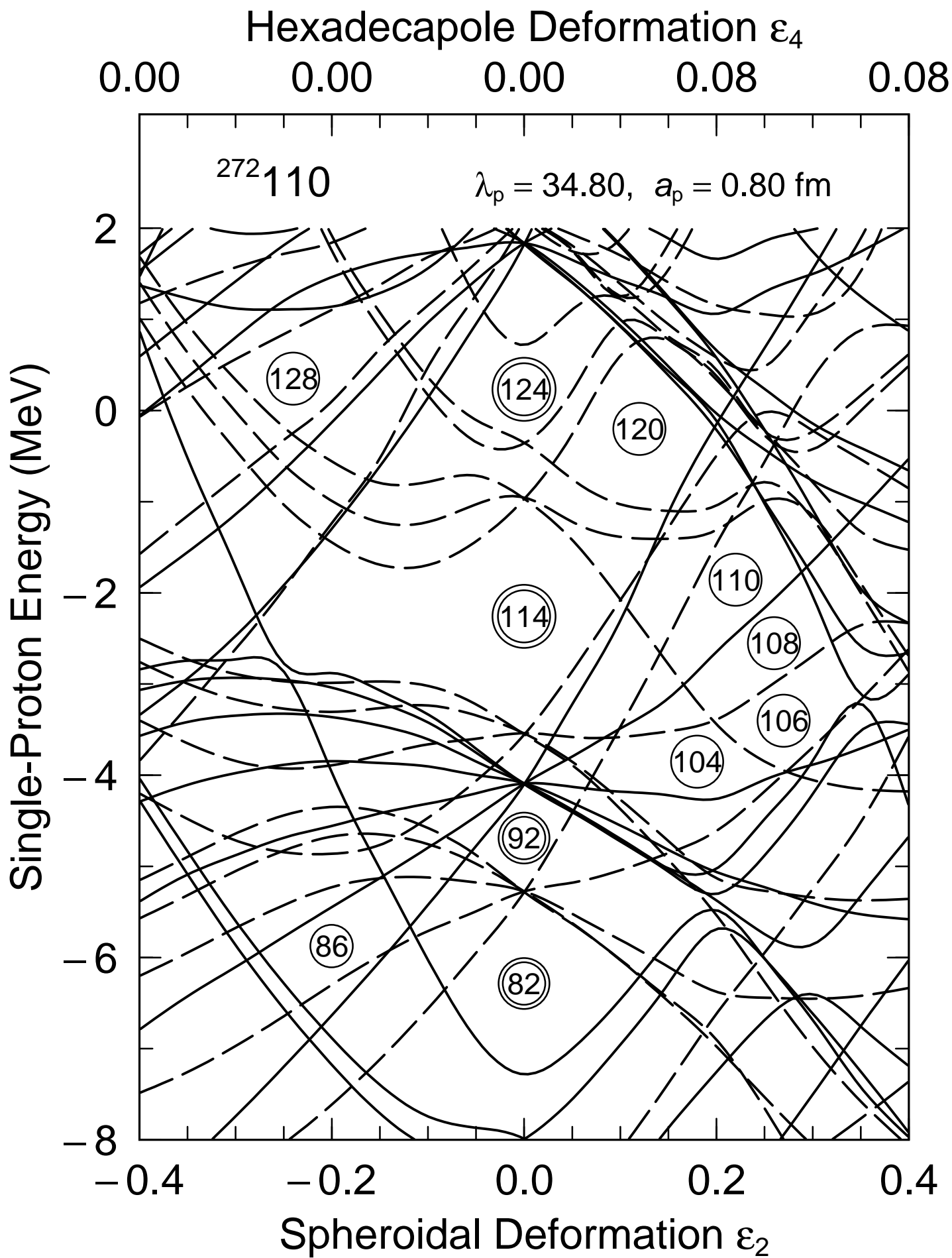


# M E T R O P O L I S

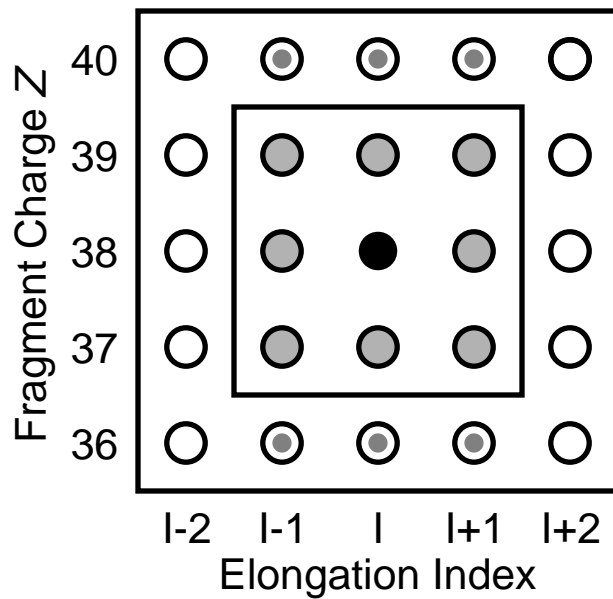
The **simplicity** of  
the algorithm nobly  
stands aside the **complexity**  
of the problems  
it **successfully** treats.

