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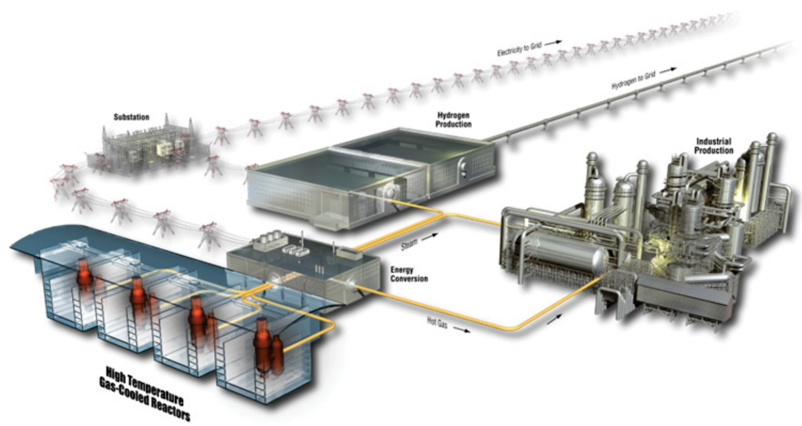

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SUMMARY

This report presents an overview of the current knowledge on diffusivities of fission products Ag, Cs, Sr, and Kr in the kernel and coating layers of a tri-structural isotropic (TRISO) particle as well as in the surrounding graphite that composes compact or pebble matrix and fuel elements. These diffusivities are used in TRISO fuel performance modeling to assess the transport and release of fission products. The majority of the data in this document originate from a report by the International Atomic Energy Agency and are completed with more recently published data. Following the first irradiation campaign of Idaho National Laboratory's Advanced Gas Reactor fuel development and qualification program and the subsequent post-irradiation examination of the irradiated fuel, tentative limits were derived on the diffusivities of these fission products in some of the layers of the TRISO particle. These limits are compared to the existing literature data. This report is meant to be a living document that will be updated and revised as new data from the Advance Gas Reactor experiments or other TRISO fuel diffusivity data become available.

CONTENTS

TABLES

ACRONYMS

AGR	Advanced Gas Reactor
HTGR	High Temperature Gas-cooled Reactor
HTI	high temperature isotropic
IAEA	International Atomic Energy Agency
INL	Idaho National Laboratory
LTI	low temperature isotropic
N/A	not applicable
PARFUME	particle fuel model
PIE	post-irradiation examination
PyC	pyrocarbon
TRISO	tristructural isotropic

Diffusivities of Ag, Cs, Sr, and Kr in TRISO Fuel Particles and Graphite

1. INTRODUCTION

Tristructural isotropic (TRISO) coated particles have been developed and studied since the late 1950s when the concept of coated particles was invented by Roy Huddle of the United Kingdom Atomic Energy Authority. When such fuel is used in modular high temperature gas-cooled reactors (HTGRs), reactor designers have decided to calculate a mechanistic source term under both normal operation and postulated accident conditions. This requirement necessitates that accurate estimates of fission product transport through and release from HTGR fuel elements can be calculated for the reactor design. As such, the DOE Advanced Gas Reactor Fuel Development and Qualification Program is performing a number of activities related to updating and improving estimates of fission product release and transport in the TRISO fuel system.

Several decades of work by half a dozen countries on fission product transport in TRISO fuel through numerous irradiation and heating experiments have led to several recommendations for transport data and to the adoption of various sets of diffusion coefficients. In 1997, the International Atomic Energy Agency (IAEA) gathered the latest of these historical results and issued a technical document (TECDOC-978 [IAEA]) that summarizes these sets of recommended diffusion coefficients. The recommendations found in TECDOC-978 reflect the consensus achieved in the early 1990s by the TRISO fuel community about the best diffusivity values to use in performance modeling calculations based on the pedigree of the available experimental data, the methods of measurement, the representativeness of the fuel samples, and the measurement uncertainties. Table 1 shows the reference literature articles for the diffusivities that have historically been recommended by the American and German TRISO fuel development programs and that are most commonly used in current U.S. models. These diffusivities are summarized in the IAEA report (see section 7 for full references of these articles).

Table 1. Diffusivities recommended by the American (USA) and German (FRG) TRISO fuel development programs ([IAEA]).

	Kernel (UO_2)		Pyrocarbon (PyC)		Silicon carbide (SiC)	
	USA	**FRG**	**USA**	**FRG**	**USA**	**FRG**
Ag	Moormann	Moormann	Amian(1)	Moormann Amian(1)	Moormann	Moormann
Cs	Moormann	Moormann	Myers(2)	Moormann	Myers(4)	Christ
Sr	Moormann	Moormann	Myers(1)	Moormann Myers(1)	Verfondern	Verfondern
Kr	-	Moormann Muller	Goodin	Goodin	-	-

	Matrix		Graphite	
	USA	**FRG**	**USA**	**FRG**
Ag	∞	Hoinkis	-	Causey
Cs	∞	Hoinkis	Myers(2)	Myers(2)
Sr	∞	Hensel	Myers(1)	Myers(1)
Kr	∞	Moormann Muller	-	Moormann

Note: a dash ("-") means no recommendation available; an infinite symbol ("∞") means instantaneous release is recommended.

In the past 20 years, new experiments have provided additional fission transport data that are compiled in this document together with the data from the IAEA TECDOC-978. In particular, the first campaign of irradiation and post-irradiation examination (PIE) of Idaho National Laboratory's (INL's) Advanced Gas Reactor (AGR) fuel development and qualification program ([INL]) led to the derivation of interim limits on the diffusivities of these fission products in the kernel and coating layers of the TRISO particle. The newer data, however, have not been subjected to a formal review by the international community and they are not part of any newer official recommendation. The IAEA diffusivities remain the preferred reference for fuel performance modeling.

INL's particle fuel model (PARFUME) code was used to calculate the predicted release of fission products from AGR-1 compacts during irradiation (Ag, Cs, and Sr) and safety testing (Ag, Cs, Sr, and Kr), and comparison to PIE data allowed, in some cases, derivation of correction factors to the diffusivities used in the code ([Collin(1,2)]). These correction factors are defined as:

$$D_c = F \times D_m \quad \text{(Eq. 1)}$$

where D_c is the corrected diffusivity, D_m is the original diffusivity used in the modeling, and F is the correction factor. When $F < 1$, smaller correction factors are indicative of original diffusivities that are over-predicted to a greater extent. Calculations performed with the corrected diffusivities lead to a better match between model predictions and AGR-1 experimental results. As the AGR program continues, it is anticipated that additional data will be collected that will allow for further refinement of the correction factors.

The assessment of fission product transport and release from TRISO fuel is obtained in fuel performance modeling through classical Fickian diffusion. "Effective" diffusion coefficients are used in this approach, meaning that all possible transport mechanisms are encompassed in a simplified single transport process. The diffusivities are parameterized using an Arrhenius type equation:

$$D = D_1 e^{-Q_1/RT} + D_2 e^{-Q_2/RT} \quad \text{(Eq. 2)}$$

where $D_{1,2}$ are pre-exponential factors (m^2/s), $Q_{1,2}$ are activation energies (J/mol), R is the universal gas constant (8.3145 J/mol-K), and T is the temperature (K).

Sections 2 through 6 summarize the diffusion coefficients that have been derived from various irradiation and heating experiments over the past few decades for each material composing the fuel. The following remarks apply to all of the diffusivity data presented below:

- Kernel data are for UO_2. Due to the lack of data for UCO, calculations by PARFUME on UCO-based AGR-1 fuel were performed using UO_2 data.
- PyC data are for low temperature isotropic (LTI) pyrocarbon, which is the current type of PyC in TRISO fuel (older particle fuel used high temperature isotropic pyrocarbon, sometimes referred to as HTI).
- SiC data are for polycrystalline silicon carbide.
- I, Kr, and Xe are considered identical with regard to their diffusion behavior. The diffusivities derived from iodine or xenon measurements are assumed to be valid for krypton.

In all of the following tables, shaded boxes show the diffusion coefficients used in PARFUME. Correction factors derived from the comparison to AGR-1 data apply to these diffusivities. Details about how these correction factors were obtained, or why they could not be derived are available in separate reports for the irradiation ([Collin(1)]) and safety testing (Collin(2)]) phases.

The diffusivities obtained using Eq. 2 from the diffusion coefficients in all of the tables are plotted against reciprocal temperature in Appendices B through F, while Appendix A gives an overview of these diffusivity data.

2. DIFFUSIVITIES IN KERNEL

2.1 Ag in Kernel

Table 2. Diffusion coefficients of silver in UO_2.

D_1 (m/s^2)	Q_1 (kJ/mol)	D_2 (m/s^2)	Q_2 (kJ/mol)	Temperature (°C)	Reference	Notes
6.7×10^{-9}	165	-	-	700 – 2400	Moormann	500 µm diameter
3.3×10^{-9}	165	-	-	-	FDDM/F	350 µm diameter
6.7×10^{-9}	165	-	-	-	FDDM/F	500 µm diameter
6.7×10^{-10}	165	-	-	1000 – 1500	Amian(1)	
3.4×10^{-9}	213	-	-	800 – 1500	Nabielek(1)	500 µm diameter
2.4×10^{-7}	269	-	-	1000 – 1400	Brown	500 µm diameter

Estimated correction factors to the diffusivity of Ag in UO_2 obtained from comparison between PARFUME and AGR-1 data:

Irradiation: None – Relatively good agreement with under-prediction at low burnup and over-prediction at high burnup. Technical rationale for the burnup relationship is not understood and still under study.

Safety Testing: Not available – Over-estimation is probable, but could not be established uniquely from AGR-1 data.

2.2 Cs in Kernel

Table 3. Diffusion coefficients of cesium in UO_2.

D_1 (m/s^2)	Q_1 (kJ/mol)	D_2 (m/s^2)	Q_2 (kJ/mol)	Temperature (°C)	Reference	Notes
5.6×10^{-8}	209	5.2×10^{-4}	362	700 – 2400	Moormann	500 µm diameter
4.7×10^{-10}	177	-	-	1000 – 1450	Fukuda(5)	500 µm diameter
4.8×10^{-14}	78	-	-	1000 – 1600	Amian(1)	
3.6×10^{-7}	362	-	-	1000 – 1500	Brown	Grain 10-50 µm
4.9×10^{-18}	78	-	-	-	FDDM/F	350 µm diameter
1.0×10^{-17}	78	-	-	-	FDDM/F	500 µm diameter

Estimated correction factors to the diffusivity of Cs in UO_2 obtained from comparison between PARFUME and AGR-1 data:

Irradiation: 4×10^{-3} to 4×10^{-2}

Safety Testing:

- 1600°C: 3.6×10^{-3} to 4.1×10^{-2}
- 1700°C: 1.0×10^{-4} to 7.0×10^{-4}
- 1800°C: 1.3×10^{-3} to 3.1×10^{-3}
- Assumes average correction factors during irradiation in kernel (1.25×10^{-2}) and SiC (0.6).

2.3 Sr in Kernel

Table 4. Diffusion coefficients of strontium in UO_2.

D_1 (m/s^2)	Q_1 (kJ/mol)	D_2 (m/s^2)	Q_2 (kJ/mol)	Temperature (°C)	Reference	Notes
$3.4\times10^{+1}$	594	-	-	-	FDDM/F	350 µm diameter
$6.9\times10^{+1}$	594	-	-	-	FDDM/F	500 µm diameter
3.5×10^{-5}	409	-	-	1000 – 1500	Amian(1)	
$2.0\times10^{+3}$	691	-	-	1500 – 1650	Brown	500 µm diameter
2.2×10^{-3}	488	-	-	700 – 2400	Moormann	500 µm diameter

Estimated correction factors to the diffusivity of Sr in UO_2 obtained from comparison between PARFUME and AGR-1 data:

Irradiation: Not available – Over-estimation is probable, but could not be established uniquely from AGR-1 data.

Safety Testing: Not available – Over-estimation is probable, but could not be established uniquely from AGR-1 data.

