UNLIMITED RELEASE

SC-RR-68-619

ANALYTICAL APPROXIMATIONS FOR TOTAL PAIR-PRODUCTION CROSS SECTIONS

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September 1968

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ABSTRACT

Analytical approximations which are efficient for use in computer programs are given for total pair-production cross sections for atomic numbers $1 \leq Z \leq 100$ in the photon energy interval $1022.012 \leq E \leq 10^5$ keV. Graphs of cross sections and approximation parameters in tabular form are included.

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ANALYTICAL APPROXIMATIONS FOR TOTAL PAIR-PRODUCTION CROSS SECTIONS

Whenever x-ray cross sections are needed in computer programs, it is convenient to have approximations for them in analytical form. It is desirable that these analytical expressions exhibit such properties as speed in computer evaluation, economy in memory storage, ease in adapting to composite materials, and as much accuracy as the "source data" justify. The term "source data" is used here to refer to the input data to the curve-fitting programs. A scheme such as this which applies to the photoelectric and Klein-Nishina cross sections is described in detail in an earlier report by the authors.[1] This report gives the results of our efforts to include the total pair production in the scheme.

Pair production is the photon-matter interaction wherein a photon of sufficient energy encounters a strong electric field and is converted into an electron-positron pair. We use the expression "total pair-production cross section" to mean the sum of the cross sections for pair production in the field of the atomic nucleus plus pair production in the fields of the atomic electrons.

The units used are keV (kiloelectron volts) for photon energies and cm^2/gm for the cross sections. The range of atomic numbers considered is $1 \leq Z \leq 100$ and the photon energy range is from threshold to 10^5 keV.

A least squares fitting technique was used to fit the analytical expressions to the source data. The technique has been described in a report by one of the authors.[2]

Source data were taken from Storm and Israel[3] who estimate that the nuclear field cross sections are accurate to within 5 percent and that the electron field cross sections are accurate to within 10 percent.

After preliminary numerical experimentation, it appeared that a suitable function to use as an approximation was

$$\mu(E) = \begin{cases} 0, \; E < B \\ C(E - B)^2, \; B \le E \le 1500 \text{ keV} \\ \dfrac{1}{1 + 1.7 \times 10^{-13} V^6} \displaystyle\sum_{n=1}^{7} A_n V^n \;, \; 1500 \text{ keV} < E \le 10^5 \text{ keV} \;, \end{cases} \tag{1}$$

where μ is the total pair-production cross section in cm^2/gm, E is photon energy in keV, $V = (E - B)^{1/2}$, $B = 2mc^2 = 1022.012$ keV (m is electronic mass and c is speed of light). A set of fitting parameters, C and A_n's, is needed for each element. These are tabulated in the parameter table, Table I, versus the atomic number Z. Since we require that the function μ be continuous at E = 1500 keV, the value of the parameter C can be calculated from the A_n's, but for convenience we give the values of C in Table I for each element.

Figures 1 through 10 are curves which represent μ of Eq. (1) for each element, using the fitting parameters given in Table I. Source data in the graphs are indicated by asterisks. Adjacent curves represent a difference of 10 in atomic number. The atomic number Z increases in going upward from one curve to the next; the top and bottom curves are labeled by the corresponding values of Z.

The part of the function of Eq. (1), applying in the interval $B < E \le 1500$ keV, was used to provide a smooth extrapolation of the approximation to zero at the nuclear field cross section threshold energy E = B. Even though the approximation for use in the interval above E = 1500 keV goes to zero at E = B, it does not always do so in a smooth manner and, indeed, would give negative values for photon energies slightly above E = B for all the elements that exhibit a negative value for A_1 in Table I.

As a measure of the average relative error involved in fitting Eq. (1) to the source data of each element, we use

$$\epsilon = \left\{ \frac{1}{M} \sum_{i=1}^{M} \left[\frac{\mu(E_i) - \hat{\mu}(E_i)}{\hat{\mu}(E_i)} \right]^2 \right\}^{1/2} , \tag{2}$$

where ϵ is the rms error, M is the number of source data cross sections, $\mu(E_i)$ is Eq. (1) evaluated at $E = E_i$, and $\hat{\mu}(E_i)$ is the source data cross section for photon energy E_i. The rms error is given for each element in Table I.

It should be noted that the fitting parameters, C and A_n's, are tabulated in Table I to fewer decimal places of accuracy than the computer (CDC 3600) uses. A calculation was made to round off the parameters as much as possible without increasing the rms error by more than 1/2 percent. It is the rounded values that appear in the table. Whenever a parameter is rounded off to less than four significant places, the printout format is such that zeros are printed in the remaining places. The curves of Figs. 1 through 10 and the rms errors of Table I were obtained by using the rounded-off parameters.

For a composite material consisting of N elements, the approximation for the total pair-production cross sections in cm^2/gm is

$$\mu(E) = \sum_{i=1}^{N} f_i \mu_i(E) \quad , \tag{3}$$

where f_i is the fraction (by mass) of element i that occurs in the material and $\mu_i(E)$ is Eq. (1), applied when the set of fitting parameters corresponding to element i is used. If one substitutes Eq. (1) into Eq. (3) and interchanges sums, $\bar{\mu}$ becomes

$$\bar{\mu}(e) = \begin{cases} 0, \; E < B \\ \bar{C}\,(E - B)^2 \;, \; B \le E \le 1500 \text{ keV} \\ \dfrac{1}{1 + 1.7 \times 10^{-13}\, V^6} \displaystyle\sum_{n=1}^{7} \bar{A}_n V^n \;, \; 1500 < E \le 10^5 \text{ keV}, \end{cases} \tag{4}$$

where

$$\bar{C} = \sum_{i=1}^{N} f_i C^i \tag{5}$$

and

$$\bar{A}_n = \sum_{i=1}^{N} f_i A_n^i \; . \tag{6}$$

We have used superscripts on the fitting parameters to designate the element, and V has the same meaning here as it did in Eq. (1). Therefore, the approximation for a composite material reduces to the same form as that of a single element, and the fitting parameters for the composite material are obtained simply by averaging the ones for the constituent elements.

REFERENCES

1. F. Biggs and R. Lighthill, Analytical Approximations for X-Ray Cross Sections, SC-RR-66-452, Sandia Laboratories, Albuquerque, New Mexico, 1967.

2. F. Biggs, A Generalized Rational Function Least-Squares Fitting Technique, SC-RR-66-2601, Sandia Laboratories, Albuquerque, New Mexico, 1967.

3. Ellery Storm and Harvey I. Israel, Photon Cross Sections From 0.001 to 100 MeV for Elements 1 through 100, LA-3753 (UC-34 Physics, TID-4500), Los Alamos Scientific Laboratory, June 1967 (distributed November 15, 1967).

