

THE TRUE POTENTIAL ENERGY CURVES AND DISSOCIATION ENERGY OF TITANIUM MONOXIDE

S. V. J. LAKSHMAN*, T. V. RAMAKRISHNA RAO AND G. T. NAIDU
Department of Physics, SVU Post-Graduate Centre, Anantapur 515 003, India

ABSTRACT

The true potential energy curves have been constructed for the different electronic states of astrophysically important molecule TiO by the method of Lakshman and Rao². The dissociation energy for the ground state of the above molecule has been estimated by fitting the H-H function to the true potential energy curves. The dissociation energy thus obtained is in good agreement with the values reported in literature.

INTRODUCTION

THE construction of accurate potential energy curves is of considerable importance for the understanding of physical problems arising in astrophysics, gas kinetics and molecular spectra. Since the molecule is of astrophysical importance whose spectra were observed in the sunspots, M and S types of stars¹, authors took up the present work. The present paper deals with the construction of experimental potential energy curves and dissociation energy of TiO for which sufficient spectroscopic data are available.

METHOD OF COMPUTATION

The present method of Lakshman and Rao² was successfully verified by them in number of cases²⁻⁷ and recently Chakraborty and Pan⁸ in their review paper gave a detailed account of different methods and the authors' method is one such reliable and accurate, which involves less complicated mathematical calculations. Since the details of this method are reported in literature², only the explicit formulae to evaluate the turning points are given below :

$$f = \left(\frac{8\pi^2 \mu c (\omega_x)_i}{h} \right)^{-1/2} \ln W_i$$

$$g = \left(\frac{2\pi^2 \mu c}{h} \right)^{1/2} \{ 2a_i (\omega_x)_i^{-1} U_i^{1/2} + (\omega_x)_i^{-1/2} [2B_i - a_i \omega_i (\omega_x)_i^{-1}] \ln W_i \}$$

where

$$W_i = \frac{[\omega_i^2 - 4(\omega_x)_i U_i]^{1/2}}{\omega_i - 2(\omega_x)_i^{1/2} U_i^{1/2}}$$

the symbols have their usual spectroscopic significance. The classical turning points are given by the relation

$$r_{\max, \min} = (f/g + f^2)^{1/2} \pm f.$$

RESULTS AND DISCUSSION

The experimental potential energy curves for three states X $^3\Delta$, A $^3\pi$, C $^3\Delta$, of TiO molecule have been constructed by Kushawaha⁹ based on the molecular constants given by Uhler¹⁰. In the present study using more accurate and reliable vibrational and rotational constants the turning points for the B $^3\pi$, a $^1\Delta$, d $^1\Sigma^+$, b $^1\pi$, c $^1\Phi$, e $^1\Sigma$ along with X $^3\Delta$ states of TiO molecule have been calculated to draw the experimental true potential energy curves. For the triplet states the rotational and vibrational constants have been taken from Collins¹¹ and for singlet states the vibrational and rotational constants were taken from Phillips¹²⁻¹⁴, Pettersson¹⁵⁻¹⁶, Linton *et al.*¹⁷, Phillips *et al.*¹⁸, Lindgren¹⁹, Linton *et al.*²⁰, Linton²¹, and summarised in Table I.

TABLE I
Spectroscopic constants of TiO molecule

State	T_e (cm ⁻¹)	ω_v (cm ⁻¹)	$\omega_r \chi_e$ (cm ⁻¹)	β (cm ⁻¹)	α_r (cm ⁻¹)	r_e (Å)
<i>TiO Molecule</i>						
X $^3\Delta$	0	1009.0208	4.4978	0.535412	0.003011	1.6201
B $^3\pi$	16214.0	871.96	4.1135	0.507812	0.0032758	1.6635
a $^1\Delta$	581.0	1016.3	3.93	0.53760	0.00298	1.6167
d $^1\Sigma^+$	1708.0	1023.8	4.64	0.5490	0.00337	1.6000
b $^1\pi$	10814.0	918.7	3.75	0.51329	0.00290	1.6540
c $^1\Phi$	18471.5	916.7	4.33	0.52301	0.00313	1.6391
e $^1\Sigma$	26005.8	853.9	4.7	0.4892	0.0025	1.6950