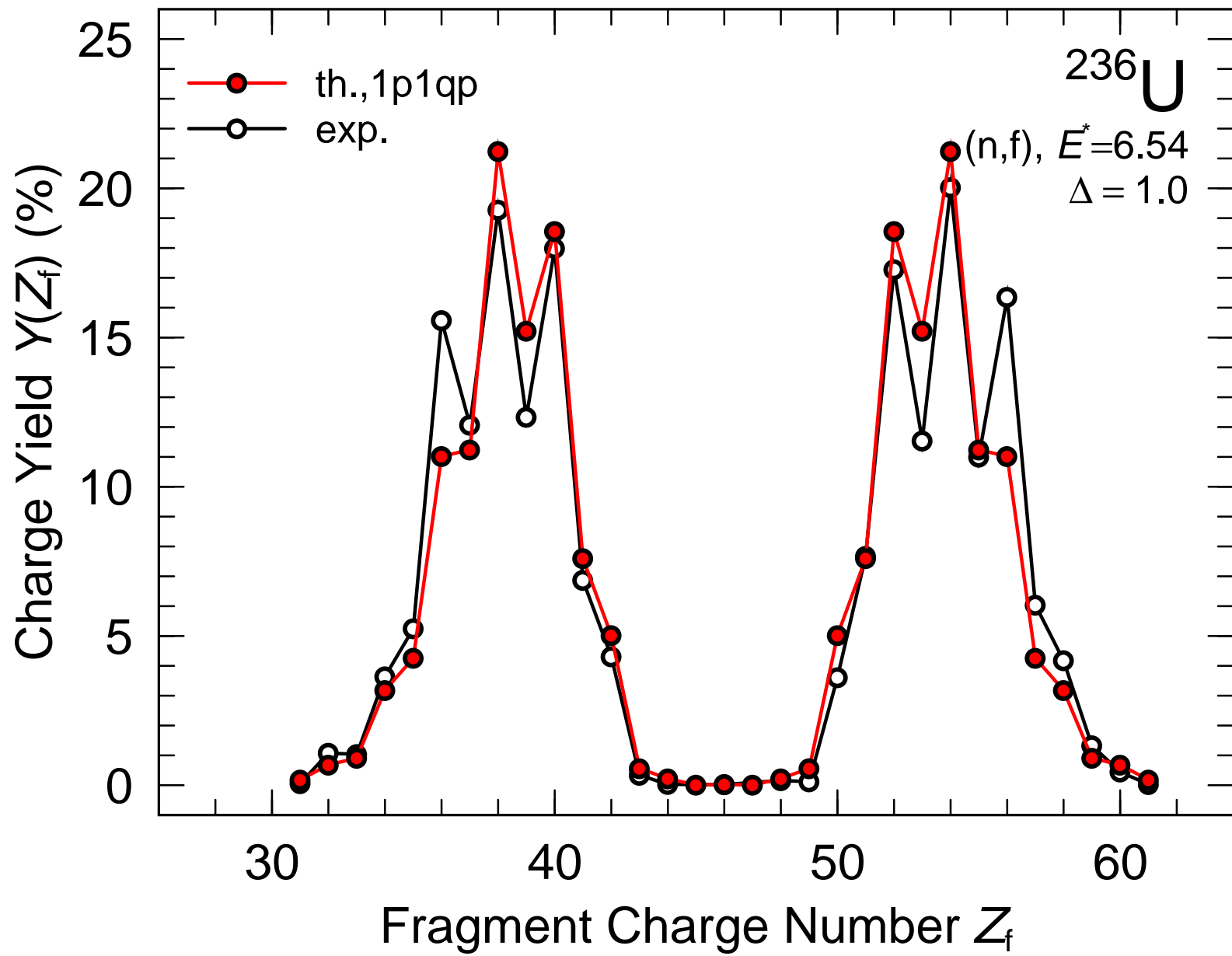
# M E T R O P O L I S

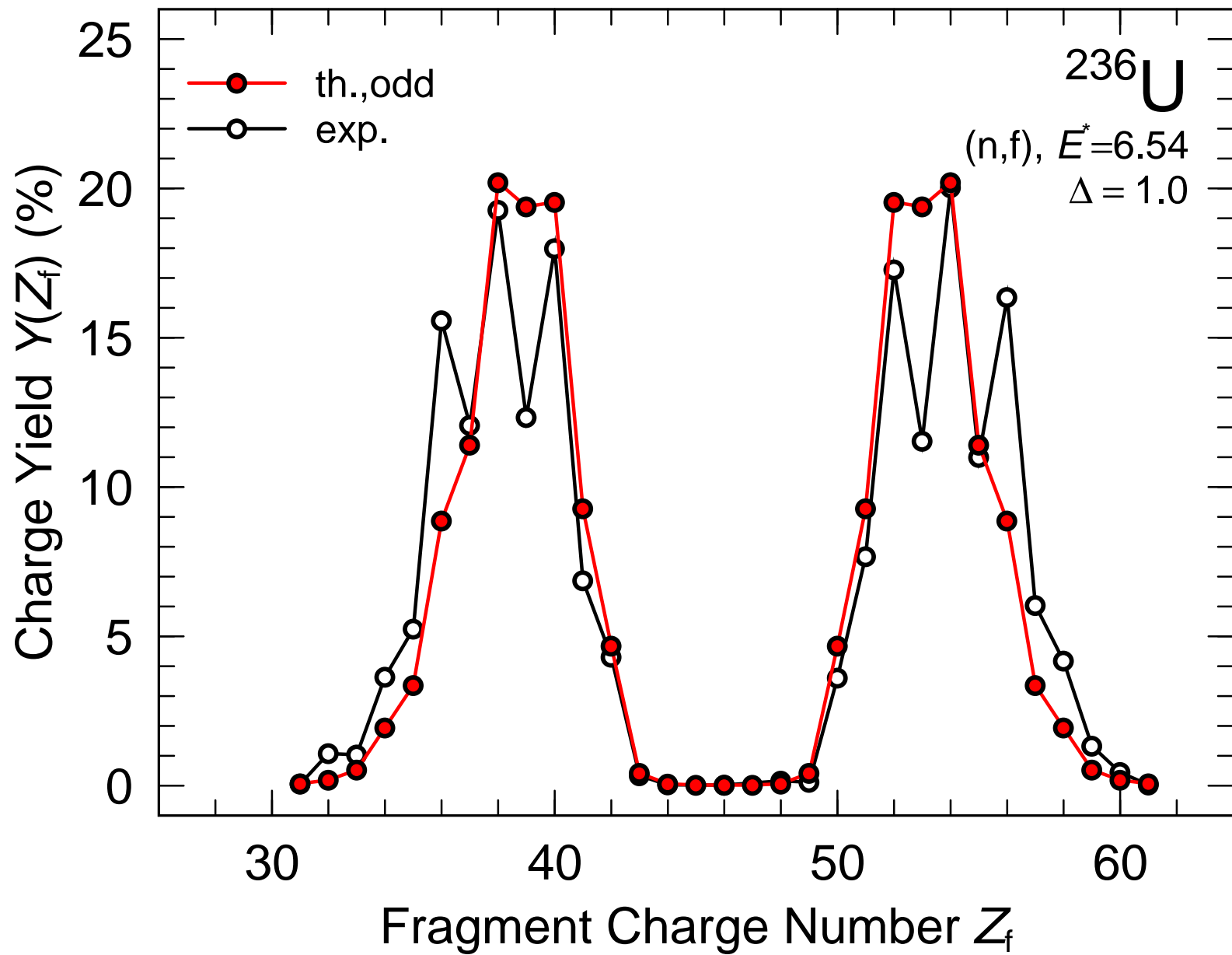