2.4 Kr in Kernel

Table 5. Diffusion coefficients of krypton in UO_2.

D_1 (m/s^2)	Q_1 (kJ/mol)	D_2 (m/s^2)	Q_2 (kJ/mol)	Temperature (°C)	Reference	Notes
8.8×10^{-15}	54	6.0×10^{-1}	480	1500 – 2400	Moormann	500 µm diameter
1.3×10^{-12}	126	-	-	700 – 1500	Moormann Muller	500 µm diameter
1.0×10^{-9}	368	-	-	1200 – 1450	Chernikov	500 µm diameter

Estimated correction factors to the diffusivity of Kr in UO_2 obtained from comparison between PARFUME and AGR-1 data:

Irradiation: no PIE data.

Safety Testing: None – Diffusivity of Kr in the kernel appears to be appropriately modeled although the estimation is based on data from one AGR-1 compact only.

3. DIFFUSIVITIES IN PYC

3.1 Ag in PyC

Table 6. Diffusion coefficients of silver in PyC.

D_1 (m/s^2)	Q_1 (kJ/mol)	D_2 (m/s^2)	Q_2 (kJ/mol)	Temperature (°C)	Reference	Notes
5.3×10^{-4}	192	-	-	1400 – 1700	Chernikov	1.84 g/cm^3
5.3×10^{-9}	154	-	-	1000 – 1500 700 – 2000	Amian(1) Moormann	
1.0×10^{-8}	164	-	-	-	Offermann	

Estimated correction factors to the diffusivity of Ag in PyC obtained from comparison between PARFUME and AGR-1 data:

Irradiation: None – Relatively good agreement with under-prediction at low burnup and over-prediction at high burnup. Technical rationale for the burnup relationship is not understood and still under study.

Safety Testing: None at this time.

3.2 Cs in PyC

Table 7. Diffusion coefficients of cesium in PyC.

D_1 (m/s^2)	Q_1 (kJ/mol)	D_2 (m/s^2)	Q_2 (kJ/mol)	Temperature(°C)	Reference	Notes
1.5×10^{-16}	-	-	-	1000	Gudkov	
1.9×10^{-6}	254	-	-	1000 – 1600	Amian(1)	
5.0×10^{-5}	318	-	-	1200 – 1850	Myers(2)	
6.3×10^{-8}	222	-	-	700 – 2000	Moormann	
1.2×10^{-3}	412	-	-	1600 – 2300	Hayashi(3)	
6.7×10^{-9}	198	-	-	1200 – 1400	Fukuda(5)	
9.7×10^{-11}	176	-	-	1000 – 1650	Gethard	
1.8×10^{-9} 9.6×10^{-10}	218 218	-	-	1000 – 1500	Brown	1.8 g/cm^3 1.9 g/cm^3

Estimated correction factors to the diffusivity of Cs in PyC obtained from comparison between PARFUME and AGR-1 data:

Irradiation: None at this time.

Safety Testing: None at this time.

3.3 Sr in PyC

Table 8. Diffusion coefficients of strontium in PyC.

D_1 (m/s^2)	Q_1 (kJ/mol)	D_2 (m/s^2)	Q_2 (kJ/mol)	Temperature (°C)	Reference
4.4×10^{-6}	201	-	-	1000 – 1600	Gethard
2.3×10^{-6}	197	-	-	700 – 2000 1200 – 1650	Moormann Myers(1)

Estimated correction factors to the diffusivity of Sr in PyC obtained from comparison between PARFUME and AGR-1 data:

Irradiation: None at this time.

Safety Testing: None at this time.

3.4 Kr in PyC

Table 9. Diffusion coefficients of krypton in PyC.

D_1 (m/s^2)	Q_1 (kJ/mol)	D_2 (m/s^2)	Q_2 (kJ/mol)	Temperature (°C)	Reference	Notes
1.1×10^{-5}	285	-	-	1000 – 1650	Chernikov	
2.9×10^{-8} 6.0×10^{-8}	255 255	-	-	1200 – 1500	Fukuda(5)	Upper limit Lower limit
2.9×10^{-8}	291	$2.0\times10^{+5}$	923	- 800 – 2400	Goodin Moorman	
2.9×10^{-11}	255	-	-	1200 – 1750	Fukuda(1)	Xe values

Estimated correction factors to the diffusivity of Kr in PyC obtained from comparison between PARFUME and AGR-1 data:

Irradiation: no PIE data.

Safety Testing: 0.8 – Based on data from one AGR-1 compact only.

4. DIFFUSIVITIES IN SIC

4.1 Ag in SiC

Table 10. Diffusion coefficients of silver in SiC.

D_1 (m/s^2)	Q_1 (kJ/mol)	D_2 (m/s^2)	Q_2 (kJ/mol)	Temperature (°C)	Reference	Notes
6.8×10^{-9}	213	-	-	800 – 1500	Nabielek(1)	Upper limit
3.6×10^{-9}	215	-	-	1000 – 1500 700 – 2400	Amian(1) Moormann	
3.5×10^{-18} 1.6×10^{-17} 3.0×10^{-15}	-	-	-	950 1150 1500	Lopez-Honorato	
6.8×10^{-11}	177	-	-	1200 – 1400	Fukuda(5)	
2.5×10^{-3}	408	-	-	1200 – 1500	Bullock	Poor SiC
3.5×10^{-10}	213	-	-	1200 – 2400	Chernikov	
4.5×10^{-9}	218	-	-	1000 – 1500	Amian(2)	
1.1×10^{-13}	109			900 – 1300	vanderMerwe	
4.3×10^{-12} 2.4×10^{-9}	241 331	-	-	1200 – 1400	Friedland(1) Friedland(2)	

Estimated correction factors to the diffusivity of Ag in SiC obtained from comparison between PARFUME and AGR-1 data:

Irradiation: None – Relatively good agreement with under-prediction at low burnup and over-prediction at high burnup. Technical rationale for the burnup relationship is not understood and still under study.

Safety Testing:

- 1600°C: 2.5×10^{-4} to 4.5×10^{-3}
- 1700°C: 8.0×10^{-4} to 2.4×10^{-3}
- 1800°C: 1.9×10^{-3} to 4.6×10^{-2}

4.2 Cs in SiC

Table 11. Diffusion coefficients of cesium in SiC.

D_1 (m/s^2)	Q_1 (kJ/mol)	D_2 (m/s^2)	Q_2 (kJ/mol)	Temperature (°C)	Reference	Notes
1.8×10^{-11}	176	-	-	700 – 1500	Moormann	
6.7×10^{-14}	106	2.4×10^{-2} 1.1×10^{-4}	482 437	-	Myers(4)	Upper limit Lower limit
2.5×10^{-2}	503	-	-	1600 – 1900	Minato	
3.5×10^{-9}	236	-	-	1000 – 1600	Amian(1,2)	
2.3×10^{-17}	-	-	-	1000	Gudkov	
6.8×10^{-12}	177	-	-	1200 – 1400	Fukuda(5)	Upper limit
2.8×10^{-4} 1.5×10^{-4}	420 422	-	-	1300 – 1500	Ogawa	Upper limit Lower limit
$5.5\times e^{\Gamma/5}$ $\times10^{-14}$	125	1.6×10^{-2}	514	-	Christ	Γ fluence, E>0.1 MeV

Estimated correction factors to the diffusivity of Cs in SiC obtained from comparison between PARFUME and AGR-1 data:

Irradiation: 0.4 to 0.8 – Assumes no correction in kernel.

Safety Testing:

- 1600°C: 1.25×10^{-2}
- Assumes correction factors during irradiation in kernel (1.25×10^{-2}) and SiC (0.6).
- 1700 and 1800°C: Not available – Not enough data, but over-estimation is probable.

4.3 Sr in SiC

Table 12. Diffusion coefficients of strontium in SiC.

D_1 (m/s^2)	Q_1 (kJ/mol)	D_2 (m/s^2)	Q_2 (kJ/mol)	Temperature (°C)	Reference
1.2×10^{-9}	205	$1.8\times10^{+6}$	791	-	Verfondern
1.2×10^{-9}	205	204×10^{-2}	482	-	Moormann
2.0×10^{-14}	-	-	-	1750	Fukuda(1)
1.2×10^{-9}	205			1650 – 1850	Fukuda(3)
4.9×10^{-16}	-	-	-	1400	Forthmann(1)

Estimated correction factors to the diffusivity of Sr in SiC obtained from comparison between PARFUME and AGR-1 data:

Irradiation: Not available – Over-estimation is probable, but could not be established uniquely from AGR-1 data.

Safety Testing: Not available – Over-estimation is probable, but could not be established uniquely from AGR-1 data.

4.4 Kr in SiC

Table 13. Diffusion coefficients of krypton in SiC.

D_1 (m/s^2)	Q_1 (kJ/mol)	D_2 (m/s^2)	Q_2 (kJ/mol)	Temperature (°C)	Reference	Notes
8.6×10^{-10} $3.7\times10^{+1}$	326 657	-	-	1200 – 1400 1400 – 1750	Fukuda(2)	Xe values
1.7×10^{0}	623	-	-	1650 – 1850	Fukuda(3)	Xe values
1.8×10^{-21} 6.5×10^{-20}	-	-	-	1100 1200	Friedland(2)	I values

Estimated correction factors to the diffusivity of Kr in SiC obtained from comparison between PARFUME and AGR-1 data:

Irradiation: no PIE data.

Safety Testing: None at this time.

5. DIFFUSIVITIES IN GRAPHITE MATRIX

5.1 Ag in graphite matrix

Table 14. Diffusion coefficients of silver in graphite matrix.

D_1 (m/s^2)	Q_1 (kJ/mol)	D_2 (m/s^2)	Q_2 (kJ/mol)	Temperature (°C)	Reference	Notes
$6.8\times10^{+1}$ 1.3×10^{0}	261 246	-	-	800 – 1300	Hoinkis	A3-3 unirradiated A3-27 unirradiated
$8.7\times10^{+7}$	414	-	-	800 – 1000	Nabielek(2)	Unirradiated (UK)
1.6×10^{0}	258	-	-	700 – 2000	Hoinkis Moormann	A3-3 irradiated

5.2 Cs in graphite matrix

Table 15. Diffusion coefficients of cesium in graphite matrix.

D_1 (m/s^2)	Q_1 (kJ/mol)	D_2 (m/s^2)	Q_2 (kJ/mol)	Temperature (°C)	Reference	Notes
4.5×10^{-7} 1.0×10^{-3}	81 170	-	-	900 – 1000 800 – 1000	Hensel	A3-3 unirrad. (vac.) A3-3 unirrad. (He)
2.0×10^{-4}	181	-	-	1000 – 1500 700 – 2000	Hoinkis Moormann	A3-3 irradiated
3.6×10^{-4}	189	-	-	1000 – 1500	Hoinkis	A3-3 irradiated (as reported in [IAEA])
2.0×10^{-5} 4.4×10^{-7}	159 109	-	-	-	Stover	A3-3 irradiated
7.6×10^{-1}	270	-	-	1000	Forthmann(2)	A3-3 unirradiated
3.5×10^{-7}	116	-	-	750 – 1550	Nabielek(2)	Unirradiated (UK)
2.0×10^{-4}	198	-	-	900 – 1100	Leyers	A3-3 unirradiated

5.3 Sr in graphite matrix

Table 16. Diffusion coefficients of strontium in graphite matrix.

D_1 (m/s^2)	Q_1 (kJ/mol)	D_2 (m/s^2)	Q_2 (kJ/mol)	Temperature (°C)	Reference	Notes
2.0×10^{-1} 1.0×10^{-2}	242 303	-	-	900 – 1270 900 – 1600	Hensel	A3-3 unirrad. (H_2) A3-3 unirrad. (vac)
2.8×10^{-4}	210	-	-	1175 – 1375	Fukuda(4)	Unirradiated
5.6×10^{-2}	312	-	-	1200 – 1600	Nabielek(2)	Unirradiated (UK)
9.1×10^{-3}	301	-	-	700 – 2000	Moormann	A3-3 irradiated

5.4 Kr in graphite matrix

Table 17. Diffusion coefficients of krypton in graphite matrix.