TABLE I APPROXIMATION PARAMETERS

Z	EL	RMS ERROR	C	A(1)	A(2)	A(3)	A(4)	A(5)	A(6)	A(7)
1	H	1.02-002	1.150-010	-5.550-007	-9.100-008	9.820-009	-9.700-011	2.770-013	4.500-016	1.640-018
2	HE	6.31-003	1.169-010	1.617-006	-3.188-007	1.860-008	-2.524-010	1.488-012	-3.750-015	6.060-018
3	LI	2.13-002	1.526-010	4.590-006	-6.320-007	3.060-008	-4.151-010	2.472-012	-6.385-015	9.000-018
4	BE	1.78-002	2.060-010	-5.080-006	1.910-007	8.770-009	-1.194-010	4.940-013	-9.000-017	2.350-018
5	B	1.68-002	2.707-010	4.160-006	-7.530-007	4.310-008	-5.970-010	3.560-012	-9.100-015	1.320-017
6	C	8.70-003	3.472-010	2.500-007	-5.217-007	4.260-008	-6.093-010	3.650-012	-9.150-015	1.410-017
7	N	2.34-002	3.999-010	-1.370-005	6.940-007	8.500-009	-1.410-010	4.900-013	9.500-016	2.900-018
8	O	1.23-002	4.600-010	1.274-006	-7.757-007	5.898-008	-8.410-010	5.035-012	-1.265-014	1.890-017
9	F	1.45-002	4.921-010	-7.920-006	5.300-008	3.450-008	-4.940-010	2.520-012	-4.700-015	9.500-018
10	NE	1.28-002	5.748-010	2.287-006	-1.034-006	7.598-008	-1.093-009	6.623-012	-1.696-014	2.470-017
11	NA	1.54-002	6.143-010	-1.226-005	2.880-007	3.627-008	-5.330-010	2.795-012	-4.650-015	1.040-017
12	MG	1.40-002	6.961-010	1.154-006	-1.090-006	8.668-008	-1.256-009	7.610-012	-1.940-014	2.834-017
13	AL	1.62-002	7.336-010	5.930-006	-1.598-006	1.059-007	-1.528-009	9.374-012	-2.460-014	3.460-017
14	SI	1.21-002	8.213-010	-5.460-006	-6.530-007	8.240-008	-1.207-009	7.130-012	-1.700-014	2.614-017
15	P	2.20-002	8.715-010	1.190-005	-2.250-006	1.329-007	-1.871-009	1.123-011	-2.873-014	3.920-017
16	S	1.26-002	9.452-010	-2.060-006	-1.138-006	1.068-007	-1.554-009	9.270-012	-2.271-014	3.340-017
17	CL	2.78-002	9.816-010	2.400-005	-3.560-006	1.840-007	-2.618-009	1.525-011	-4.410-014	5.800-017
18	A	1.20-002	9.733-010	-1.050-005	-3.700-007	8.440-008	-1.264-009	7.495-012	-1.770-014	2.810-017
19	K	9.82-003	1.110-009	-3.800-006	-1.177-006	1.200-007	-1.776-009	1.080-011	-2.730-014	4.030-017
20	CA	1.68-002	1.205-009	6.250-006	-2.166-006	1.548-007	-2.217-009	1.330-011	-3.350-014	4.700-017
21	SC	1.65-002	1.180-009	-2.458-005	6.906-007	6.507-008	-1.006-009	5.360-012	-1.050-014	2.100-017
22	TI	1.48-002	1.217-009	-2.057-005	2.830-007	8.0[illegible]-008	-1.208-009	6.770-012	-1.363-014	2.440-017
23	V	1.63-002	1.275-009	1.075-005	-2.700-006	1.787-007	-2.615-009	1.633-011	-4.400-014	6.100-017
24	CR	1.96-002	1.377-009	2.010-005	-3.610-006	2.111-007	-3.038-009	1.883-011	-5.060-014	6.850-017
25	MN	1.51-002	1.416-009	3.600-006	-2.130-006	1.674-007	-2.435-009	1.479-011	-3.780-014	5.370-017
26	FE	1.22-002	1.508-009	-6.900-006	-1.309-006	1.900-007	-2.235-009	1.358-011	-3.410-014	5.030-017
27	CO	1.67-002	1.550-009	5.000-006	-2.458-006	1.892-007	-2.790-009	1.724-011	-4.515-014	6.300-017
28	NI	1.56-002	1.677-009	-3.565-005	1.128-006	8.674-008	-1.410-009	8.220-012	-1.730-014	3.260-017
29	CU	1.44-002	1.672-009	-3.230-005	8.300-007	9.570-008	-1.539-009	9.342-012	-1.965-014	3.464-017
30	ZN	1.32-002	1.765-009	-3.000-005	5.700-007	1.079-007	-1.700-009	1.000-011	-2.230-014	3.840-017
31	GA	1.27-002	1.778-009	-2.530-005	9.000-008	1.255-007	-1.981-009	1.210-011	-2.940-014	4.700-017
32	GE	1.48-002	1.813-009	-4.169-005	1.513-006	9.558-008	-1.460-009	8.770-012	-1.920-014	3.560-017
33	AS	1.84-002	1.889-009	-4.449-005	1.749-006	8.997-008	-1.385-009	8.070-012	-1.630-014	3.200-017
34	SE	1.37-002	1.932-009	-1.080-005	-1.457-006	1.897-007	-2.874-009	1.816-011	-4.810-014	5.970-017
35	BR	2.44-002	2.019-009	-8.280-005	5.100-006	-1.20[illegible]-008	-1.600-010	2.200-013	7.700-015	5.600-018
36	KR	1.80-002	2.057-009	-4.676-005	1.730-006	9.572-008	-1.682-009	1.041-011	-2.417-014	4.300-017
37	RB	1.80-002	2.151-009	-3.382-005	5.200-007	1.30[illegible]-007	-2.283-009	1.350-011	-3.250-014	5.200-017
38	SR	1.53-002	2.228-009	-4.930-005	1.855-006	1.03-007	-1.743-009	1.054-011	-2.320-014	4.170-017
39	Y	2.30-002	2.325-009	-9.670-005	8.080-006	-2.3[illegible]-008	-9.000-011	-2.100-013	9.800-015	4.500-018
40	ZR	1.40-002	2.428-009	-3.770-005	6.700-007	1.47[illegible]-007	-2.394-009	1.464-011	-3.470-014	5.580-017

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TABLE I (Cont)