* Department of Physics, S.V. University, Tirupati,

Employing the method of Lakshman and Rao², the turning points for different vibrational levels of X ³Δ, B ³π, a ¹Δ, d ¹Σ+, b ¹π, e ¹Φ and e ¹Σ states of TiO molecule have been calculated and presented in Table II. The extrapolated energy values for the highest bound level v_1 and the corresponding turning points are evaluated and included in this table at the end of observed levels in each state.

TABLE II

The true potential energy curves for different states of TiO Molecule

v	$U(\text{cm}^{-1})$	$U + \text{Te}$	$r_{\min}(\text{\AA})$	$r_{\max}(\text{\AA})$
		(cm^{-1})		
1	100	100	1.5	2.5
2	150	150	1.5	2.5
3	200	200	1.5	2.5
4	250	250	1.5	2.5
5	300	300	1.5	2.5
6	350	350	1.5	2.5
7	400	400	1.5	2.5
8	450	450	1.5	2.5
9	500	500	1.5	2.5
10	550	550	1.5	2.5
11	600	600	1.5	2.5
12	650	650	1.5	2.5
13	700	700	1.5	2.5
14	750	750	1.5	2.5
15	800	800	1.5	2.5
16	850	850	1.5	2.5
17	900	900	1.5	2.5
18	950	950	1.5	2.5
19	1000	1000	1.5	2.5
20	1050	1050	1.5	2.5
21	1100	1100	1.5	2.5
22	1150	1150	1.5	2.5
23	1200	1200	1.5	2.5
24	1250	1250	1.5	2.5
25	1300	1300	1.5	2.5
26	1350	1350	1.5	2.5
27	1400	1400	1.5	2.5
28	1450	1450	1.5	2.5
29	1500	1500	1.5	2.5
30	1550	1550	1.5	2.5
31	1600	1600	1.5	2.5
32	1650	1650	1.5	2.5
33	1700	1700	1.5	2.5
34	1750	1750	1.5	2.5
35	1800	1800	1.5	2.5
36	1850	1850	1.5	2.5
37	1900	1900	1.5	2.5
38	1950	1950	1.5	2.5
39	2000	2000	1.5	2.5
40	2050	2050	1.5	2.5
41	2100	2100	1.5	2.5
42	2150	2150	1.5	2.5
43	2200	2200	1.5	2.5
44	2250	2250	1.5	2.5
45	2300	2300	1.5	2.5
46	2350	2350	1.5	2.5
47	2400	2400	1.5	2.5
48	2450	2450	1.5	2.5
49	2500	2500	1.5	2.5
50	2550	2550	1.5	2.5
51	2600	2600	1.5	2.5
52	2650	2650	1.5	2.5
53	2700	2700	1.5	2.5
54	2750	2750	1.5	2.5
55	2800	2800	1.5	2.5
56	2850	2850	1.5	2.5
57	2900	2900	1.5	2.5
58	2950	2950	1.5	2.5
59	3000	3000	1.5	2.5
60	3050	3050	1.5	2.5
61	3100	3100	1.5	2.5
62	3150	3150	1.5	2.5
63	3200	3200	1.5	2.5
64	3250	3250	1.5	2.5
65	3300	3300	1.5	2.5
66	3350	3350	1.5	2.5
67	3400	3400	1.5	2.5
68	3450	3450	1.5	2.5
69	3500	3500	1.5	2.5
70	3550	3550	1.5	2.5
71	3600	3600	1.5	2.5
72	3650	3650	1.5	2.5
73	3700	3700	1.5	2.5
74	3750	3750	1.5	2.5
75	3800	3800	1.5	2.5
76	3850	3850	1.5	2.5
77	3900	3900	1.5	2.5
78	3950	3950	1.5	2.5
79	4000	4000	1.5	2.5
80	4050	4050	1.5	2.5
81	4100	4100	1.5	2.5
82	4150	4150	1.5	2.5
83	4200	4200	1.5	2.5
84	4250	4250	1.5	2.5
85	4300	4300	1.5	2.5
86	4350	4350	1.5	2.5
87	4400	4400	1.5	2.5
88	4450	4450	1.5	2.5