D_1 (m/s^2)	Q_1 (kJ/mol)	D_2 (m/s^2)	Q_2 (kJ/mol)	Temperature (°C)	Reference	Notes
6.0×10^{-6} 2.5×10^{-11} 10^{-6}	- 71 -	-	-	700 – 2000 (a) 700 – 1250 (b) 1250-200	Moormann Muller Muller	A3-3 irradiated / I values (a) pore surface (b) bulk
3.1×10^{-8}	151	-	-	900 – 1400	Chernikov	Irradiated

6. DIFFUSIVITIES IN STRUCTURAL GRAPHITE

6.1 Ag in structural graphite

Table 18. Diffusion coefficients of silver in structural graphite.

D_1 (m/s^2)	Q_1 (kJ/mol)	D_2 (m/s^2)	Q_2 (kJ/mol)	Temperature (°C)	Reference	Notes
$1.7\times10^{+1}$ 1.6×10^{0}	184 258	-	-	480 – 800 -	Causey	H-451 unirradiated (as reported in [IAEA])
1.4×10^{-2}	226	-	-	-	FDDM/F	
$1.6\times10^{+2}$	364	-	-	850 – 1100	Nabielek(2)	Unirradiated (UK)
6.3×10^{-3}	264	-	-	900 – 1030	Hayashi(1)	IG-110 irradiated

6.2 Cs in structural graphite

Table 19. Diffusion coefficients of cesium in structural graphite.

D_1 (m/s^2)	Q_1 (kJ/mol)	D_2 (m/s^2)	Q_2 (kJ/mol)	Temperature (°C)	Reference	Notes
1.2×10^{-4} 1.7×10^{-4}	112 95	-	-	600 – 1000	Hayashi(2)	IG-110 unirradiated
5.8×10^{-2}	151	-	-	450 – 750	Nabielek(2)	Unirradiated (UK)
2.2×10^{-10} 1.1×10^{-9} 1.2×10^{-9} 1.3×10^{-9}	-	-	-	854 943 951 952	Myers(3)	H-451 unirradiated
1.0×10^{-7}	110	-	-	820 – 1020	Carter(1)	IG-110 unirradiated
9.0×10^{-6}	157	-	-	750 – 1030	Hayashi(1)	IG-110 irradiated
1.7×10^{-6}	149	-	-	-	Moormann	H-451 irradiated
1.7×10^{-6}	149	-	-	550 – 1450	Myers(2)	Various irradiated
1.0×10^{-7}	123	-	-	820 – 1020	Carter(2)	NBG-18 unirradiated

6.3 Sr in structural graphite

Table 20. Diffusion coefficients of strontium in structural graphite.

D_1 (m/s^2)	Q_1 (kJ/mol)	D_2 (m/s^2)	Q_2 (kJ/mol)	Temperature (°C)	Reference	Notes
1.7×10^{-2}	268	-	-	-	Moormann	H-451 irradiated
1.7×10^{-2}	268	-	-	800 – 2200	Myers(2)	Various irradiated
8.3×10^{-1}	324	-	-	850 – 1400	Nabielek(2)	Unirradiated (UK)

6.4 Kr in structural graphite

Table 21. Diffusion coefficients of krypton in structural graphite.

D_1 (m/s^2)	Q_1 (kJ/mol)	D_2 (m/s^2)	Q_2 (kJ/mol)	Temperature (°C)	Reference	Notes
6.0×10^{-6}	-	-	-	700 – 2000	Moormann	H-451 irradiated / I values
2.8×10^{-3}	205	-	-	900 – 1600	Cubiciotti	Xe values (Canada)

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Appendix A

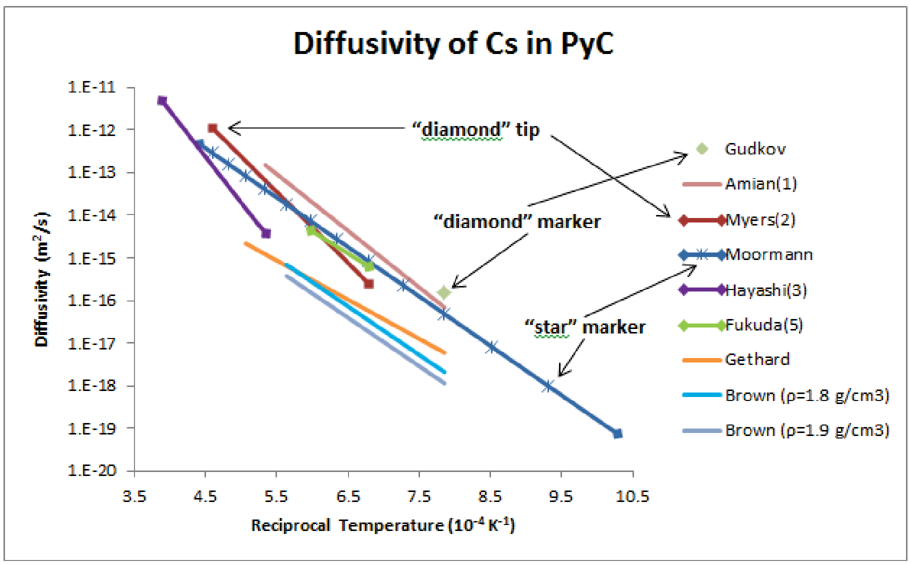
Plots of Diffusivities

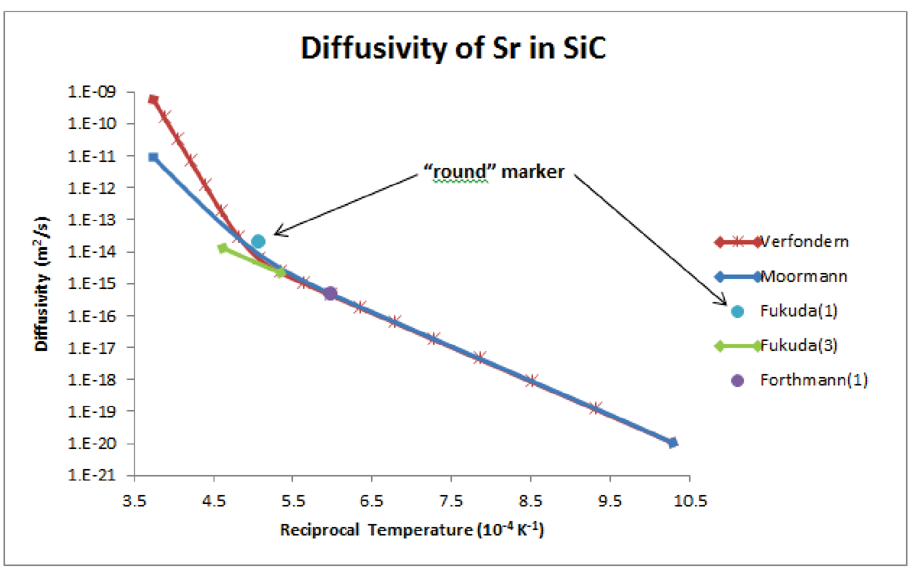
Appendix A
Plots of Diffusivities

Appendices B through F show plots of the diffusivities against reciprocal temperature obtained using Eq. 2 and the diffusion coefficients in Tables 2 to 21.

Below are examples of the plots found in the following Appendices. They show the nomenclature used in the legend for the various diffusivity data:

- Diffusivity curves plotted with "diamond" tips correspond to data that are reported in the IAEA TECDOC-978.
- Diffusivities used in PARFUME are plotted with "star" markers.
- For single-point diffusivities, data shown as "diamond" markers are data that are reported in the IAEA TECDOC-978, while data shown with "round" markers are not found in the IAEA report.





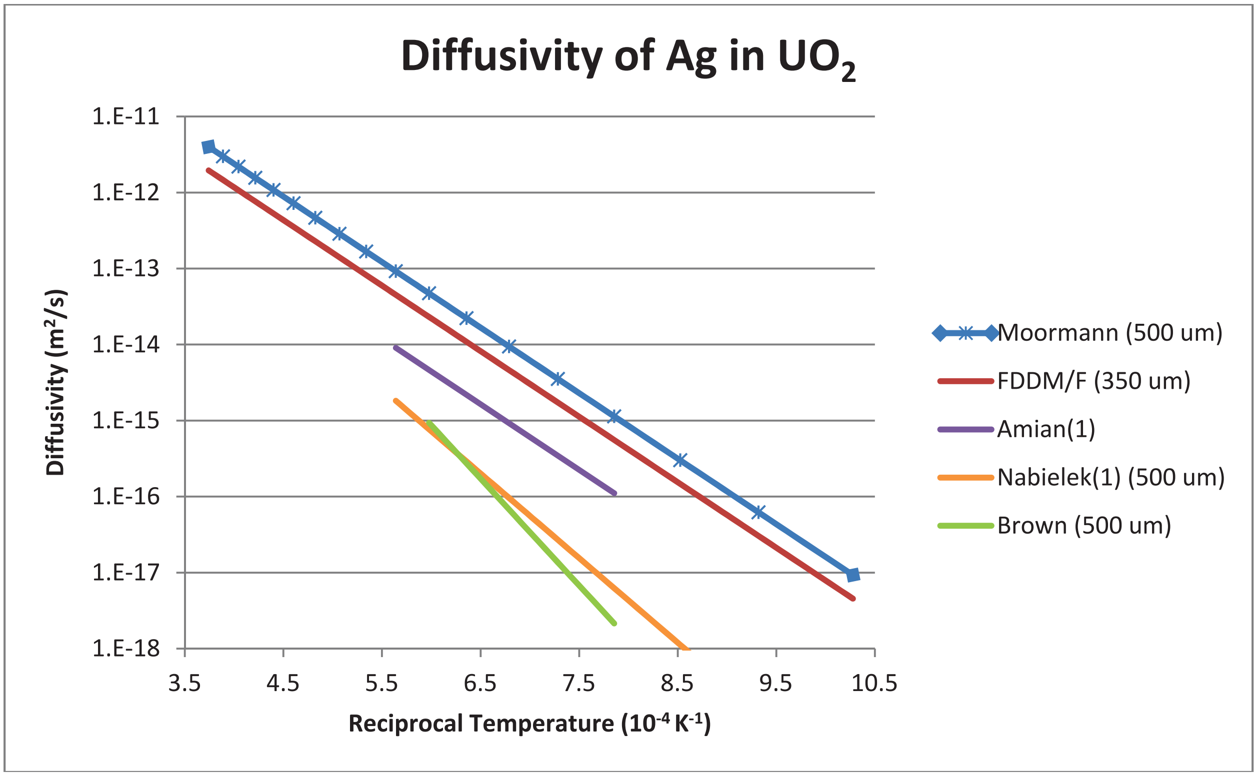
In addition to literature data, some plots include "prediction" curves obtained by applying the correction factors assessed by PARFUME to the diffusivities implemented in its source code. Because the comparison between PARFUME and AGR-1 data was made on several fuel compacts, it resulted in a range of correction factors for each fission product in each material (when deriving such correction factors was possible) from which minimum and maximum corrections, and subsequent minimum and maximum predictions, were calculated.