Z	E_b	RMS ERROR	C	A(1)	A(2)	A(3)	A(4)	A(5)	A(6)	A(7)
41	NB	1.66-002	2.559-00*	-2,280-005	-6,760-007	1,912-007	-2,964-009	1,800-011	-4,380-014	6,500-017
42	MO	1.86-002	2.594-00*	-8,510-005	4,390-006	2,710-008	-8,350-010	4,800-012	-5,400-015	2,360-017
43	TC	1.48-002	2.678-00*	-4,760-005	1,470-006	1,342-007	-2,270-009	1,390-011	-3,230-014	5,370-017
44	RU	1.71-002	2.789-00*	-5,870-005	2,480-006	1,063-007	-1,876-009	1,108-011	-2,270-014	4,200-017
45	RH	2.20-002	2.851-00*	-1,112-004	7,220-006	-3,570-008	4,600-011	-1,530-012	1,640-014	-2,700-018
46	PD	2.56-002	3.002-00*	1,813-005	-4,576-006	3,318-007	-4,984-009	3,148-011	-8,520-014	1,150-016
47	AG	1.80-002	3.082-00*	-4,230-005	8,800-007	1,680-007	-2,738-009	1,545-011	-3,750-014	5,900-017
48	CD	1.80-002	3.095-00*	-9,240-005	5,397-006	3,320-008	-9,960-010	5,770-012	-6,900-015	2,540-017
49	IN	1.53-002	3.204-00*	-4,900-005	1,370-006	1,630-007	-2,794-009	1,760-011	-4,320-014	6,800-017
50	SN	1.86-002	3.277-00*	-2,640-005	-6,200-007	2,233-007	-3,580-009	2,259-011	-5,844-014	8,600-017
51	SB	1.86-002	3.386-00*	-1,170-005	-1,980-006	2,698-007	-4,250-009	2,702-011	-7,160-014	1,006-016
52	TE	1.32-002	3.349-00*	-5,680-005	2,110-006	1,450-007	-2,609-009	1,673-011	-4,147-014	6,705-017
53	I	1.38-002	3.517-00*	-9,180-005	5,170-006	6,100-008	-1,505-009	9,570-012	-1,940-014	4,300-017
54	XE	2.21-002	3.553-00*	-1,440-004	9,920-006	-8,250-008	4,000-010	-2,550-012	1,660-014	3,100-018
55	CS	2.92-002	3.656-00*	-1,790-004	1,295-005	-1,655-007	1,440-009	-8,900-012	3,514-014	-1,680-017
56	BA	2.54-002	3.717-00*	-1,670-004	1,197-005	-1,384-007	1,130-009	-7,300-012	3,160-014	-1,400-017
57	LS	2.69-002	3.838-00*	-1,840-004	1,338-005	-1,720-007	1,510-009	-9,500-012	3,800-014	-2,100-017
58	CE	2.73-002	3.983-00*	-1,952-004	1,442-005	-2,006-007	1,918-009	-1,243-011	4,800-014	-3,300-017
59	PR	3.01-002	4.152-00*	-2,150-004	1,613-005	-2,454-007	2,423-009	-1,540-011	5,664-014	-4,150-017
60	ND	1.51-002	4.281-00*	-1,280-004	8,360-006	-8,200-009	-6,730-010	4,020-012	-4,000-016	2,200-017
61	PM	1.54-002	4.469-00*	-9,660-005	5,460-006	8,800-008	-2,000-009	1,266-011	-2,650-014	5,200-017
62	SM	1.48-002	4.513-00*	-1,074-004	6,500-006	5,600-008	-1,580-009	1,000-011	-1,843-014	4,270-017
63	EU	1.48-002	4.635-00*	-1,373-004	9,130-006	-1,700-008	-6,375-010	4,027-012	-5,000-016	2,300-017
64	GD	1.44-002	4.663-00*	-1,503-004	1,040-005	-5,760-008	-9,500-011	5,700-013	9,900-015	1,100-017
65	TB	1.77-002	4.765-00*	-1,906-004	1,393-005	-1,572-007	1,207-009	-7,900-012	3,650-014	-2,000-017
66	DY	1.33-002	4.900-00*	-1,400-004	9,360-006	-1,400-008	-7,530-010	5,000-012	-3,600-015	2,700-017
67	HO	1.44-002	4.956-00*	-1,692-004	1,194-005	-8,770-008	1,900-010	-8,200-013	1,340-014	9,000-018
68	ER	1.68-002	5.079-00*	-1,931-004	1,399-005	-1,410-007	8,260-010	-4,560-012	2,400-014	-2,000-018
69	TM	1.55-002	5.251-00*	-2,001-004	1,466-005	-1,573-007	1,045-009	-6,200-012	2,994-014	-9,000-018
70	YB	1.27-002	5.366-00*	-1,830-004	1,317-005	-1,105-007	4,200-010	-2,290-012	1,870-014	3,000-018
71	LU	1.25-002	5.478-00*	-2,000-004	1,457-005	-1,430-007	7,460-010	-3,700-012	2,100-014	3,000-018
72	HF	1.38-002	5.634-00*	-1,212-004	7,540-006	7,170-008	-2,130-009	1,483-011	-3,510-014	6,700-017
73	TA	1.03-002	5.709-00*	-1,836-004	1,313-005	-9,300-008	4,000-011	8,400-013	7,800-015	1,800-017
74	W	9.96-003	5.860-00*	-1,870-004	1,330-005	-8,700-008	-1,500-010	2,640-012	1,050-015	2,700-017
75	RE	1.18-002	5.962-00*	-2,076-004	1,510-005	-1,350-007	4,200-010	-6,000-013	9,770-015	1,870-017
76	OS	1.00-002	6.069-00*	-2,020-004	1,462-005	-1,176-007	1,640-010	1,140-012	4,200-015	2,500-017
77	IR	1.32-002	6.291-00*	-1,535-004	1,043-005	8,000-009	-1,430-009	1,066-011	-2,210-014	5,300-017
78	PT	1.11-002	6.317-00*	-2,485-004	1,882-005	-2,370-007	1,750-009	-9,370-012	3,750-014	-1,360-017
79	AU	1.33-002	6.511-00*	-2,692-004	2,068-005	-2,860-007	2,350-009	-1,300-011	4,810-014	-2,500-017
80	HG	1.08-002	6.651-00*	-2,709-004	2,096-005	-2,947-007	2,485-009	-1,403-011	5,190-014	-3,000-017

(continued on next page)

TABLE I (Cont)

Z	EL	RMS ERROR	C	A(1)	A(2)	A(3)	A(4)	A(5)	A(6)	A(7)
81	TL	1.2[illegible]*002	6.723-00[illegible]	-2,788-004	2,158-005	-3,064-007	2,550-009	-1,393-011	5,020-014	-2,600-017
82	PB	1.15-002	6.962-00[illegible]	-2,320-004	1,750-005	-1,80[illegible]-007	8,360-010	-2,740-012	1,570-014	1,400-017
83	BI	1.07-002	7.115-00[illegible]	-2,680-004	2,066-005	-2,67[illegible]-007	1,945-009	-9,722-012	3,690-014	-1,000-017
84	PO	9.27-003	7.342-00[illegible]	-2,680-004	2,065-005	-2,58[illegible]-007	1,750-009	-8,190-012	3,165-014	-2,000-018
85	AT	7.78-003	7.572-00[illegible]	-2,880-004	2,249-005	-3,083-007	2,444-009	-1,304-011	4,820-014	-2,300-017
86	RN	7.64-003	7.426-00[illegible]	-2,870-004	2,258-005	-3,21[illegible]-007	2,610-009	-1,377-011	4,880-014	-2,300-017
87	FR	9.87-003	7.560-00[illegible]	-3,300-004	2,628-005	-4,214-007	3,872-009	-2,168-011	7,290-014	-5,022-017
88	RA	9.10-003	7.809-00[illegible]	-2,900-004	2,290-005	-3,194-007	2,523-009	-1,306-011	4,670-014	-1,940-017
89	AC	1.02-002	8.012-00[illegible]	-2,750-004	2,146-005	-2,65[illegible]-007	1,700-009	-7,398-012	2,900-014	2,000-018
90	TH	9.40-003	8.143-00[illegible]	-2,940-004	2,334-005	-3,24[illegible]-007	2,530-009	-1,307-011	4,750-014	-2,200-017
91	PA	8.40-003	8.446-00[illegible]	-3,190-004	2,562-005	-3,83[illegible]-007	3,240-009	-1,730-011	5,960-014	-3,300-017
92	U	1.11-002	8.415-00[illegible]	-2,965-004	2,360-005	-3,23[illegible]-007	2,430-009	-1,200-011	4,310-014	-1,500-017
93	NP	1.58-002	8.754-00[illegible]	-2,660-004	2,080-005	-2,25[illegible]-007	1,037-009	-2,760-012	1,490-014	1,850-017
94	PU	1.45-002	8.907-00[illegible]	-2,660-004	2,105-005	-2,36[illegible]-007	1,190-009	-3,750-012	1,800-014	1,500-017
95	AM	9.05-003	9.153-00[illegible]	-3,340-004	2,700-005	-3,99[illegible]-007	3,201-009	-1,594-011	5,334-014	-2,360-017
96	CM	8.39-003	9.270-00[illegible]	-3,720-004	3,046-005	-5,0[illegible]-007	4,501-009	-2,406-011	7,750-014	-5,100-017
97	BK	8.43-003	9.454-00[illegible]	-3,480-004	2,837-005	-4,34[illegible]-007	3,630-009	-1,860-011	5,160-014	-3,300-017
98	CF	1.39-002	9.789-00[illegible]	-3,250-004	2,657-005	-3,787-007	2,913-009	-1,430-011	4,962-014	-2,000-017
99	ES	1.20-002	9.931-00[illegible]	-3,330-004	2,718-005	-3,87[illegible]-007	2,910-009	-1,360-011	4,500-014	-1,300-017
100	FM	9.99-003	1.022-00[illegible]	-3,810-004	3,140-005	-5,0[illegible]-007	4,307-009	-2,215-011	7,100-014	-4,107-017