89	4500	4500	1.5	2.5
90	4550	4550	1.5	2.5
91	4600	4600	1.5	2.5
92	4650	4650	1.5	2.5
93	4700	4700	1.5	2.5
94	4750	4750	1.5	2.5
95	4800	4800	1.5	2.5
96	4850	4850	1.5	2.5
97	4900	4900	1.5	2.5
98	4950	4950	1.5	2.5
99	5000	5000	1.5	2.5
100	5050	5050	1.5	2.5
101	5100	5100	1.5	2.5
102	5150	5150	1.5	2.5
103	5200	5200	1.5	2.5
104	5250	5250	1.5	2.5
105	5300	5300	1.5	2.5
106	5350	5350	1.5	2.5
107	5400	5400	1.5	2.5
108	5450	5450	1.5	2.5
109	5500	5500	1.5	2.5
110	5550	5550	1.5	2.5
111	5600	5600	1.5	2.5
112	5650	5650	1.5	2.5
113	5700	5700	1.5	2.5
114	5750	5750	1.5	2.5
115	5800	5800	1.5	2.5
116	5850	5850	1.5	2.5
117	5900	5900	1.5	2.5
118	5950	5950	1.5	2.5
119	6000	6000	1.5	2.5
120	6050	6050	1.5	2.5
121	6100	6100	1.5	2.5
122	6150	6150	1.5	2.5
123	6200	6200	1.5	2.5
124	6250	6250	1.5	2.5
125	6300	6300	1.5	2.5
126	6350	6350	1.5	2.5
127	6400	6400	1.5	2.5
128	6450	6450	1.5	2.5
129	6500	6500	1.5	2.5
130	6550	6550	1.5	2.5
131	6600	6600	1.5	2.5
132	6650	6650	1.5	2.5
133	6700	6700	1.5	2.5
134	6750	6750	1.5	2.5
135	6800	6800	1.5	2.5
136	6850	6850	1.5	2.5
137	6900	6900	1.5	2.5
138	6950	6950	1.5	2.5
139	7000	7000	1.5	2.5
140	7050	7050	1.5	2.5
141	7100	7100	1.5	2.5
142	7150	7150	1.5	2.5
143	7200	7200	1.5	2.5
144	7250	7250	1.5	2.5
145	7300	7300	1.5	2.5
146	7350	7350	1.5	2.5
147	7400	7400	1.5	2.5
148	7450	7450	1.5	2.5
149	7500	7500	1.5	2.5
150	7550	7550	1.5	2.5
151	7600	7600	1.5	2.5
152	7650	7650	1.5	2.5
153	7700	7700	1.5	2.5
154	7750	7750	1.5	2.5
155	7800	7800	1.5	2.5
156	7850	7850	1.5	2.5
157	7900	7900	1.5	2.5
158	7950	7950	1.5	2.5
159	8000	8000	1.5	2.5
160	8050	8050	1.5	2.5
161	8100	8100	1.5	2.5
162	8150	8150	1.5	2.5
163	8200	8200	1.5	2.5
164	8250	8250	1.5	2.5
165	8300	8300	1.5	2.5
166	8350	8350	1.5	2.5
167	8400	8400	1.5	2.5
168	8450	8450	1.5	2.5
169	8500	8500	1.5	2.5
170	8550	8550	1.5	2.5
171	8600	8600	1.5	2.5
172	8650	8650	1.5	2.5
173	8700	8700	1.5	2.5
174	8750	8750	1.5	2.5
175	8800	8800	1.5	2.5
176	8850	8850	1.5	2.5
177	8900	8900	1.5	2.5
178	8950	8950	1.5	2.5
179	9000	9000	1.5	2.5
180	9050	9050	1.5	2.5
181	9100	9100	1.5	2.5
182	9150	9150	1.5	2.5
183	9200	9200	1.5	2.5
184	9250	9250	1.5	2.5
185	9300	9300	1.5	2.5
186	9350	9350	1.5	2.5
187	9400	9400	1.5	2.5
188	9450	9450	1.5	2.5
189	9500	9500	1.5	2.5
190	9550	9550	1.5	2.5
191	9600	9600	1.5	2.5
192	9650	9650	1.5	2.5
193	9700	9700	1.5	2.5
194	9750	9750	1.5	2.5
195	9800	9800	1.5	2.5
196	9850	9850	1.5	2.5
197	9900	9900	1.5	2.5
198	9950	9950	1.5	2.5
199	10000	10000	1.5	2.5