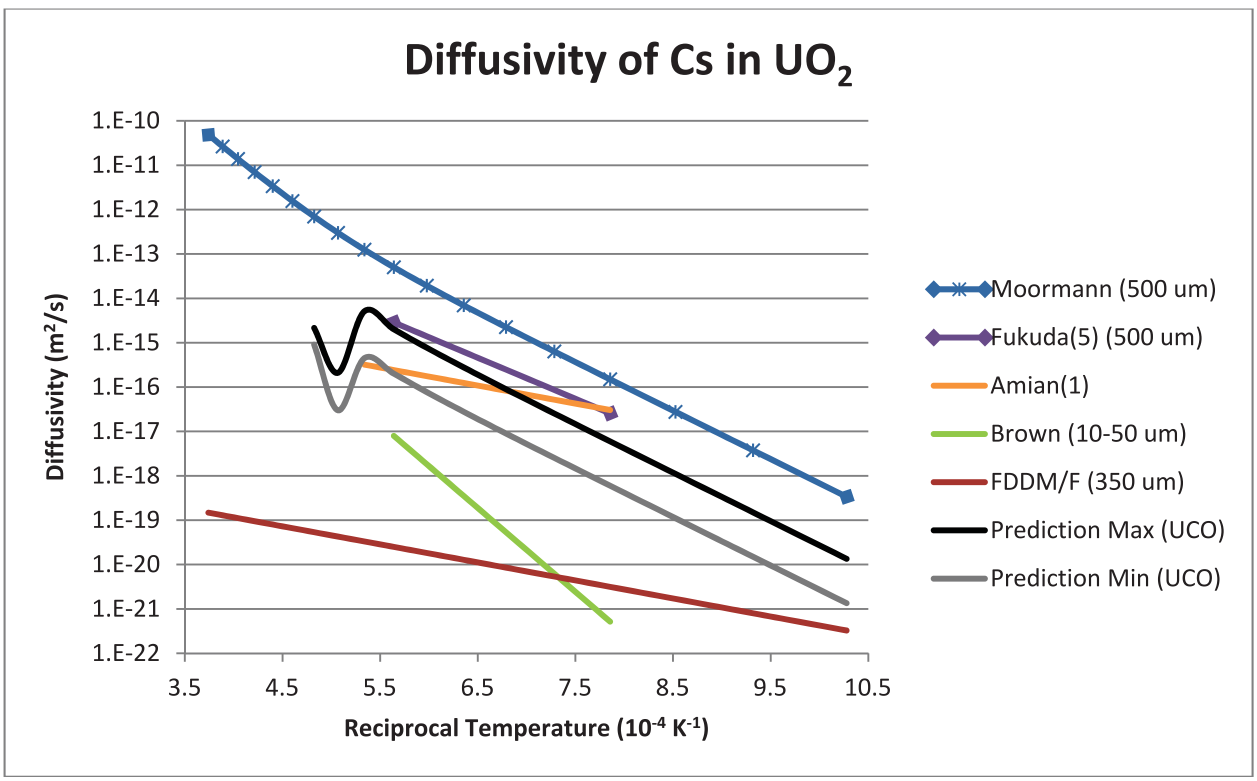
These "prediction" curves can apply to both the irradiation and safety testing phases (e.g. Cs in UO_2 or Cs in SiC) or to the safety testing phase only (e.g. Ag in SiC). For the irradiation phase, a correction factor consists of a constant and global value that applies to a range of temperatures obtained from the overlap of the applicability range of the IAEA recommendations and the range of irradiation temperatures of the AGR-1 experiment, i.e. 700 to1500°C. For safety testing temperatures, diffusivities have temperature-dependent correction factors, i.e. the correction factors are different at 1600, 1700, and 1800°C (reciprocal temperatures of 5.3, 5.1, and 4.8×10^{-4} K^{-1}, respectively). In some cases, this can result in "hooked" curves because the correction factor at 1700°C is proportionally small compared to the correction factors at the other two safety testing temperatures. This underlines the large inaccuracies associated with the determination of these correction factors that are also reflected in the wide spread between the minimum and maximum predictions at each safety testing temperature.

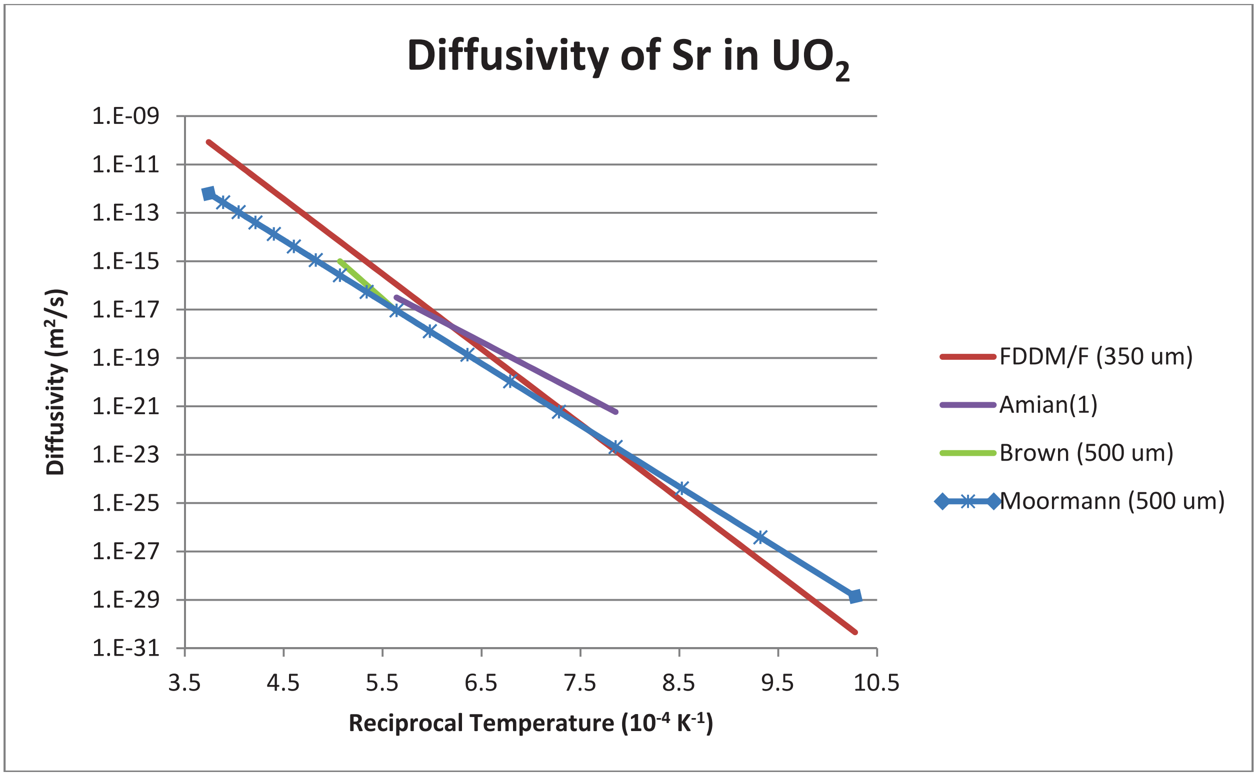
Appendix B

Diffusivities in Kernel

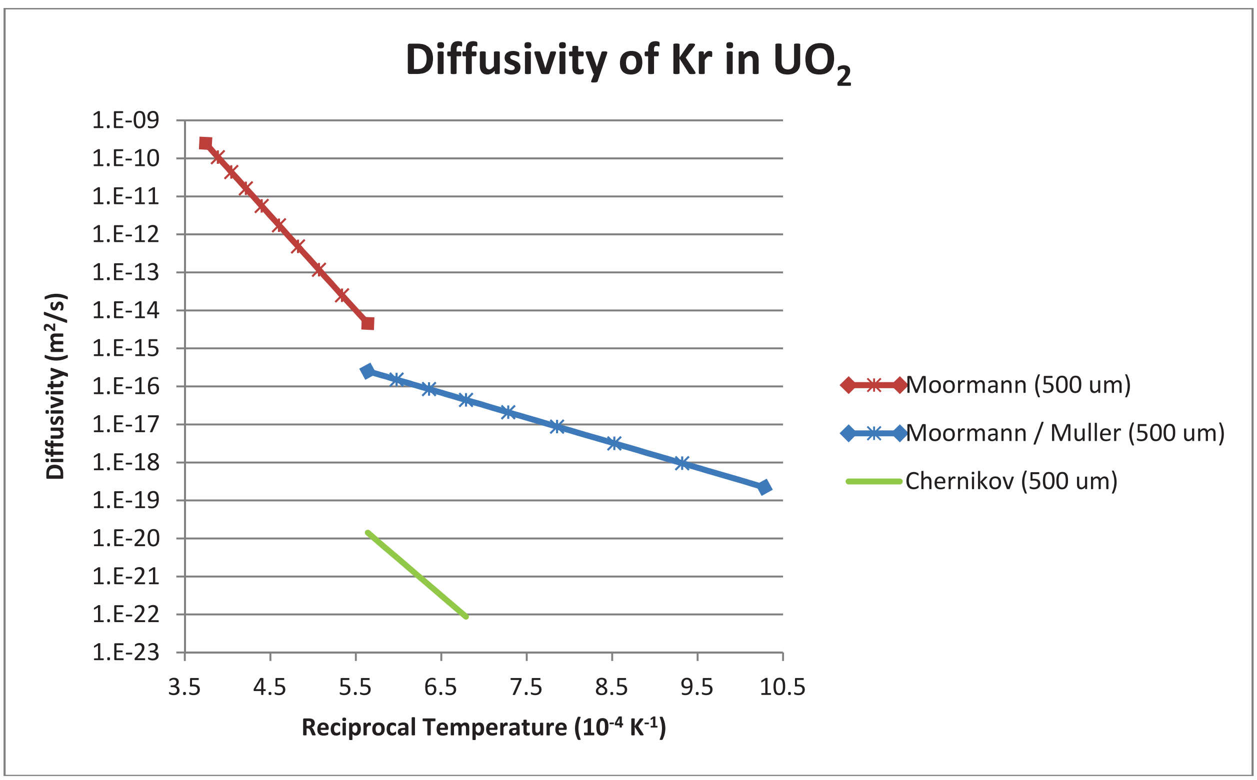
Appendix B
Diffusivities in Kernel







Diffusivity of Sr in UO_2
1.E-09
1.E-11
1.E-13
1.E-15
1.E-17
1.E-19
1.E-21
1.E-23
1.E-25
1.E-27
1.E-29
1.E-31
3.5
4.5
5.5
6.5
7.5
8.5
9.5
10.5
Diffusivity (m^2/s)
Reciprocal Temperature (10^{-4} K^{-1})
FDDM/F (350 um)
Amian(1)
Brown (500 um)
Moormann (500 um)