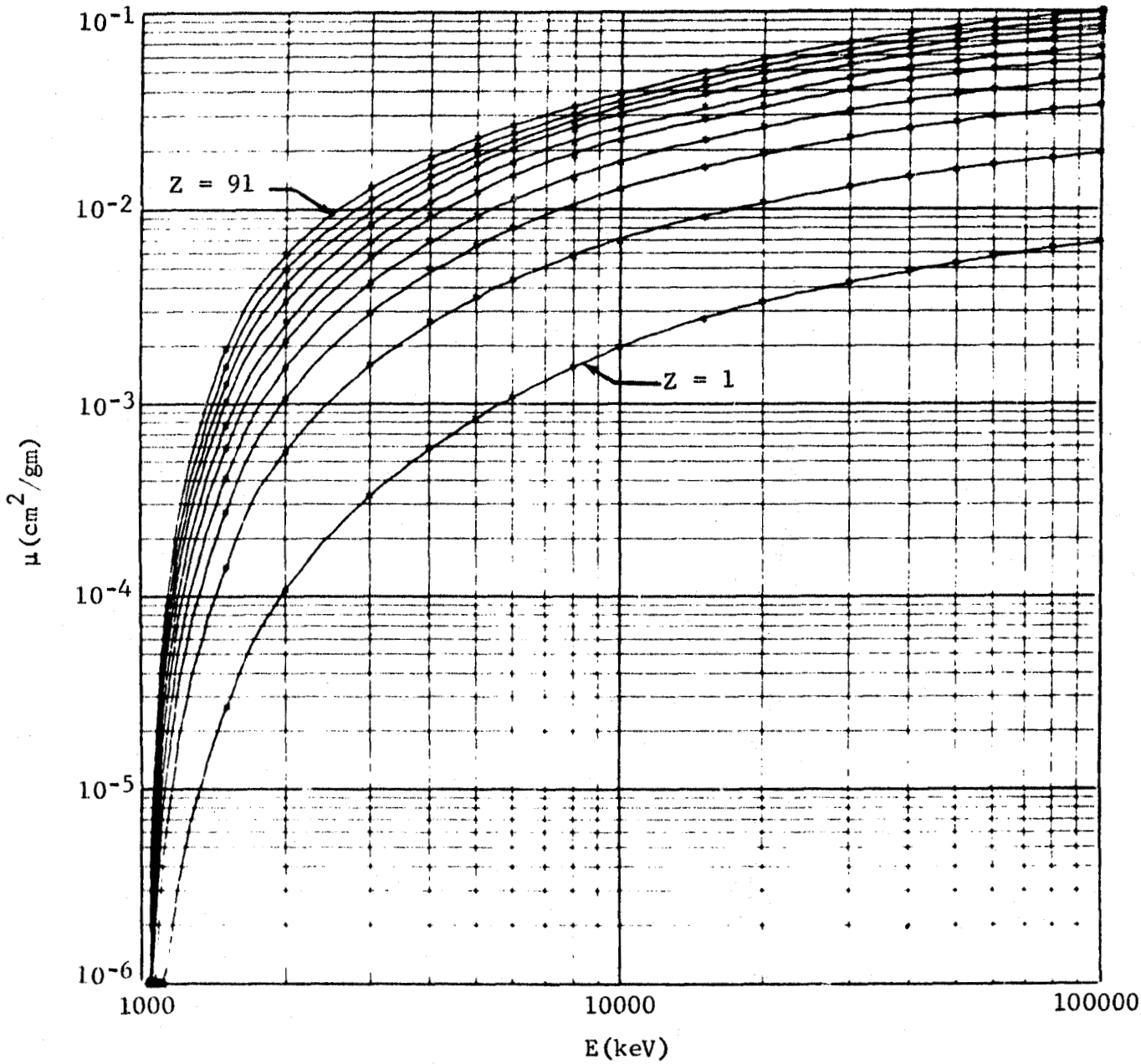

Fig. 1 Pair-production cross section as a function of energy for the elements with atomic numbers Z = 1, 11, 21, 31, 41, 51, 61, 71, 81, 91. Cross sections increase monotonically with atomic numbers.

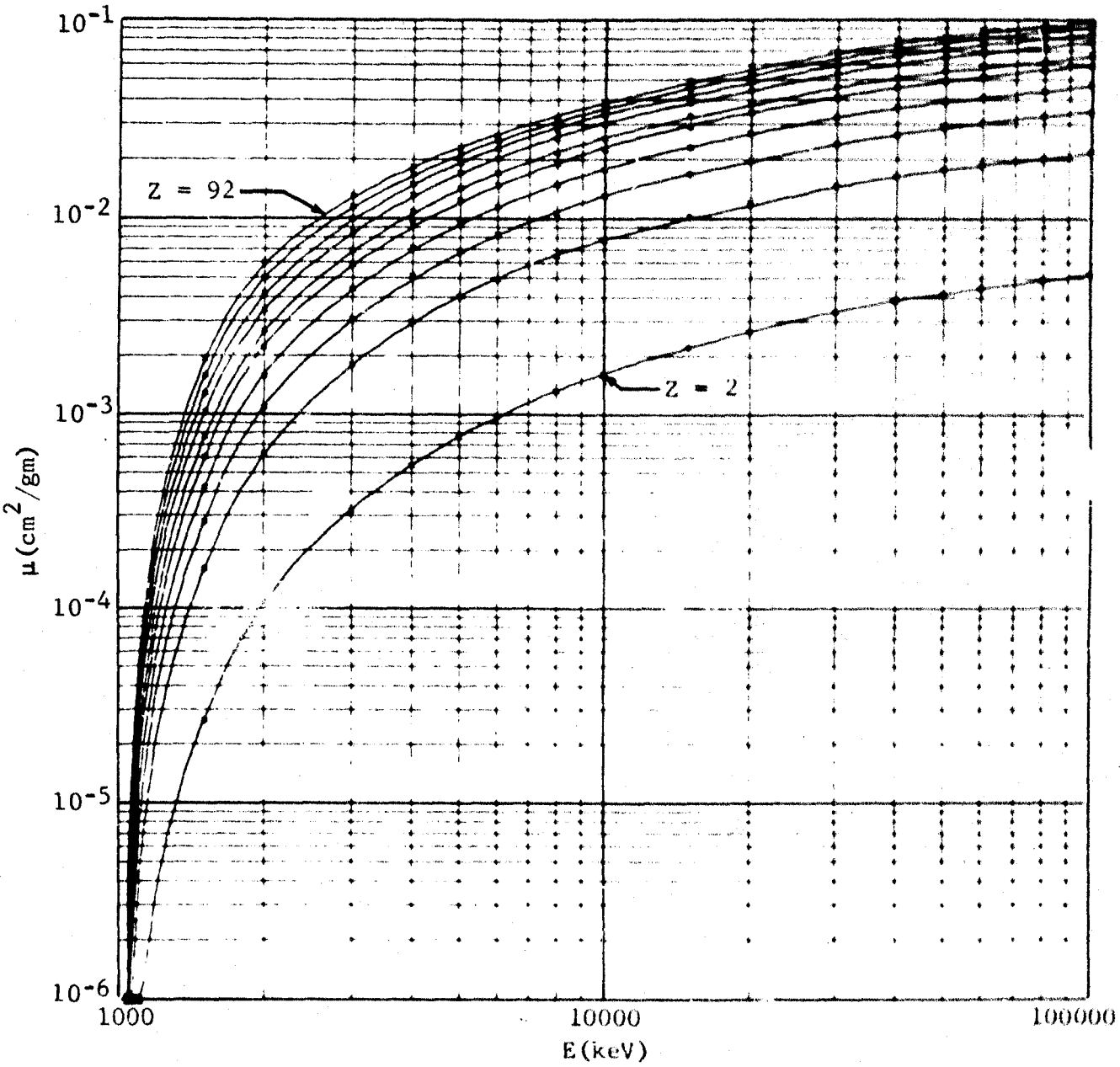

Fig. 2 Pair-production cross section as a function of energy for the elements with atomic numbers Z = 2, 12, 22, 32, 42, 52, 62, 72, 82, 92. Cross sections increase monotonically with atomic numbers.