$X^3 \wedge$ state

$$T_e = 0$$

0	503·4	503·4	1·569	1·675
1	1503·4	1503·4	1·535	1·719
2	2494·4	2494·4	1·513	1·751
3	3476·5	3476·5	1·495	1·778
4	4449·5	4449·5	1·480	1·802
5	5413·6	5413·6	1·468	1·825
6	6368·6	6368·6	1·456	1·846
7	7314·7	7314·7	1·446	1·867
8	8251·7	8251·7	1·437	1·886
9	9179·8	9179·8	1·428	1·905
10	10098·8	10098·8	1·420	1·923
11	11008·9	11008·9	1·413	1·941
12	11910·0	11910·0	1·406	1·959
13	12802·1	12802·1	1·399	1·976
14	13685·1	13685·1	1·392	1·993
15	14559·2	14559·2	1·386	2·010
16	15424·3	15424·3	1·380	2·027
17	16280·4	16280·4	1·374	2·044
18	17127·5	17127·5	1·369	2·060
19	17965·6	17965·6	1·364	2·076
20	18794·7	18794·7	1·359	2·092
21	19614·8	19614·8	1·354	2·108
111(v_1)	56588·0	56588·0	0·823	6·465

$$B^3\pi^{-SKIP}$$

$$T_e = 16214 \cdot 0 \text{ cm}^{-1}$$

0	435·0	16649·0	1·609	1·723
1	1298·7	17512·7	1·572	1·770
2	2154·2	18368·2	1·549	1·805
3	3001·5	19215·5	1·530	1·835
4	3840·5	20054·5	1·515	1·862
5	4671·3	20885·3	1·502	1·886
105(v_s)	46207·5	62421·5	0·815	7·939

TABLE II (Contd.)