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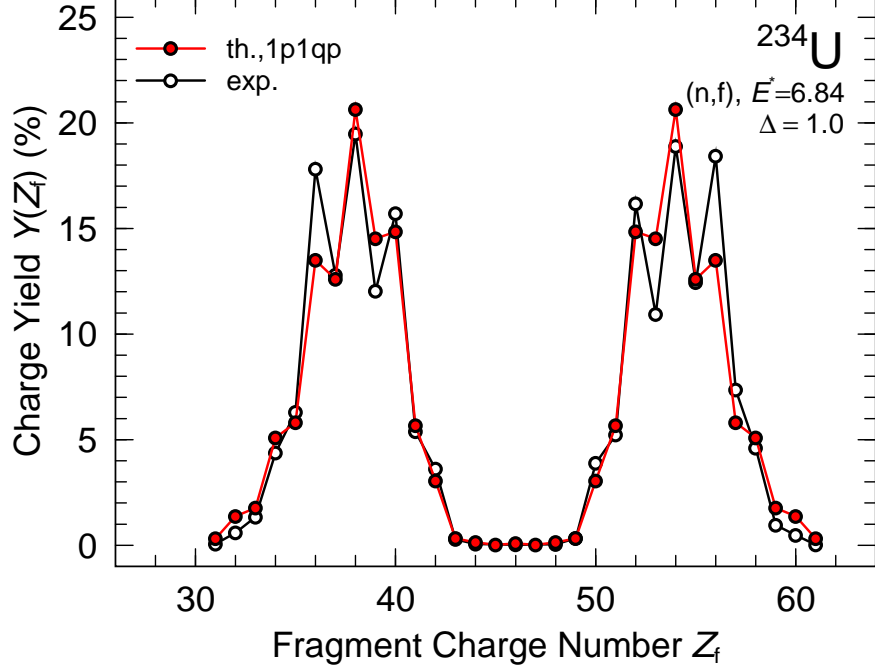