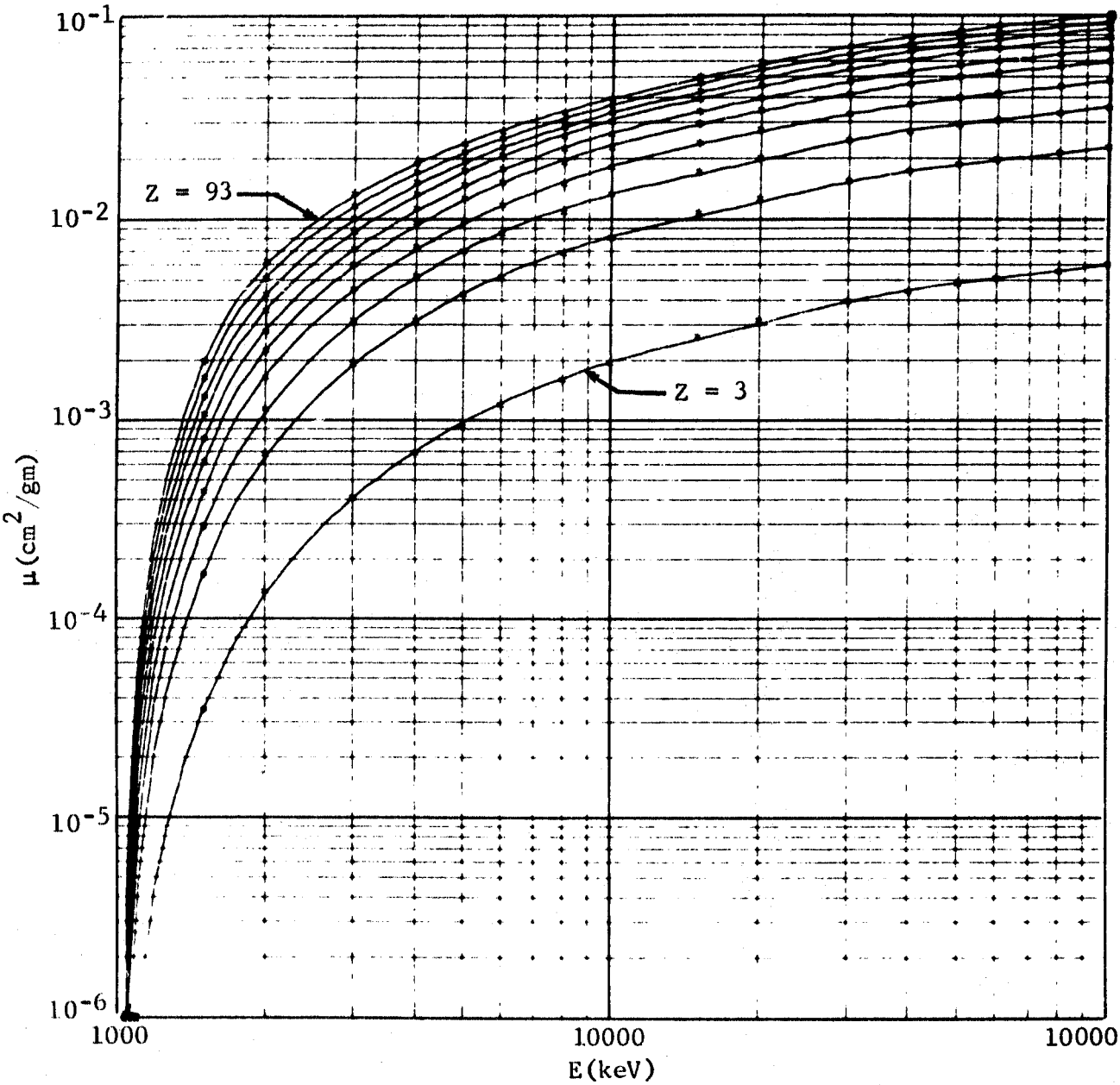

Fig. 3 Pair-production cross section as a function of energy for the elements with atomic numbers Z = 3, 13, 23, 33, 43, 53, 63, 73, 83, 93. Cross sections increase monotonically with atomic numbers.

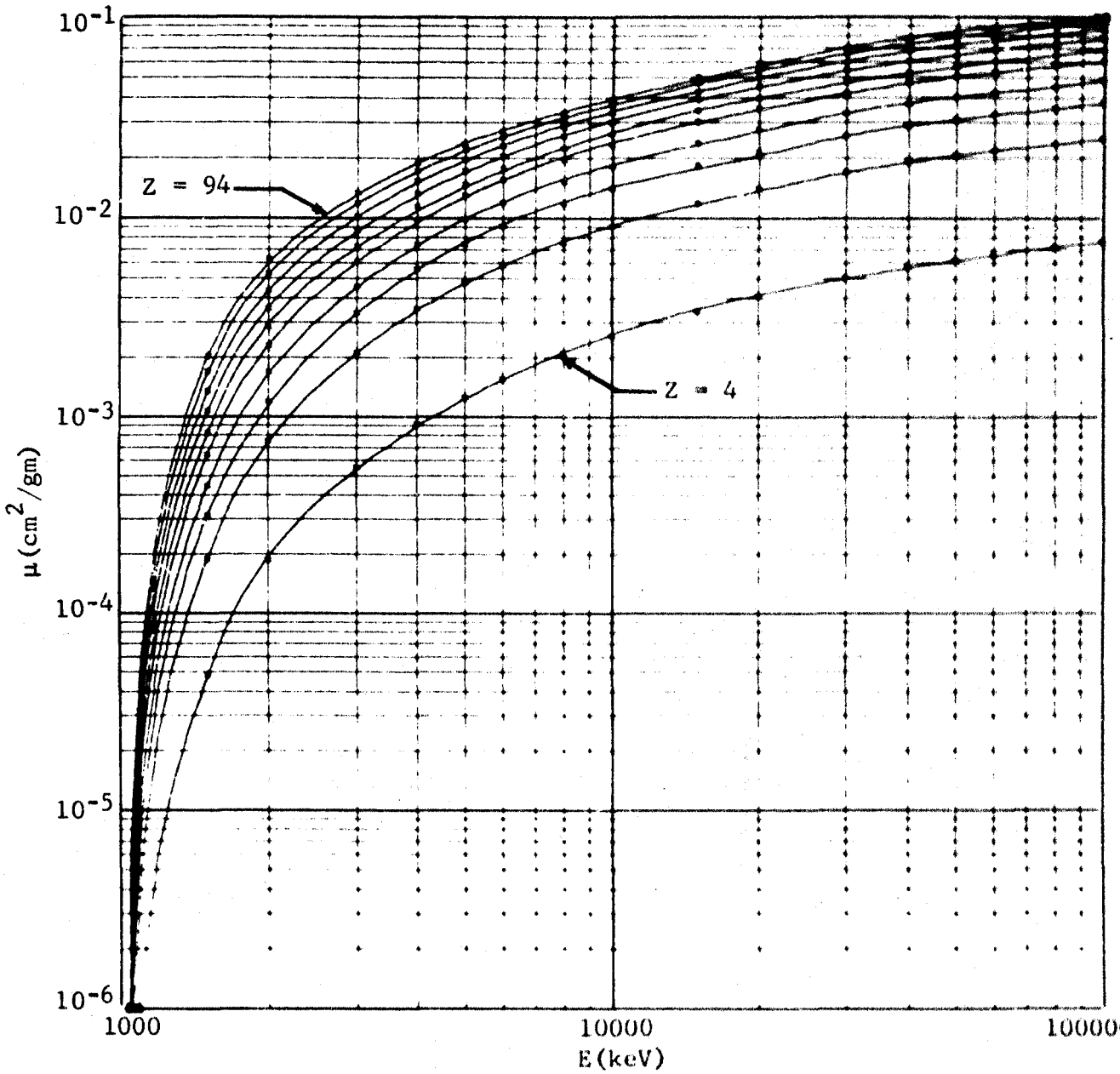

Fig. 4 Pair-production cross section as a function of energy for the elements with atomic numbers Z = 4, 14, 24, 34, 44, 54, 64, 74, 84, 94. Cross sections increase monotonically with atomic numbers.