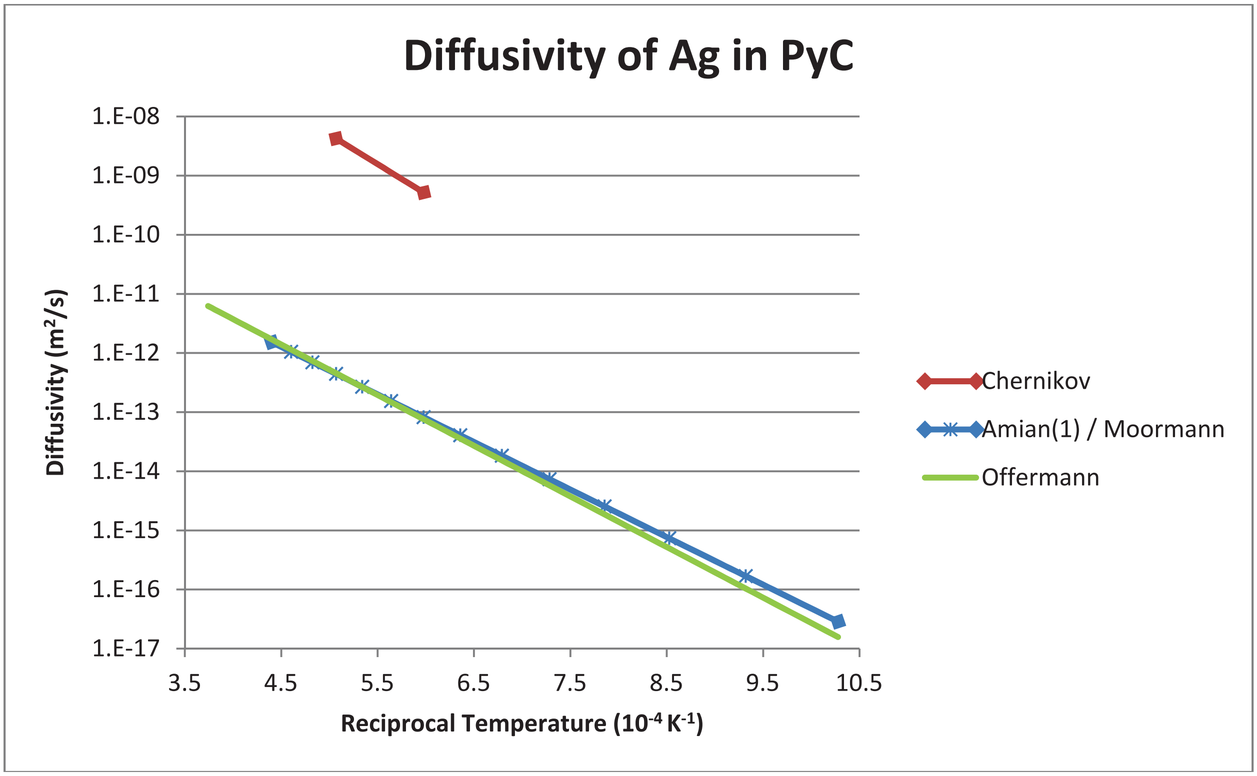


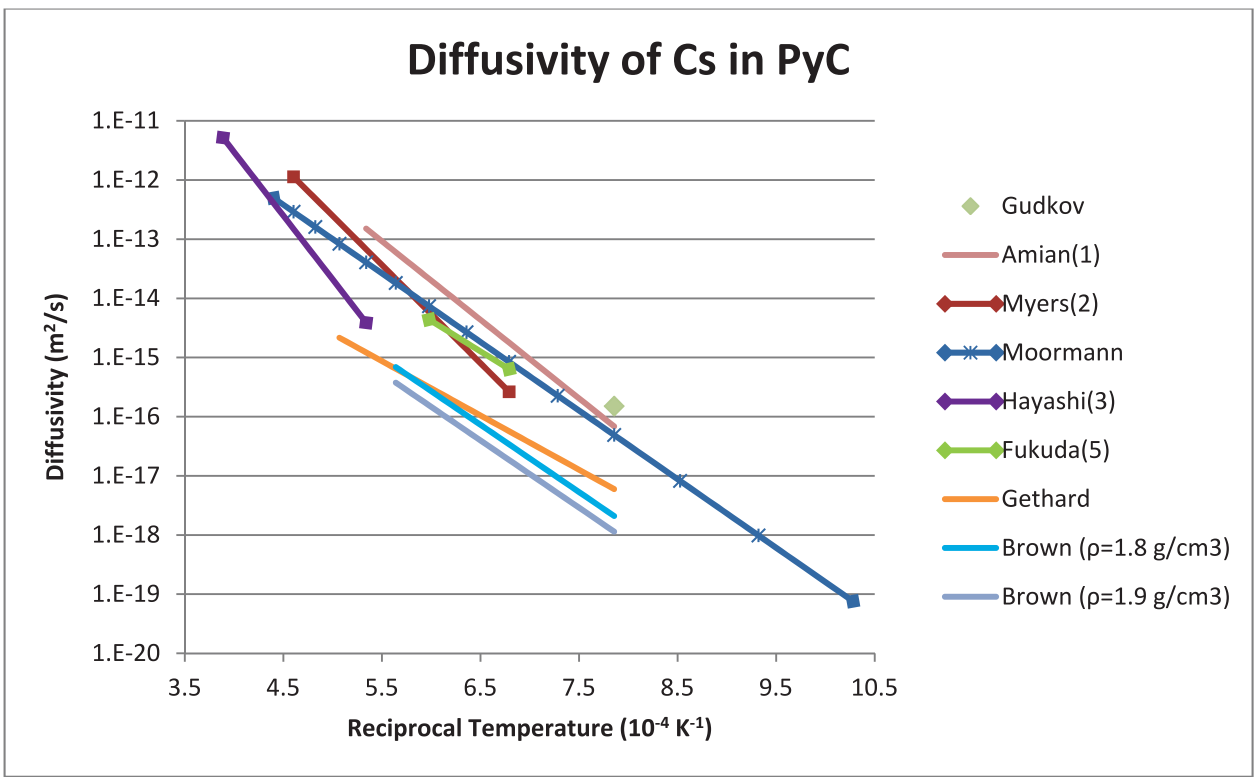
Diffusivity of Kr in UO_2
1.E-09
1.E-10
1.E-11
1.E-12
1.E-13
1.E-14
1.E-15
1.E-16
1.E-17
1.E-18
1.E-19
1.E-20
1.E-21
1.E-22
1.E-23
3.5
4.5
5.5
6.5
7.5
8.5
9.5
10.5
Diffusivity (m^2/s)
Reciprocal Temperature (10^{-4} K^{-1})
Moormann (500 um)
Moormann / Muller (500 um)
Chernikov (500 um)

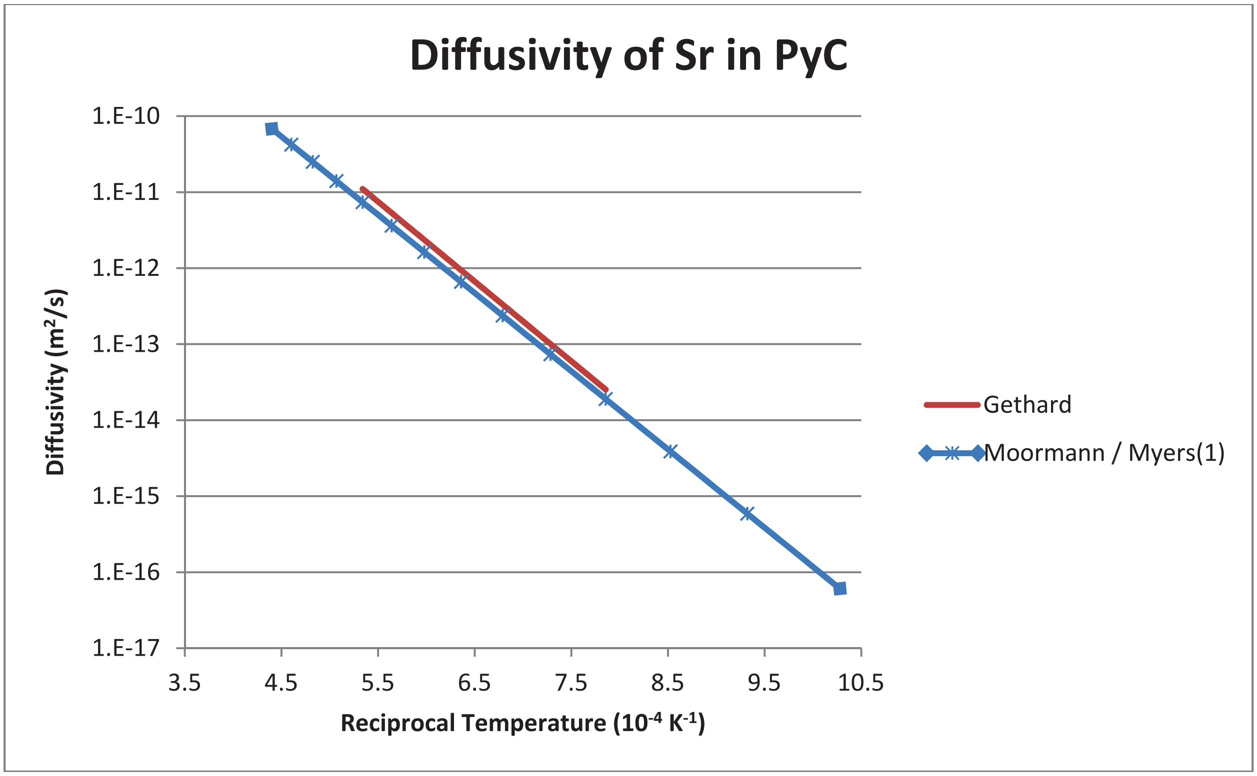
Appendix C

Diffusivities in PyC

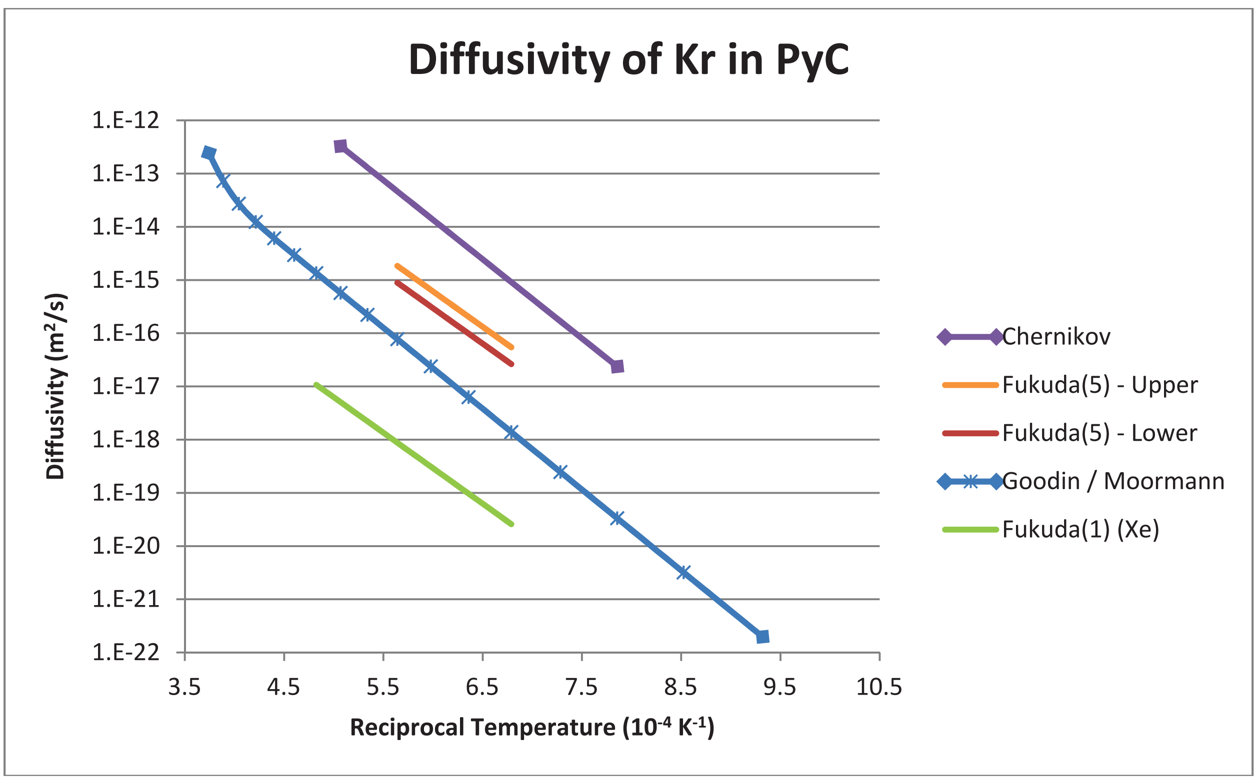
Appendix C
Diffusivities in PyC







Diffusivity of Sr in PyC
Diffusivity (m²/s)
1.E-10
1.E-11
1.E-12
1.E-13
1.E-14
1.E-15
1.E-16
1.E-17
3.5
4.5
5.5
6.5
7.5
8.5
9.5
10.5
Reciprocal Temperature (10⁻⁴ K⁻¹)
Gethard
Moormann / Myers(1)