v	$U(\text{cm}^{-1})$	$U + \text{Te}$ (cm^{-1})	$r_{\min}(\text{\AA})$	$r_{\max}(\text{\AA})$
$a^1\Delta \text{ state}$				
$\text{Te} = 581 \cdot 0 \text{ cm}^{-1}$				
0	507·2	1088·2	1·566	1·671
1	1515·6	2096·6	1·532	1·715
2	2516·2	3097·2	1·510	1·747
3	3508·9	4089·9	1·492	1·774
4	4493·8	5074·8	1·478	1·798
5	5470·8	6051·8	1·465	1·820
129(v_c)	65703·8	66284·8	0·736	9·247
$d^1\Sigma^+ \text{ state}$				
$\text{Te} = 1708 \cdot 0 \text{ cm}^{-1}$				
0	510·7	2218·7	1·549	1·654
1	1525·3	3233·3	1·516	1·698
2	2530·5	4238·5	1·494	1·730
3	3526·5	5234·5	1·477	1·758
4	4513·1	6221·1	1·462	1·782
5	5490·5	7198·5	1·447	1·800
6	6458·7	8166·7	1·439	1·826
7	7417·5	9125·5	1·429	1·847
110(v_c)	56474·3	58182·3	0·717	8·535
$b^1\pi \text{ state}$				
$\text{Te} = 10814 \cdot 4 \text{ cm}^{-1}$				
0	458·4	11272·0	1·601	1·712
1	1369·6	12184·0	1·565	1·758
2	2273·3	13087·7	1·542	1·791
3	3169·4	13983·8	1·524	1·820
4	4058·0	14872·4	1·508	1·845
5	4939·1	15753·5	1·495	1·869
122(v_c)	56267·3	67081·7	0·666	10·406
$c^1\Phi \text{ state}$				
$\text{Te} = 18471 \cdot 5 \text{ cm}^{-1}$				
0	457·3	18928·8	1·586	1·697
1	1365·3	19836·8	1·550	1·743
2	2264·8	20736·3	1·527	1·777
3	3155·5	21627·0	1·508	1·805
105(v_c)	48517·9	66989·4	0·721	7·992
$e^1\Sigma \text{ state}$				
$\text{Te} = 26005 \cdot 8 \text{ cm}^{-1}$				
0	425·8	26431·6	1·639	1·754
1	1270·3	27276·1	1·602	1·802
2	2105·4	28111·2	1·577	1·836
3	2931·1	28936·9	1·557	1·866
4	3747·4	29753·2	1·541	1·892
5	4554·3	30560·1	1·526	1·917
6	5351·8	31357·6	1·513	1·940
90(v_c)	38783·8	64789·6	0·347	7·216

The true potential energy curves (RKR) have been used to estimate the dissociation energies of diatomic molecules in a number of cases by fitting an empirical potential energy curve²²⁻²⁵. The Hulbert-Hirschfelder function has been shown to fit to a good extent the RKR curves wherever these are known over a wide range of energy for a number of diatomic molecules (Steele *et al.*²²).

Hulbert-Hirschfelder function²⁶.

$$U = D_e [(1 - e^{-x})^2 + cx^3 e^{-2x} (1 + bx)]$$

where

$$x = \frac{\omega_e}{2(B_e D_e)^{1/2}} \frac{r - r_e}{r_e}; \quad c = 1 + a_1 \left(\frac{D_e}{a_0} \right)^{1/2}$$

$$b = 2 - \left(\frac{7}{12} - \frac{D_e a_0}{a_0} \right) / c$$

and a_0 , a_1 , a_2 are constants given by

$$a_0 = \frac{\omega_e^2}{4B_e}, \quad a_1 = -1 - \frac{\omega_e a_e}{6B_e^2}$$

$$a_2 = \frac{5}{4} a_1^2 - \frac{2\omega_e x_e}{3B_e} \quad \text{and} \quad D_e = \frac{\omega_e^2}{4\omega_e x_e}$$

being five parameter function gives best average results and in general gives the best fit of the potential for all the cases studied whereas Lippincott 3-parameter potential function gives nearly good results. Varshni III and Lippincott functions, the best of the three-parameter functions in fitting the potential energy curves, both give good prediction of dissociation energy values. On the other hand, the Lippincott function gives fairly reliable values of D_e , while Varshni III function does not. According to the study of comparison of potential functions by Steele, Lippincott and Vanderslice²² the better 3-parameter functions give potential curves with an average error of 2 to 3% in $|V - V_{RKR}|/D_e$, whereas the better five-parameter function should give only average error of 1 to 2%.

The most prominent feature of these curves is that these are narrow well type potentials which indicate that the molecule behaves approximately like a harmonic oscillator rather than an anharmonic oscillator as has been observed by Kushawaha⁹. The true potential energy curves are lying approximately one above the other indicating the structure of the molecule in the ground and the upper states should be nearly the same as is evident from the approximately equal r_e values for all these states.