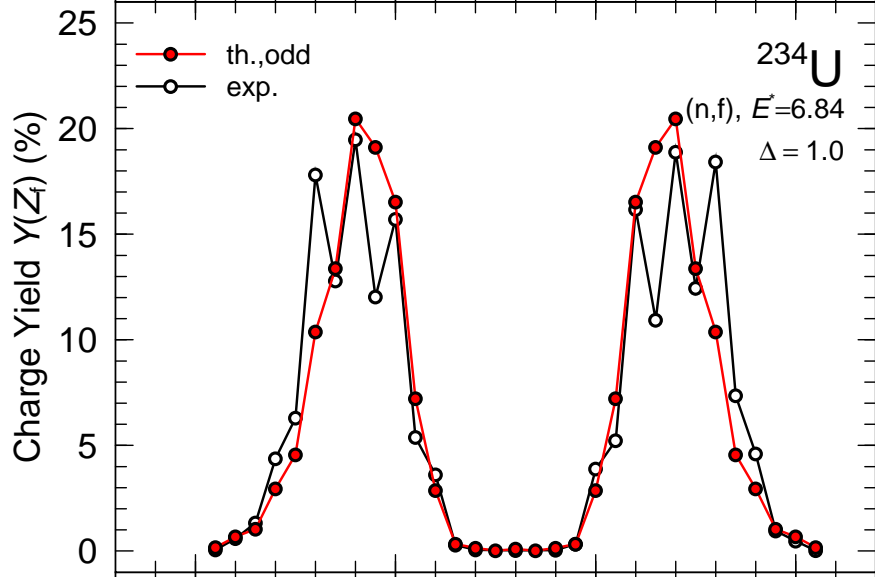
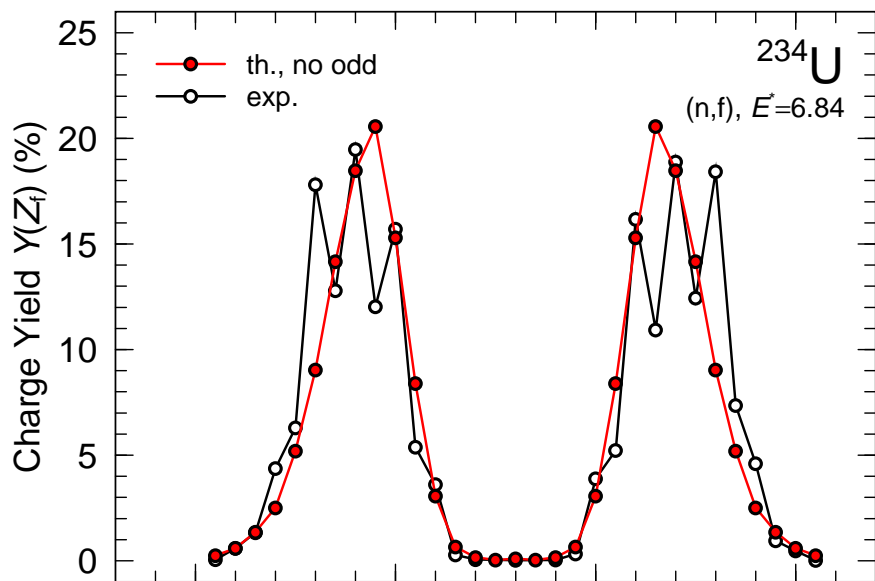


### Next Track-Point