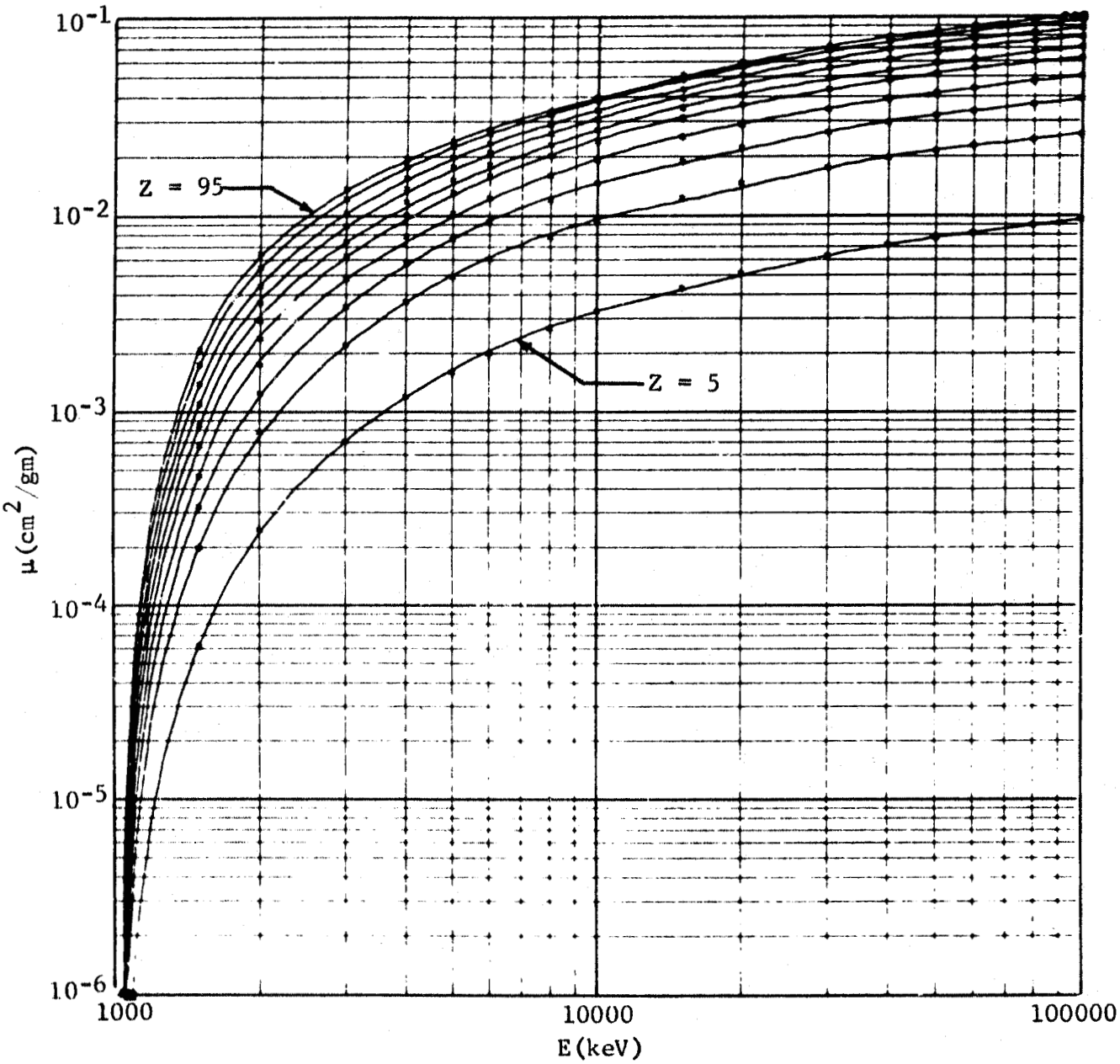

Fig. 5 Pair-production cross section as a function of energy for the elements with atomic numbers Z = 5, 15, 25, 35, 45, 55, 65, 75, 85, 95. Cross sections increase monotonically with atomic numbers.

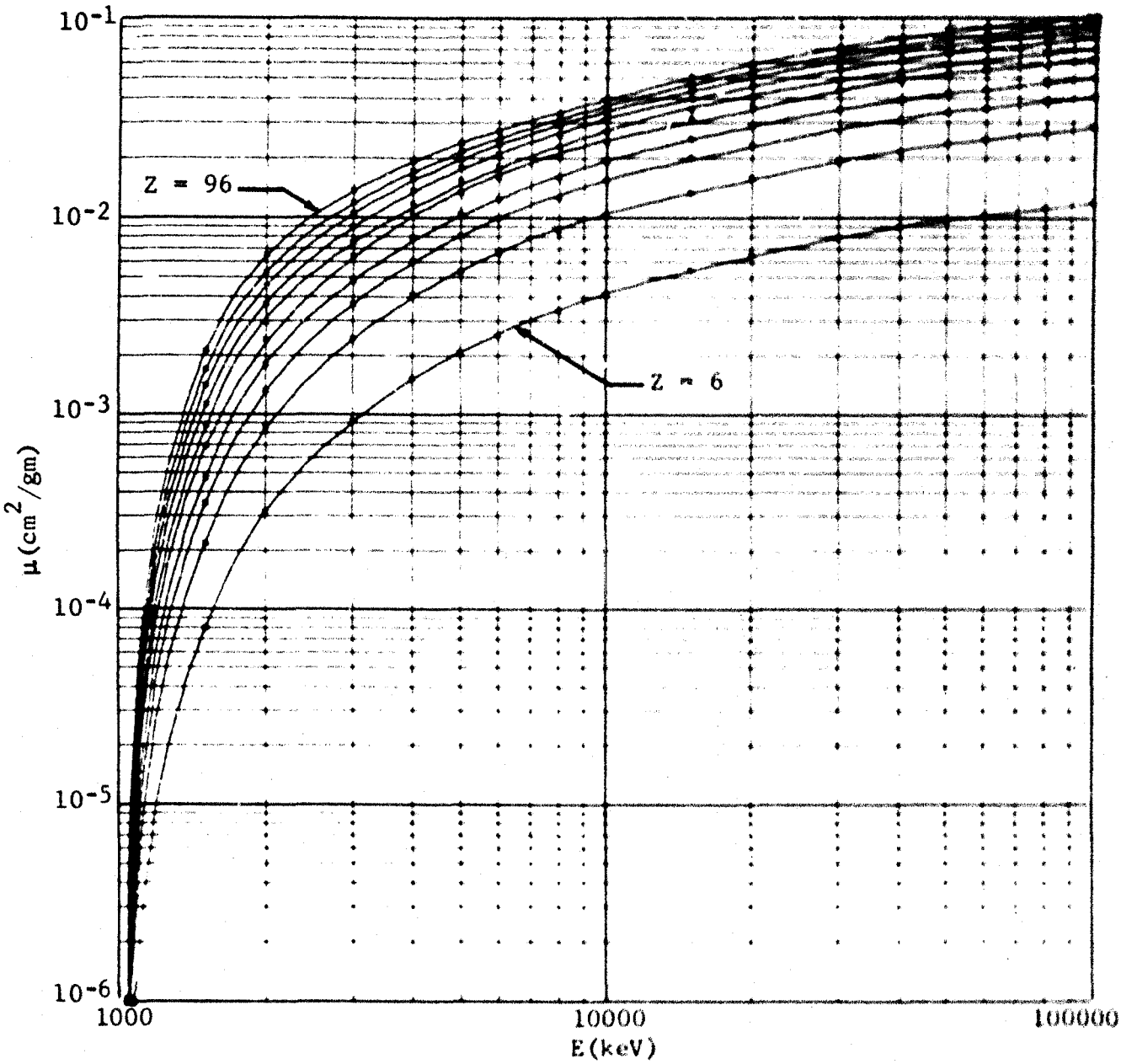

Fig. 6 Pair-production cross section as a function of energy for the elements with atomic numbers Z = 6, 16, 26, 36, 46, 56, 66, 76, 86, 96. Cross sections increase monotonically with atomic numbers.