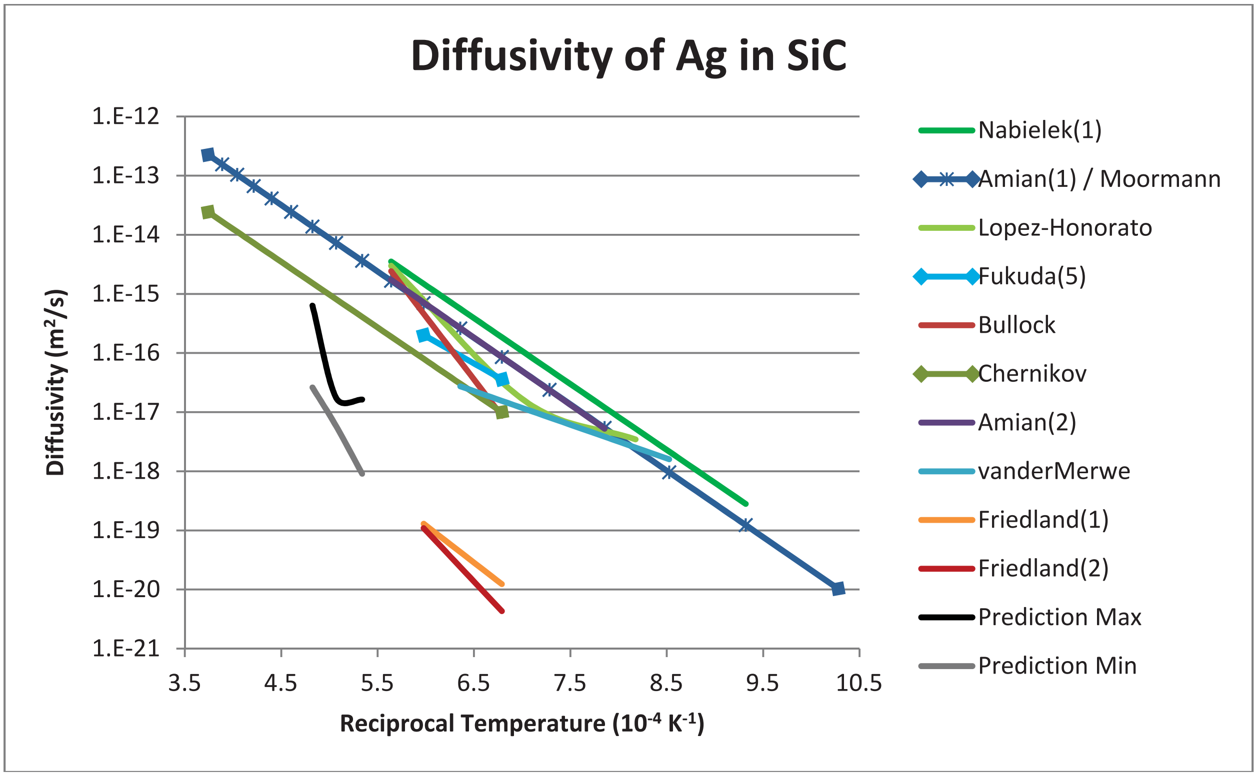


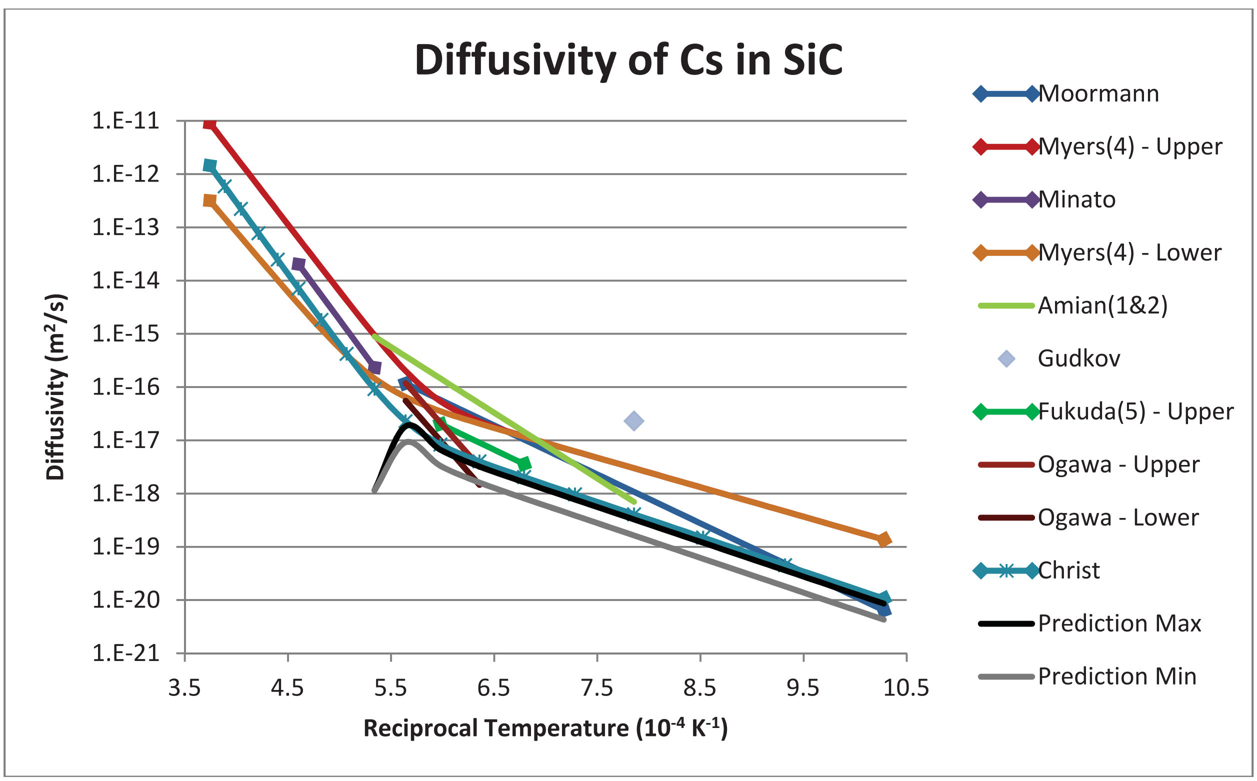
Diffusivity of Kr in PyC
Diffusivity (m²/s)
1.E-12
1.E-13
1.E-14
1.E-15
1.E-16
1.E-17
1.E-18
1.E-19
1.E-20
1.E-21
1.E-22
3.5
4.5
5.5
6.5
7.5
8.5
9.5
10.5
Reciprocal Temperature (10⁻⁴ K⁻¹)
Chernikov
Fukuda(5) - Upper
Fukuda(5) - Lower
Goodin / Moormann
Fukuda(1) (Xe)