Candidates

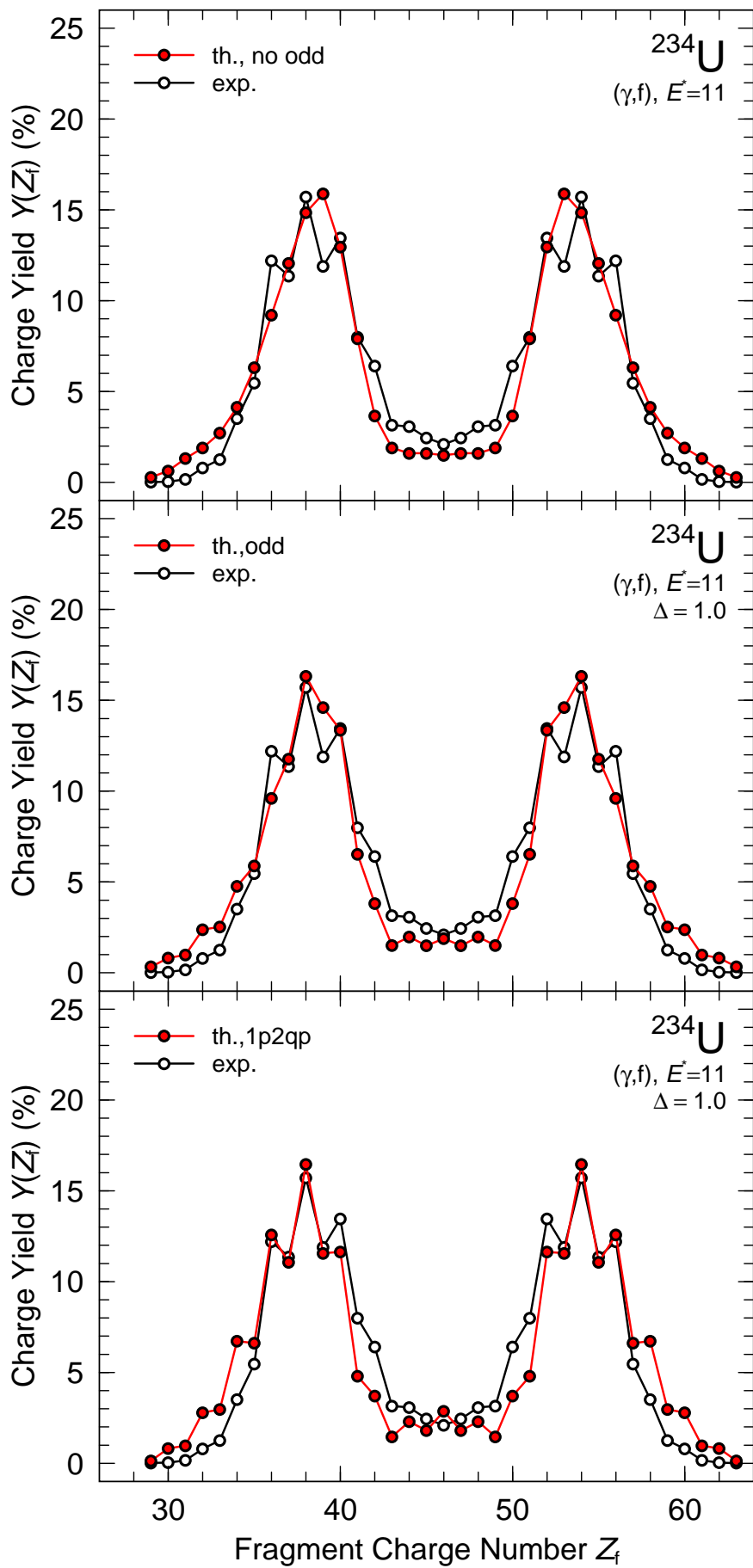




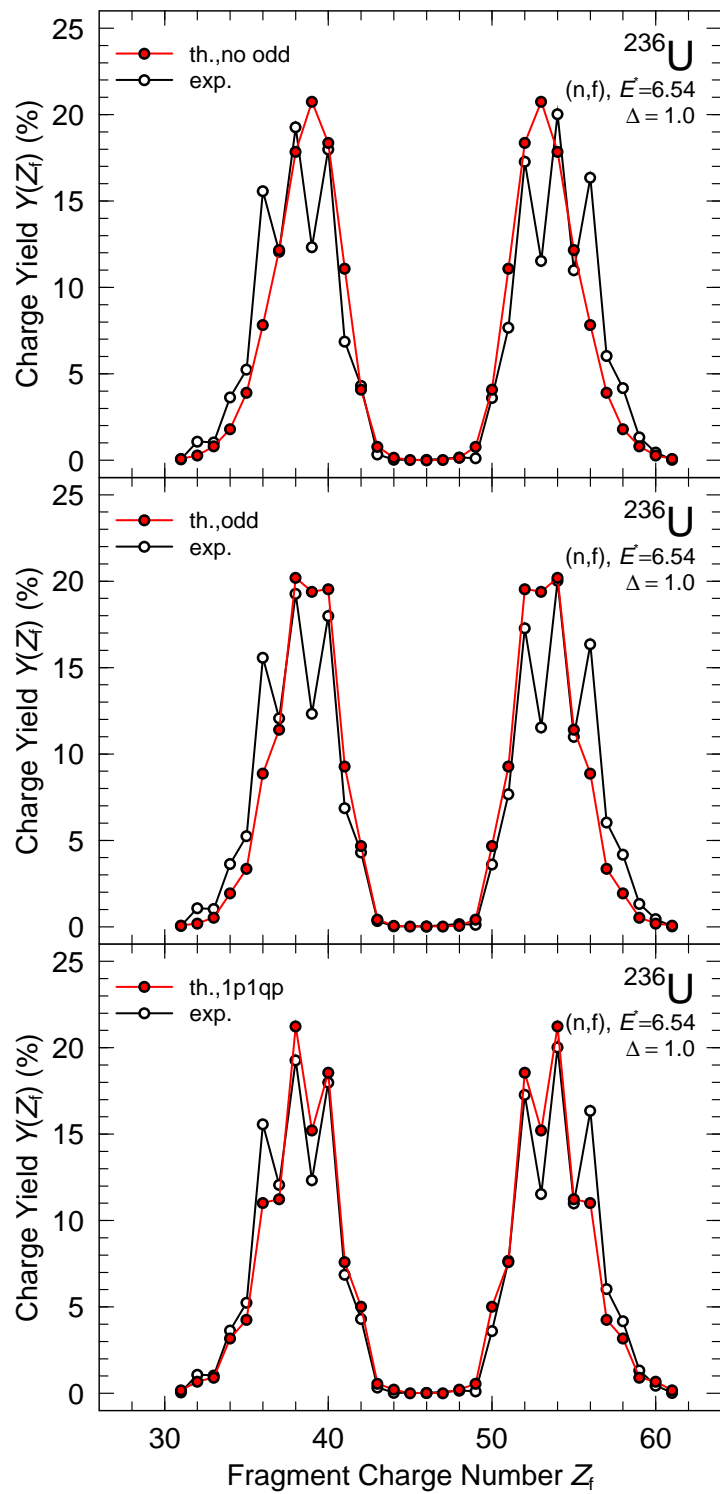