The results of the calculation for the ground state dissociation energy is given in Table III. From this table one can conclude that the best fit to the RKR curve is obtained when we put $D = 56,500 \text{ cm}^{-1}$ (7.005 eV). The most probable value of D_e from our calculations is 7.005 eV since $|V - V_{RKR}|/D_e$ is 0.3%. The value obtained by

TABLE III
Calculations for the ground-state dissociation energy of TiO molecule using the H-H function

$r(\text{\AA})$	$D_e = 56,000 \text{ cm}^{-1}$	$D_e = 56,500 \text{ cm}^{-1}$	$D_e = 58,000 \text{ cm}^{-1}$	RKR cm^{-1}
1.675	492.1	496.5	509.7	503.4
1.719	1483.3	1496.6	1536.3	1503.4
1.778	3428.2	3458.8	3550.6	3476.5
1.802	4373.4	4412.5	4529.6	4449.5
1.846	6277.7	6333.7	6501.9	6368.6
1.867	7248.3	7313.0	7507.2	7314.7
1.905	9078.9	9160.1	9403.2	9179.8
1.923	9971.4	10060.4	10327.5	10098.8
1.976	12657.8	12770.8	13109.8	12802.1
1.993	13529.9	13650.7	14013.1	13685.1
2.027	15277.5	15413.9	15823.1	15424.3
2.044	16149.1	16293.3	16725.8	16280.4
2.076	17782.0	17940.8	18417.1	17965.6
1.513	2469.1	2491.2	2557.3	2494.4
1.468	5377.6	5425.6	5569.6	5413.6
1.437	8215.0	8288.4	8508.4	8251.7
1.413	10945.9	11043.7	11336.9	11008.9
1.406	11837.7	11943.4	12260.5	11910.0
1.386	14629.9	14760.5	15388.5	14559.2
1.369	17150.0	17303.1	17947.3	17127.5
1.359	18853.9	19022.3	19732.6	18794.7
1.354	19849.9	20032.9	20667.4	19614.8

Kushawaha⁹ is based on the curve fitting, using the old rotational constants and also the uncertainty of $\pm 20 \text{ K cal/mol}$ (experimental value) for which unconvincing explanation in his article and only the main value included in the text and assumes the uncertainty of the D of TiO with that of Wahlbeck's²⁷ uncertainty value, since these two are independent works the uncertainty cannot be the same even though main value be the same.

The dissociation energy of TiO molecule has been given by different authors (Gaydon²⁶, Herzberg²⁸, Drowart *et al.*²⁹, Gilles *et al.*³⁰, and Kushawaha⁹). In the present work using the Hulbert-Hirschfelder function, the dissociation energy for the ground state of TiO molecule is estimated to be 7.005 eV which is in very good agreement with the value given by Gaydon²⁶ ($7.2 \pm 0.1 \text{ eV}$).

ACKNOWLEDGEMENTS

The authors are thankful to Prof. S. V. Subrahmanyam for his interest and encouragement in the present work. One of the authors (GTN) wishes to thank U.G.C., New Delhi, for financial assistance.

1. Davis, D. N., *Astrophys. J.*, 1947, 106, 28.
2. Lakshman, S. V. J. and Ramakrishna Rao, T. V., *J. Phys. B*, 1971, 4, 269.
3. Ramakrishna Rao, T. V. and Lakshman, S. V. J., *J. Quant. Spectro. Radiat. Transfer.*, 1972, 12, 1063.
4. — and —, *Physica*, 1971, 56, 322.
5. — and —, *Ind. J. Pure and Appl. Phys.*, 1973, 11, 539.
6. Lakshman, S. V. J., Ramakrishna Rao, T. V. and Naidu, G. T., *Pramāṇa*, 1976, 7, 369.
7. —, — and —, *Curr. Sci.*, 1977, 46, 33.
8. Chakraborty, B. and Pan, Y. K., *Applied Spectro.*, 1973, 7, 283.
9. Kushawaha, V. S., *J. Phys. Chem.*, 1973, 77, 2885.
10. Uhler, U., *Ph.D. Thesis*, University of Stockholm, Sweden, 1954.
11. Collins, J. G., *J. Phys. B*, 1975, 8, 304.
12. Phillips, J. G., *Astrophys. J.*, 1950, 111, 314.
13. —, *Ibid.*, 1969, 157, 449.
14. —, *Appl. J.*, 1973, 26, 313.