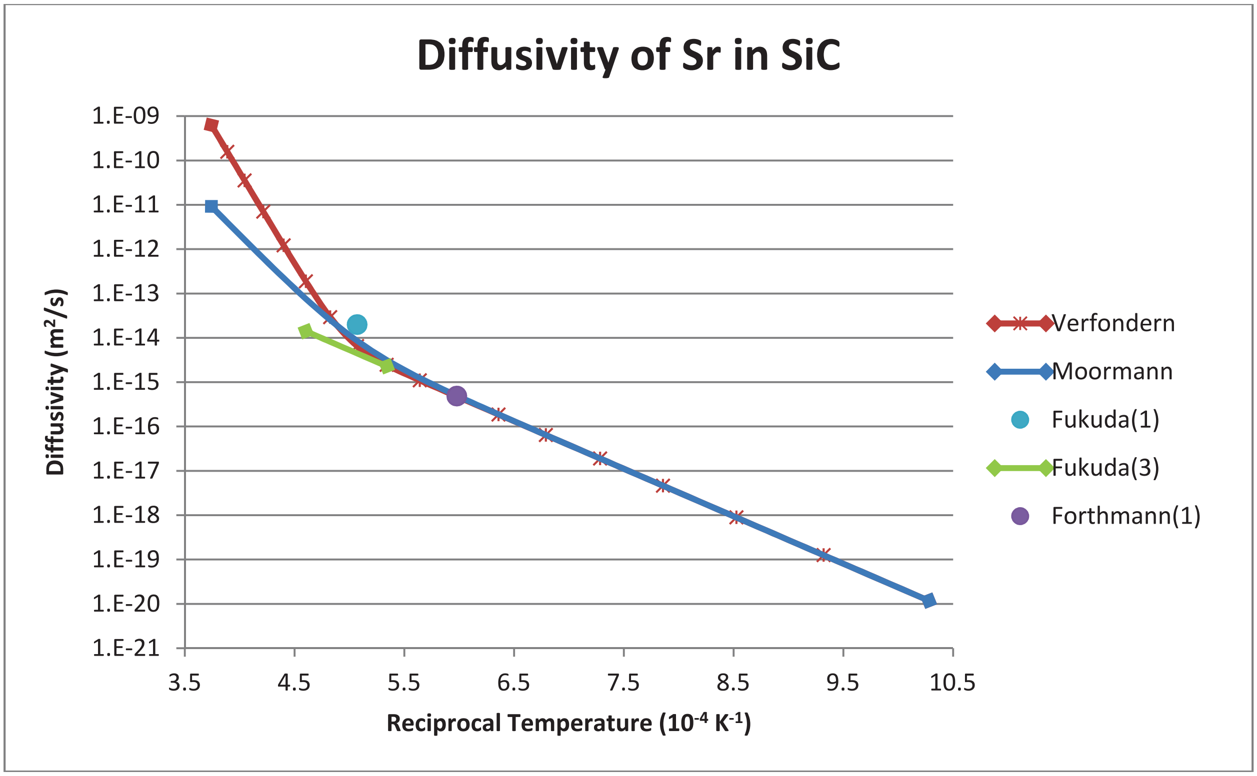
Appendix D

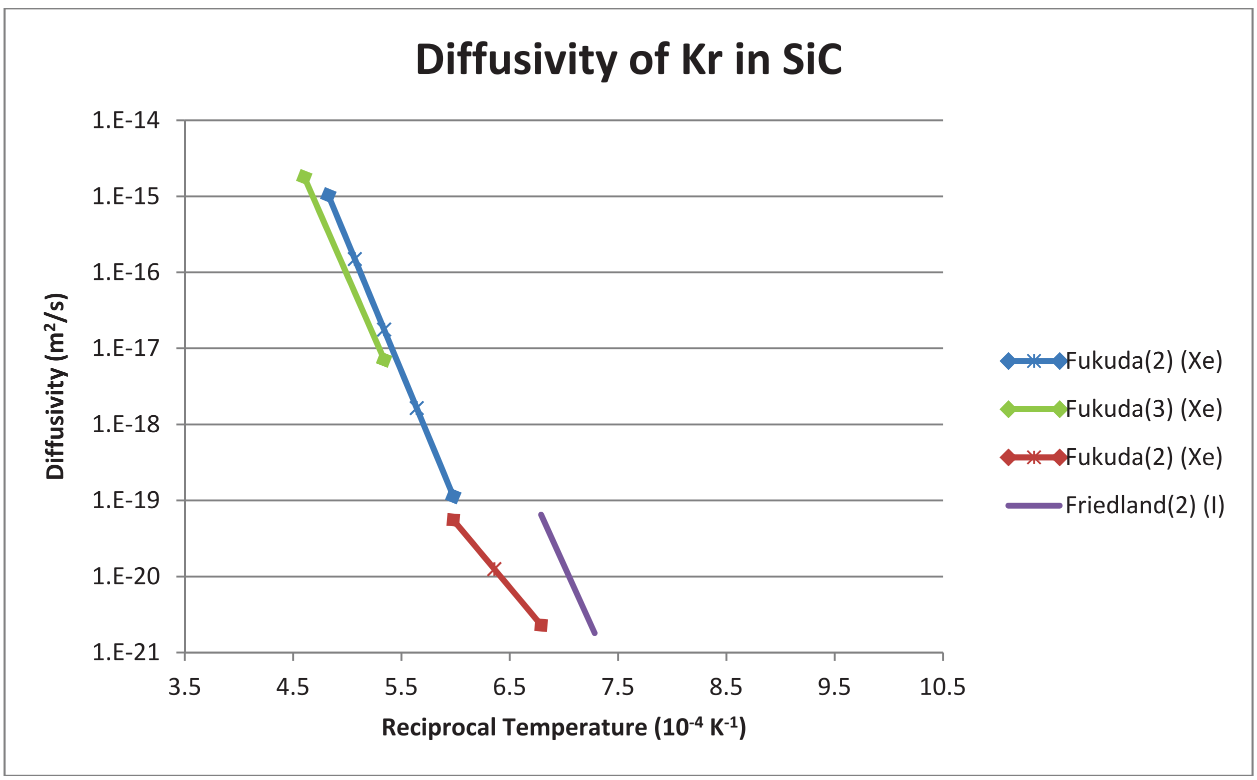
Diffusivities in SiC

Appendix D
Diffusivities in SiC





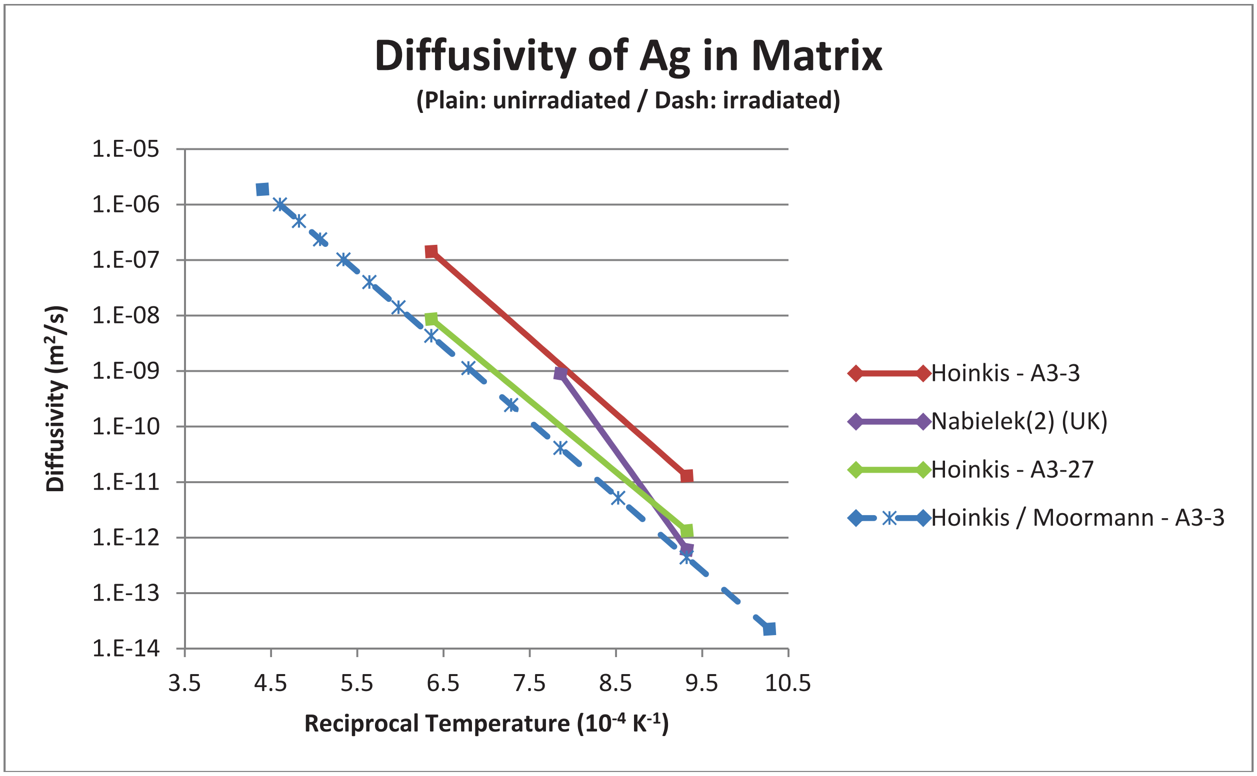

Diffusivity of Sr in SiC
Diffusivity (m²/s)
1.E-09
1.E-10
1.E-11
1.E-12
1.E-13
1.E-14
1.E-15
1.E-16
1.E-17
1.E-18
1.E-19
1.E-20
1.E-21
3.5
4.5
5.5
6.5
7.5
8.5
9.5
10.5
Reciprocal Temperature (10⁻⁴ K⁻¹)
Verfondern
Moormann
Fukuda(1)
Fukuda(3)
Forthmann(1)

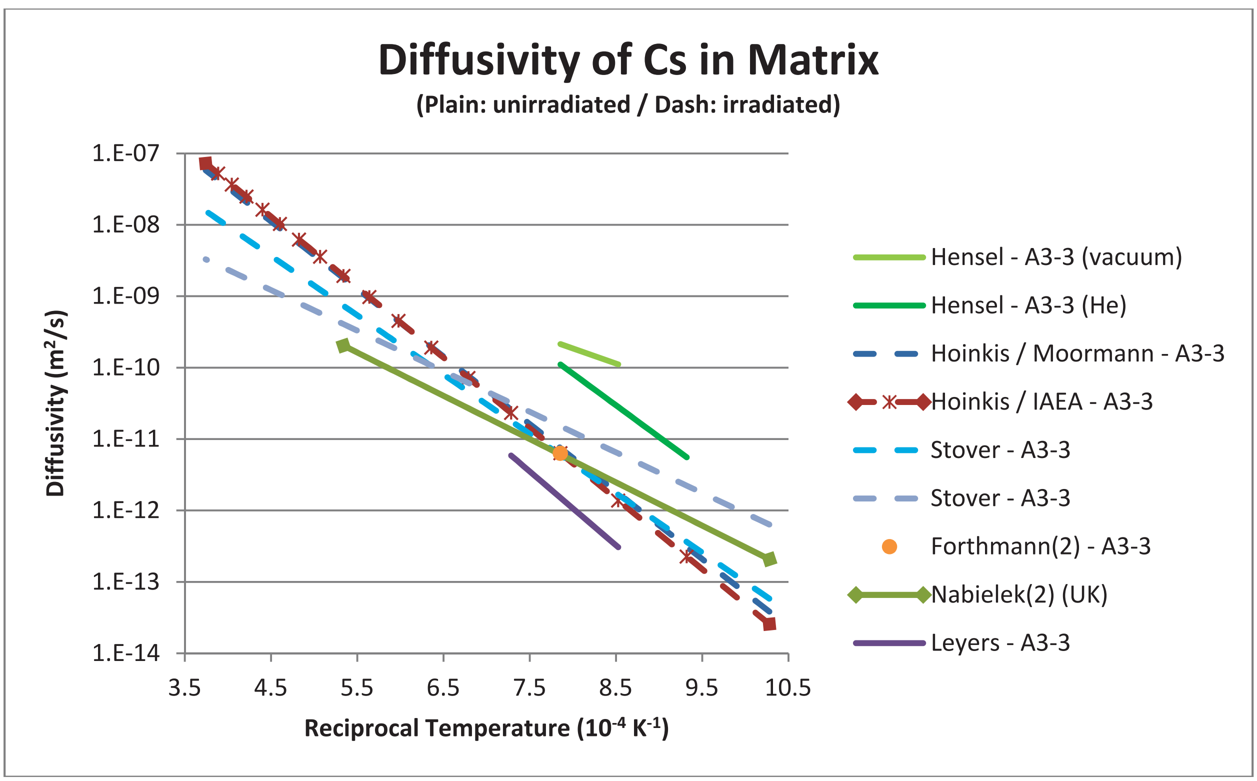

Diffusivity of Kr in SiC
Diffusivity (m²/s)
1.E-14
1.E-15
1.E-16
1.E-17
1.E-18
1.E-19
1.E-20
1.E-21
3.5
4.5
5.5
6.5
7.5
8.5
9.5
10.5
Reciprocal Temperature (10⁻⁴ K⁻¹)
Fukuda(2) (Xe)
Fukuda(3) (Xe)
Fukuda(2) (Xe)
Friedland(2) (I)