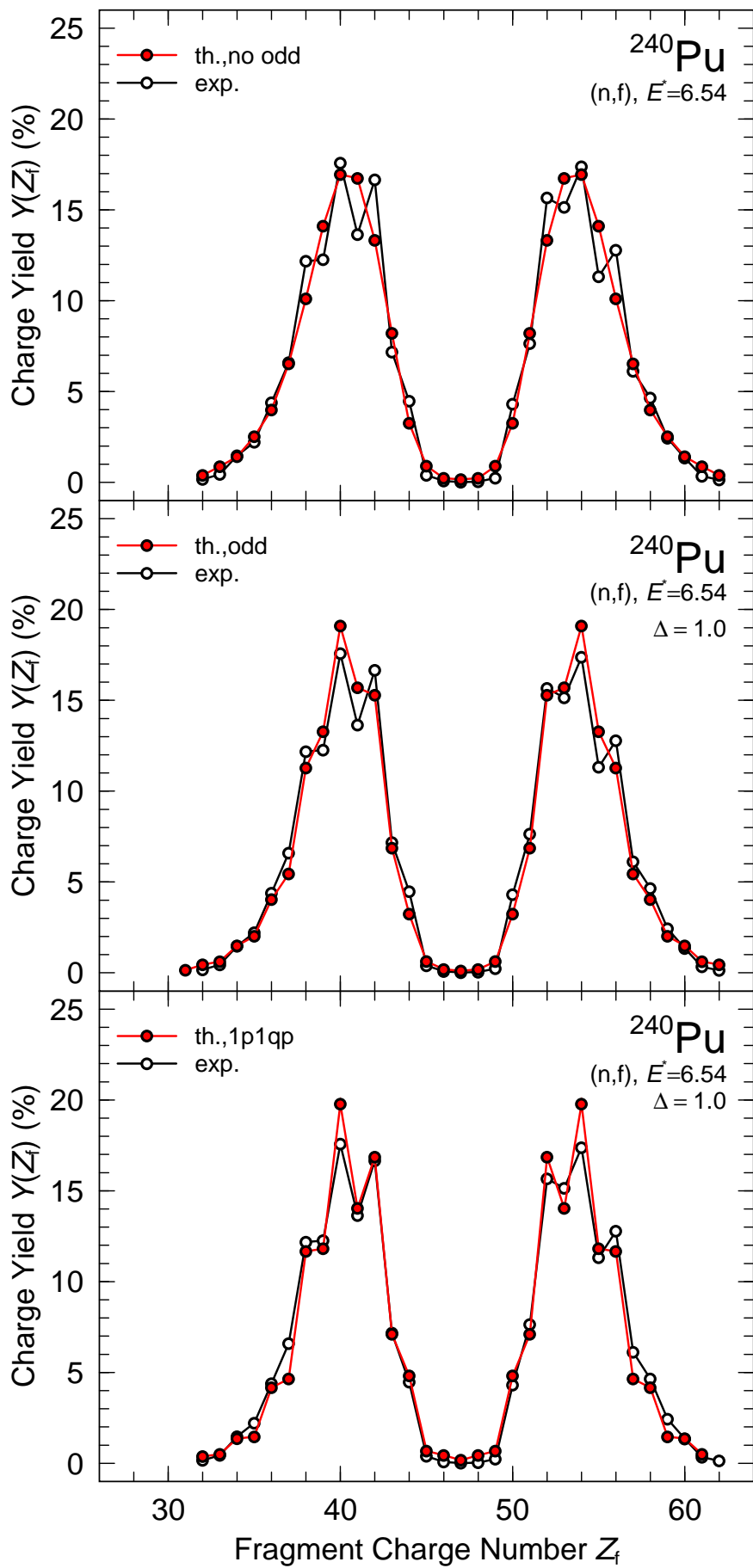


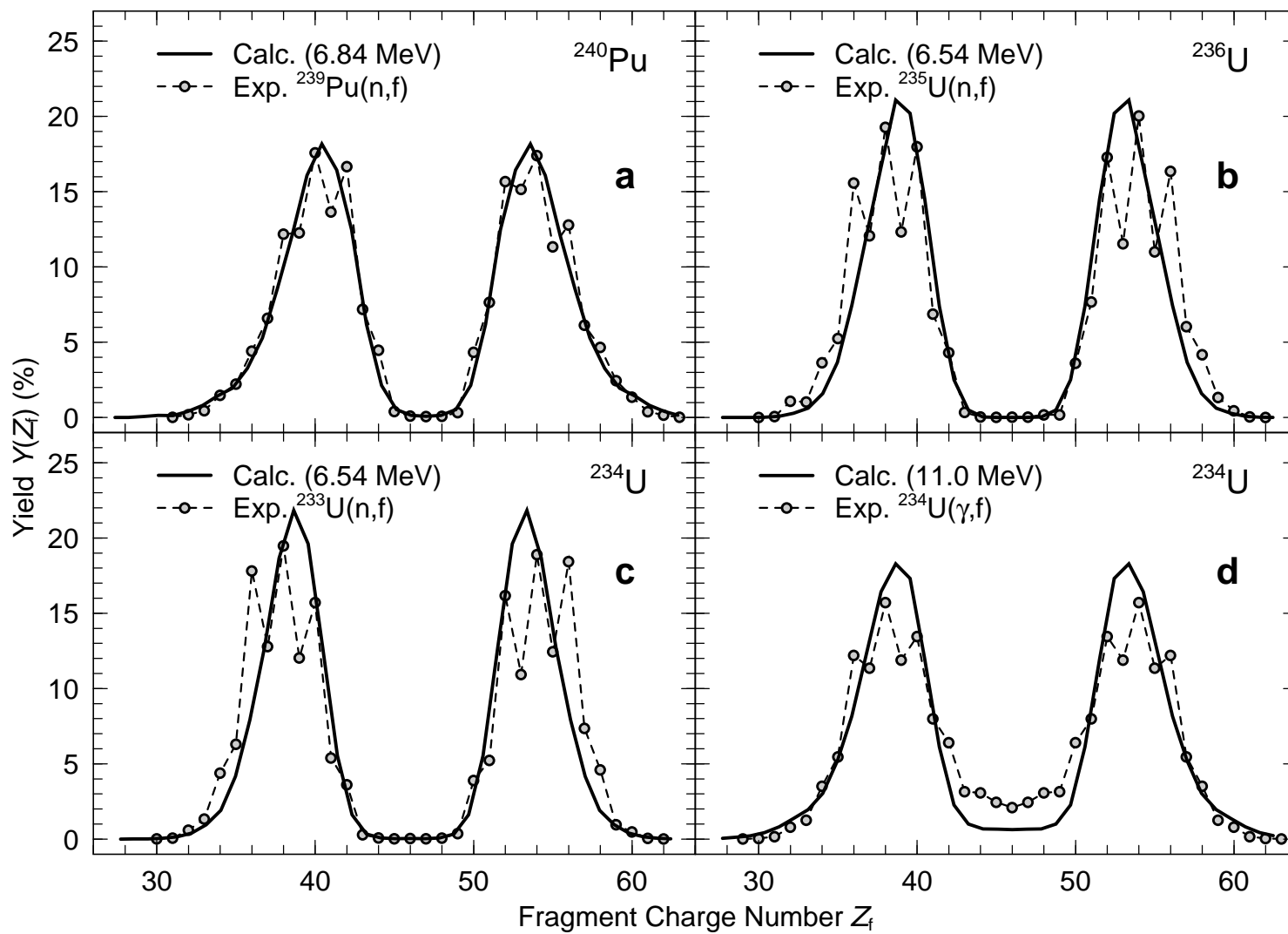
Fragment Charge Number  $Z_f$