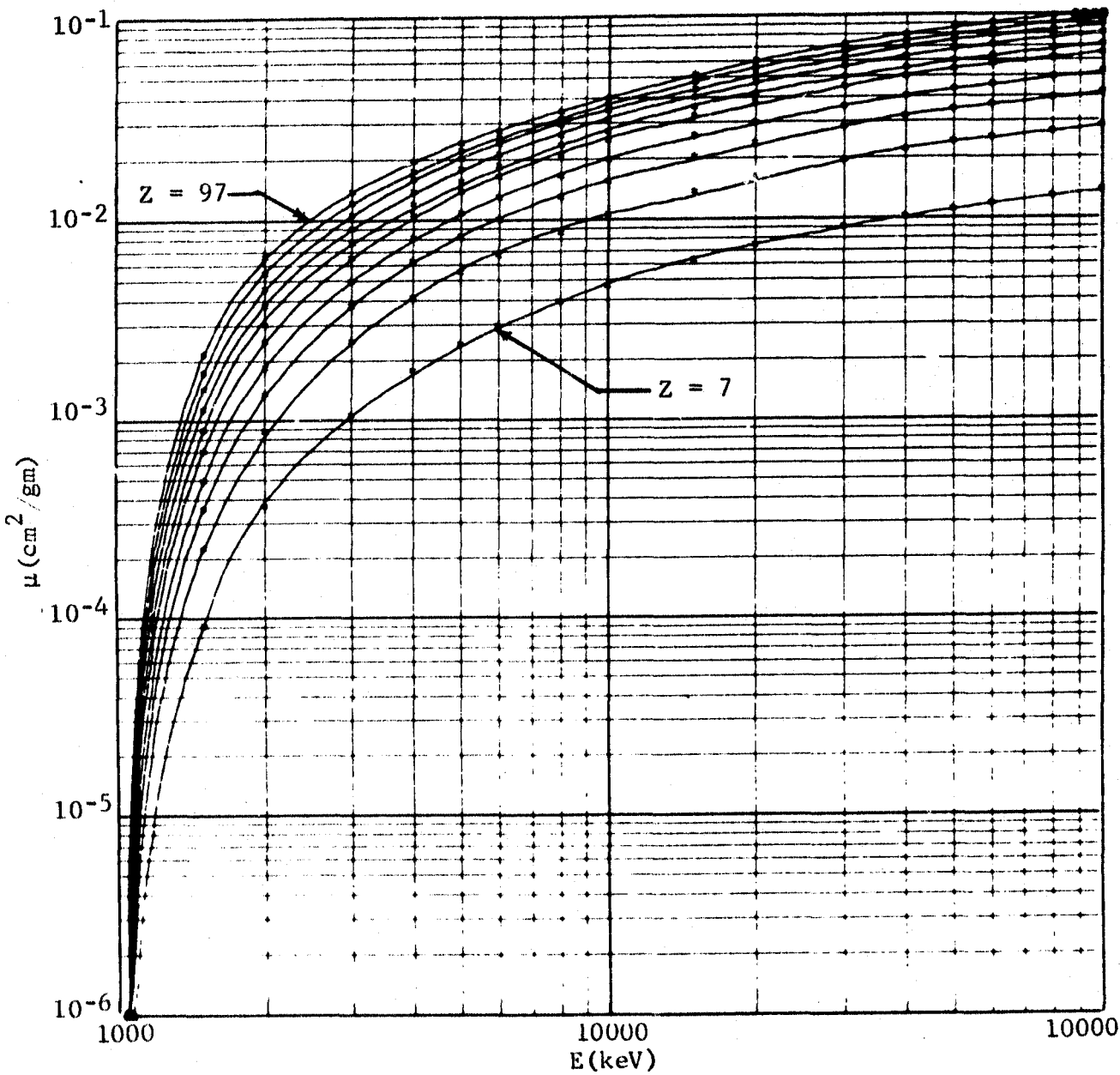

Fig. 7 Pair-production cross section as a function of energy for the elements with atomic numbers Z = 7, 17, 27, 37, 47, 57, 67, 77, 87, 97. Cross sections increase monotonically with atomic numbers.

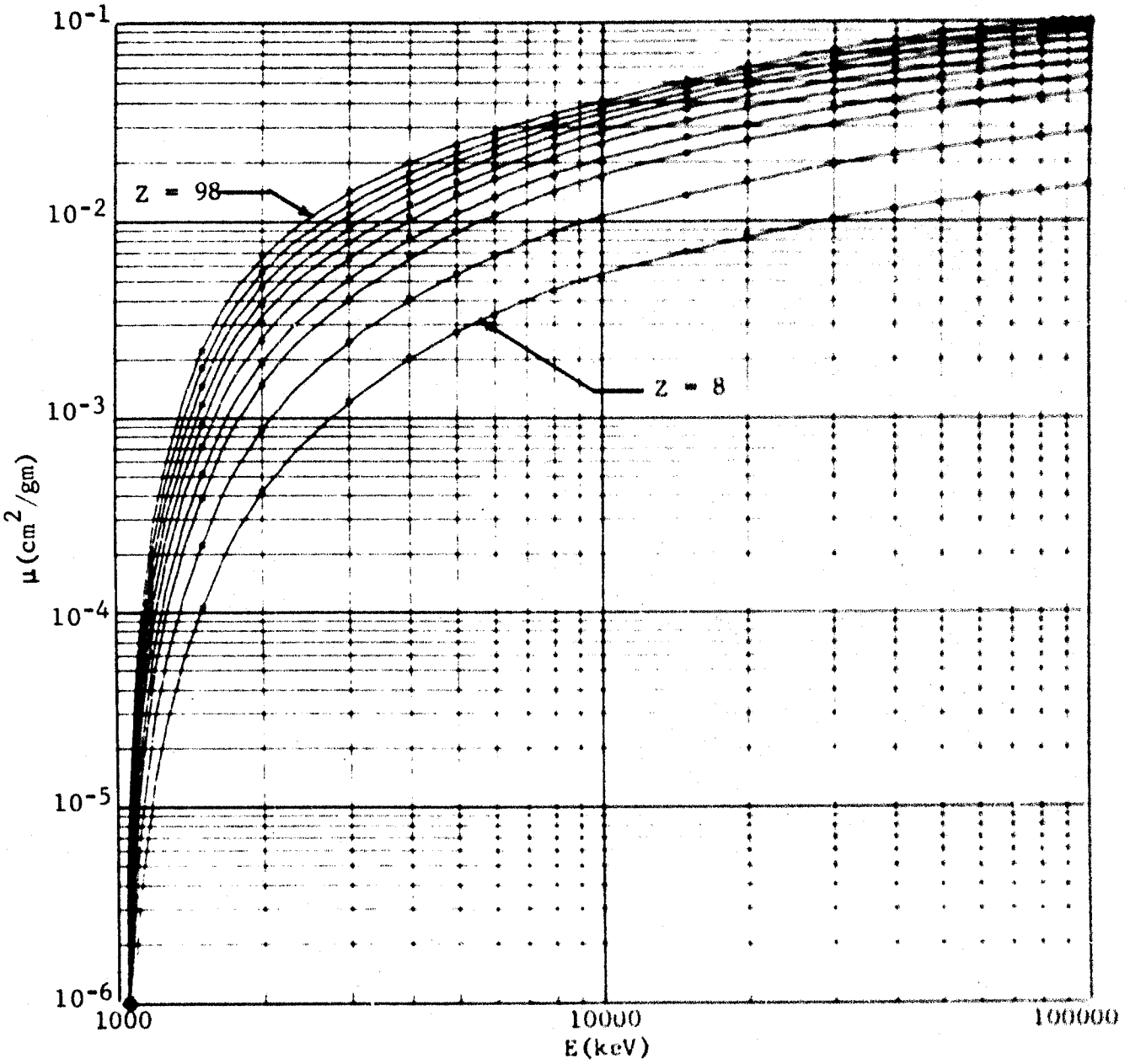

Fig. 8 Pair-production cross section as a function of energy for the elements with atomic numbers Z = 8, 18, 28, 38, 48, 58, 68, 78, 88, 98. Cross sections increase monotonically with atomic numbers.