15. Pettersson, A. V., *Ark. Fys.*, 1959, 16, 185.
16. — and Lindgren, B., *Ibid.*, 1962, 22, 491.
17. Linton, C. and Nicholls, R. W., *J. Phys. B*, 1969, 2, 490.
18. Phillips, J. G. and Davis, S. P., *Astrophys. J.*, 1971, 167, 209.
19. Lindgren, B., *J. Mol. Spectro.*, 1972, 43, 474.
20. Linton, C. and Singhal, S. R., *Ibid.*, 1974, 51, 194.
21. —, *Ibid.*, 1974, 50, 235.
22. Steele, D., Lippincott, E. R. and Vanderslice, J. T., *Rev. Mod. Phys.*, 1962, 34, 239.
23. Singh, R. B. and Rai, D. K., *Canad. J. Phys.*, 1965, 43, 829.
24. Singh, J., Nair, K. P. R. and Rai, D. K., *J. Mol. Struct.*, 1970, 5, 492.
25. Nair, K. P. R., Singh, R. B. and Rai, D. K., *J. Chem. Phys.*, 1965, 43, 3570.
26. Gaydon, A. G., *Dissociation Energies*, Chapman and Hall, Ltd. (London), 1968.
27. Wahlbeck, P. G. and Gilles, P. W., *J. Chem. Phys.*, 1967, 46, 2465.
28. Herzberg, G., *Mol. Spectra and Mol. Structure—I*, Van Nostrand Company, New York, 1967.
29. Drowart, J., Coppens, P. and Smoes, S., *J. Chem. Phys.*, 1969, 50, 1046.
30. Gilles, P. W., Hamson, P. J. and Wahlbeck, P. G., *Ibid.*, 1969, 50, 1048.

DETERMINATION OF URANIUM TRACE IN SOME SEMICONDUCTING MATERIALS BY NUCLEAR TRACK DETECTORS

S. K. CHAKARVARTI

Department of Applied Physics, Regional Engineering College, Kurukshetra 132119, Haryana, India

AND

M. M. DHAWAN AND K. K. NAGPAUL

Department of Physics, Kurukshetra University, Kurukshetra 132119, Haryana, India

ABSTRACT

Fission track counting method has been applied to the trace determination of uranium in some semiconductors Se, Te, As₂-S₃ (Glass), CdS, PbS, Pb-As-S and Pb-Sb-S in amorphous form. It has been found that the uranium is not uniformly distributed. Results indicate uranium concentration as low as 0.43 ppm in the homogeneous region and 77 ppm on the higher side in the heterogeneous region.

INTRODUCTION

ONE of the significant applications of solid state nuclear track detectors (SSNTD) lies in determining some trace elements¹ (U²³⁵, B¹⁰, Li⁷, Li⁶, O¹⁷, K³⁹, Fe⁵⁷, S³³, Zn⁶⁶, etc.), in various materials. In the present investigations, attempt has been made to apply this technique to semiconductors for the determination of traces of uranium.

EXPERIMENTAL PROCEDURE

The method consists of placing suitable plastic detectors in close and intimate contact on both sides of the sample under investigation. A standard sample with known uranium content or other isotope of interest is also included. All the samples are then enclosed in an aluminium capsule and the whole assembly irradiated to thermal neutrons of