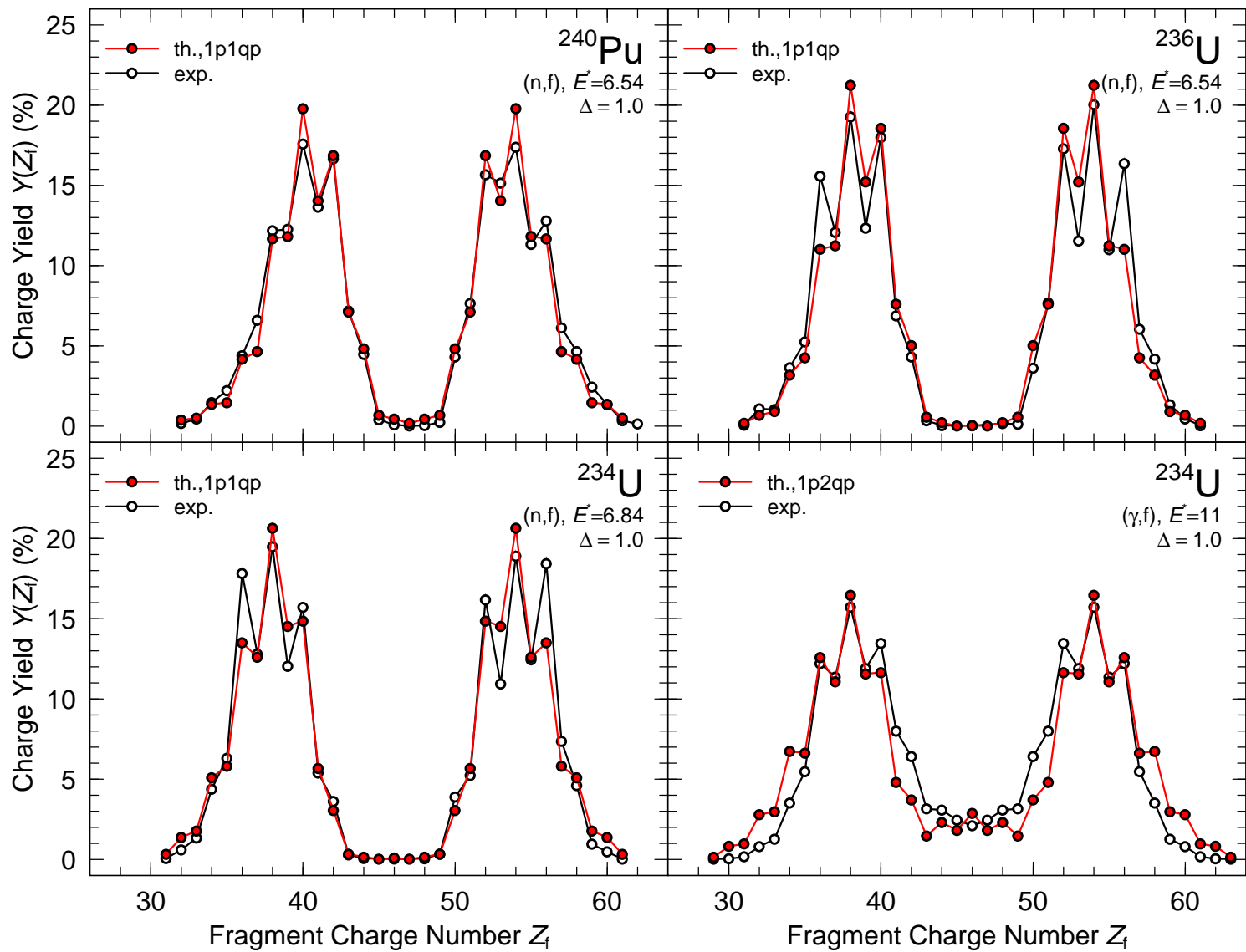












# M E T R O P O L I S

The **simplicity** of  
the algorithm nobly  
stands aside the **complexity**  
of the problems  
it **successfully** treats.