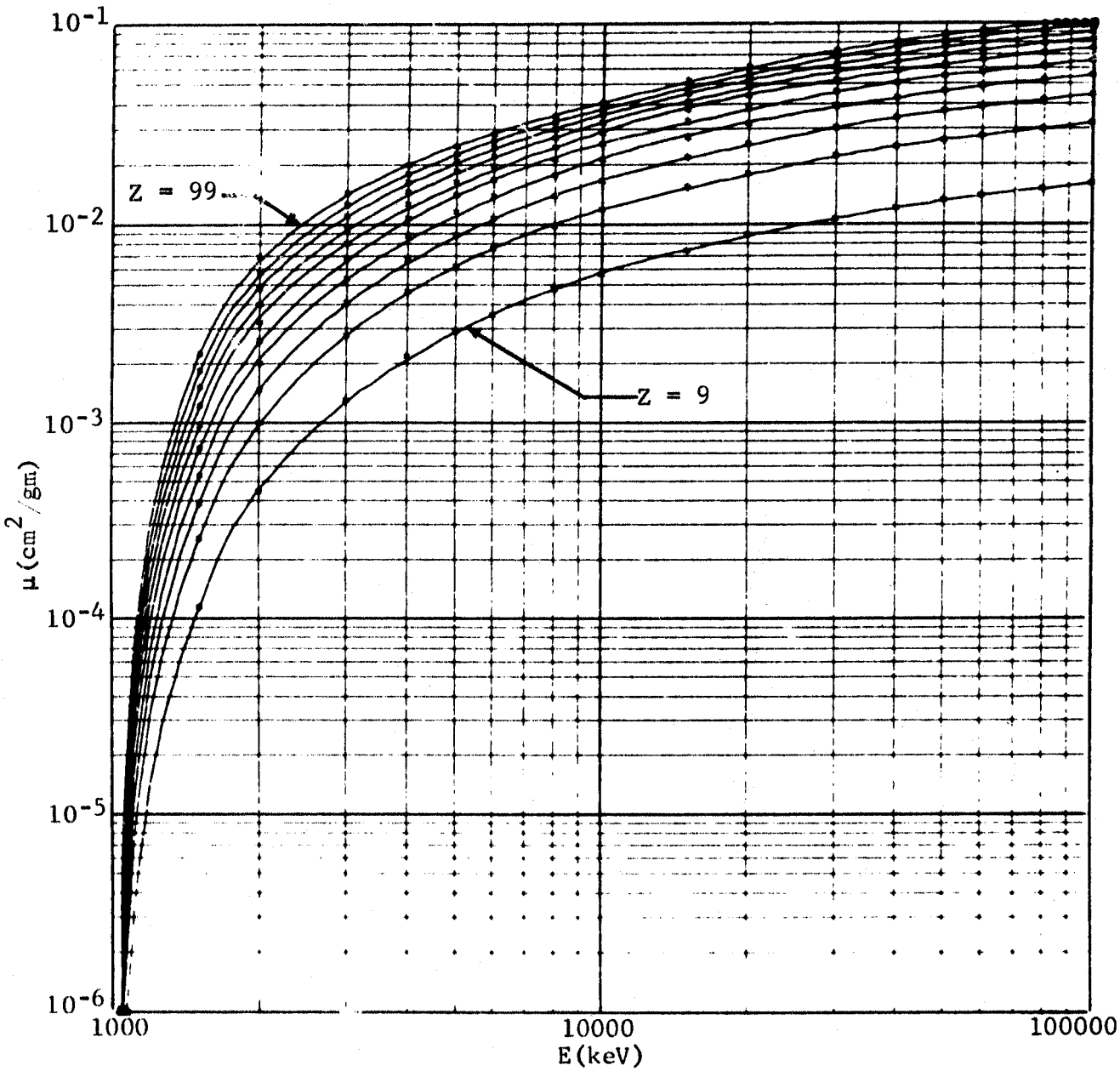

Fig. 9 Pair-production cross section as a function of energy for the elements with atomic numbers Z = 9, 19, 29, 39, 49, 59, 69, 79, 89, 99. Cross sections increase monotonically with atomic numbers.

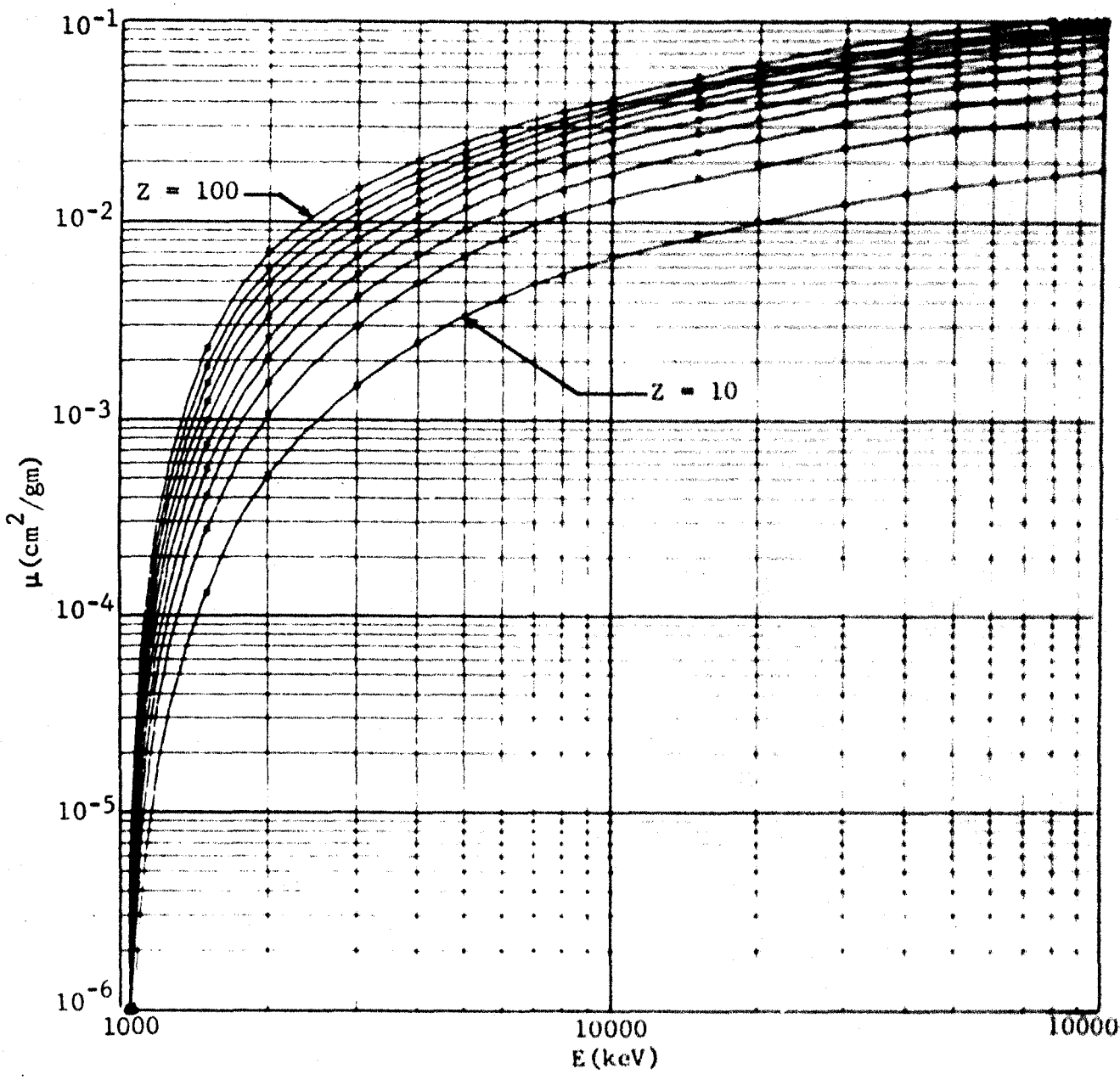

Fig. 10 Pair-production cross section as a function of energy for the elements with atomic numbers Z = 10, 20, 30, 40, 50, 60, 70, 80, 90, 100. Cross sections increase monotonically with atomic numbers.

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