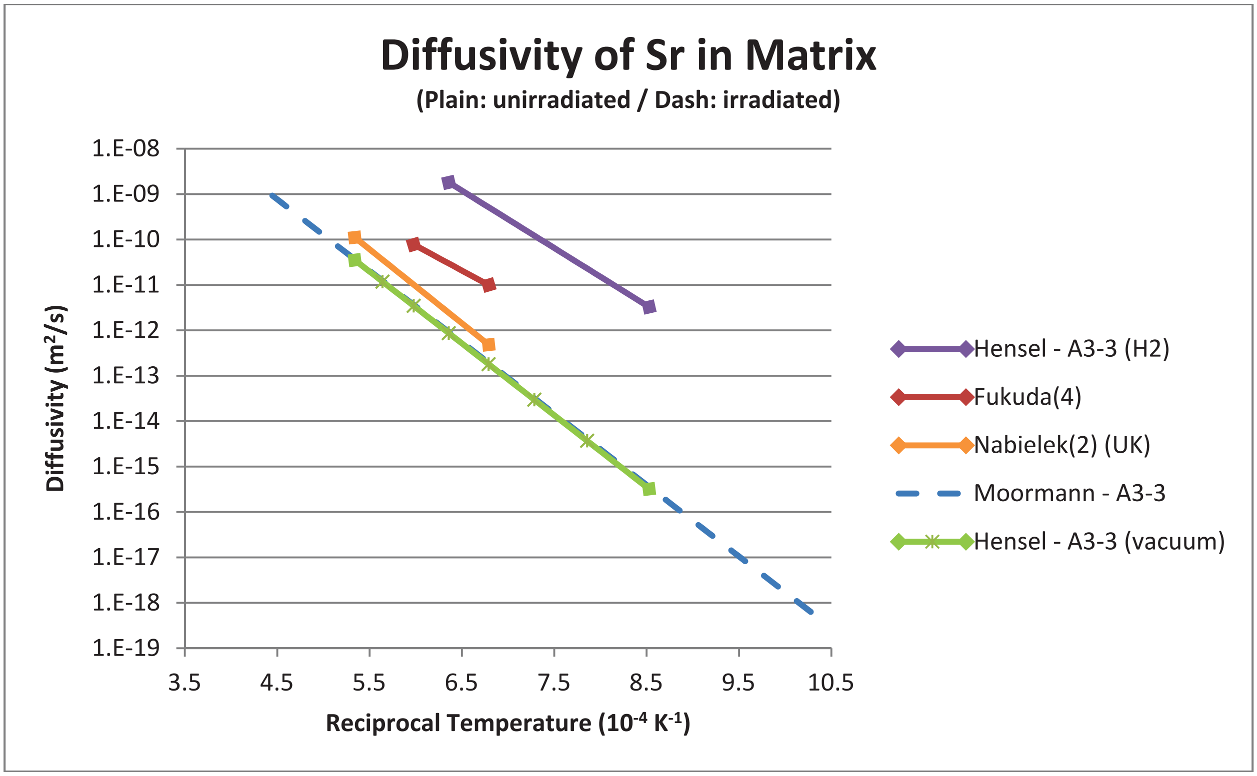
Appendix E

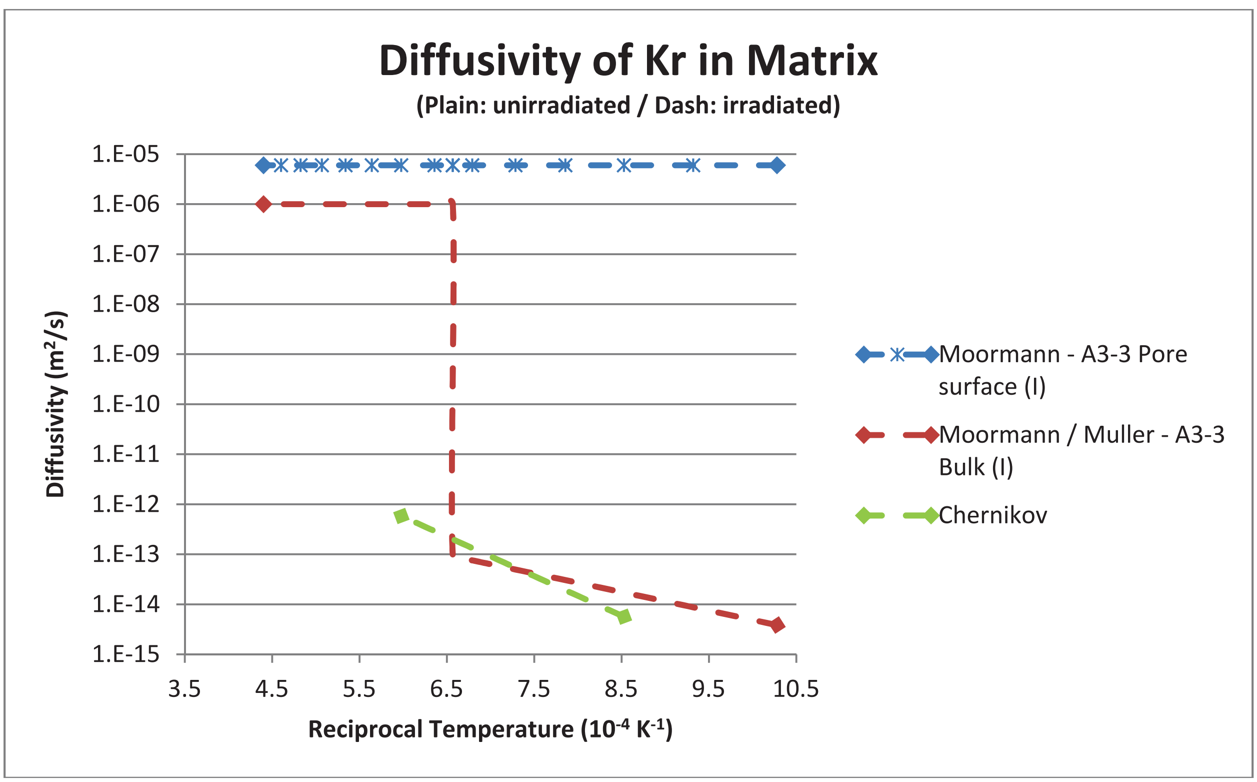
Diffusivities in graphite matrix

Appendix E
Diffusivities in graphite matrix





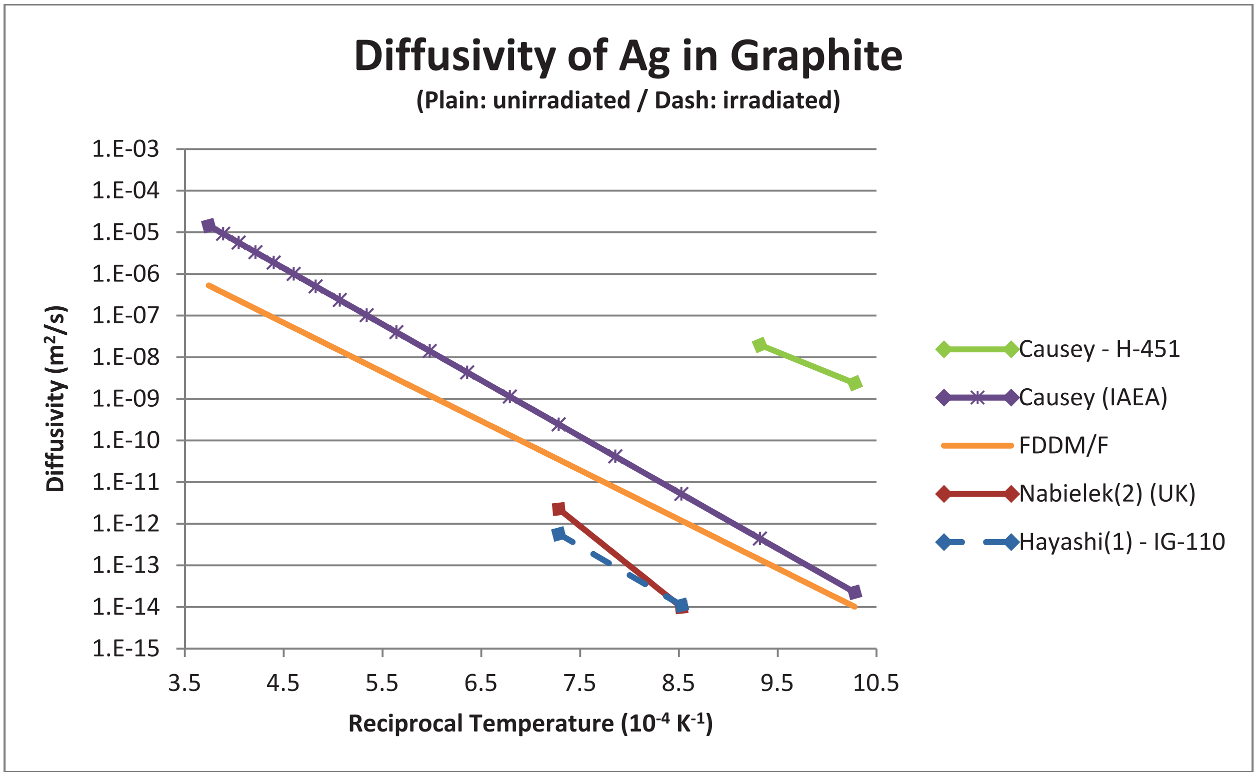

Diffusivity of Sr in Matrix
(Plain: unirradiated / Dash: irradiated)
Diffusivity (m²/s)
1.E-08
1.E-09
1.E-10
1.E-11
1.E-12
1.E-13
1.E-14
1.E-15
1.E-16
1.E-17
1.E-18
1.E-19
3.5
4.5
5.5
6.5
7.5
8.5
9.5
10.5
Reciprocal Temperature (10-4 K-1)
Hensel - A3-3 (H2)
Fukuda(4)
Nabielek(2) (UK)
Moormann - A3-3
Hensel - A3-3 (vacuum)

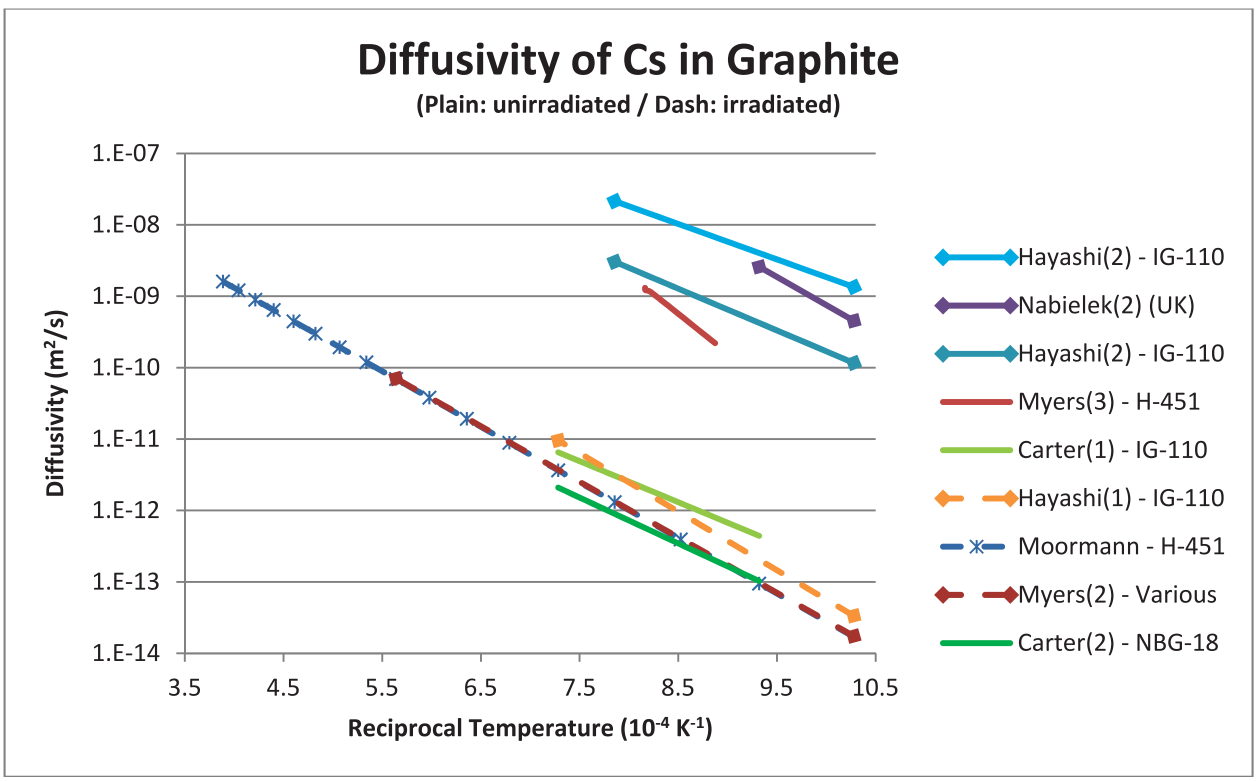

Diffusivity of Kr in Matrix
(Plain: unirradiated / Dash: irradiated)
Diffusivity (m²/s)
1.E-05
1.E-06
1.E-07
1.E-08
1.E-09
1.E-10
1.E-11
1.E-12
1.E-13
1.E-14
1.E-15
3.5
4.5
5.5
6.5
7.5
8.5
9.5
10.5
Reciprocal Temperature (10-4 K-1)
Moormann - A3-3 Pore surface (I)
Moormann / Muller - A3-3 Bulk (I)
Chernikov

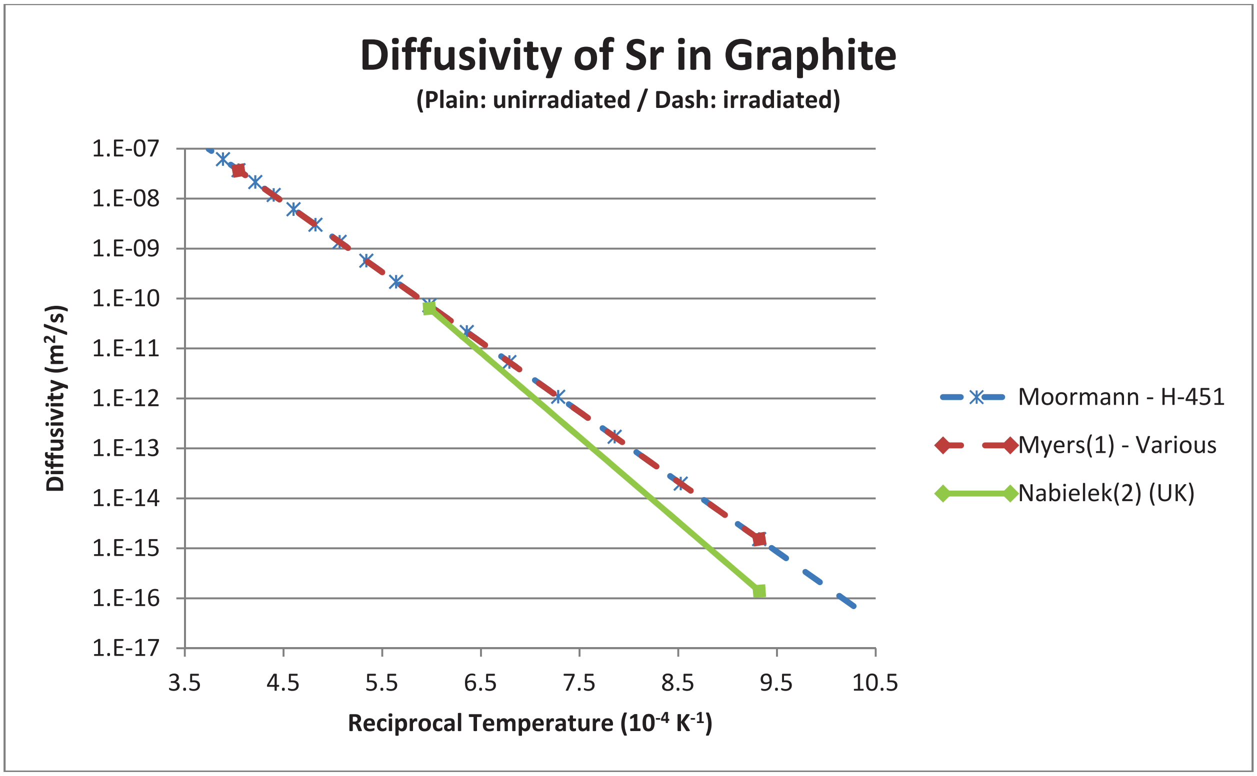
Appendix F

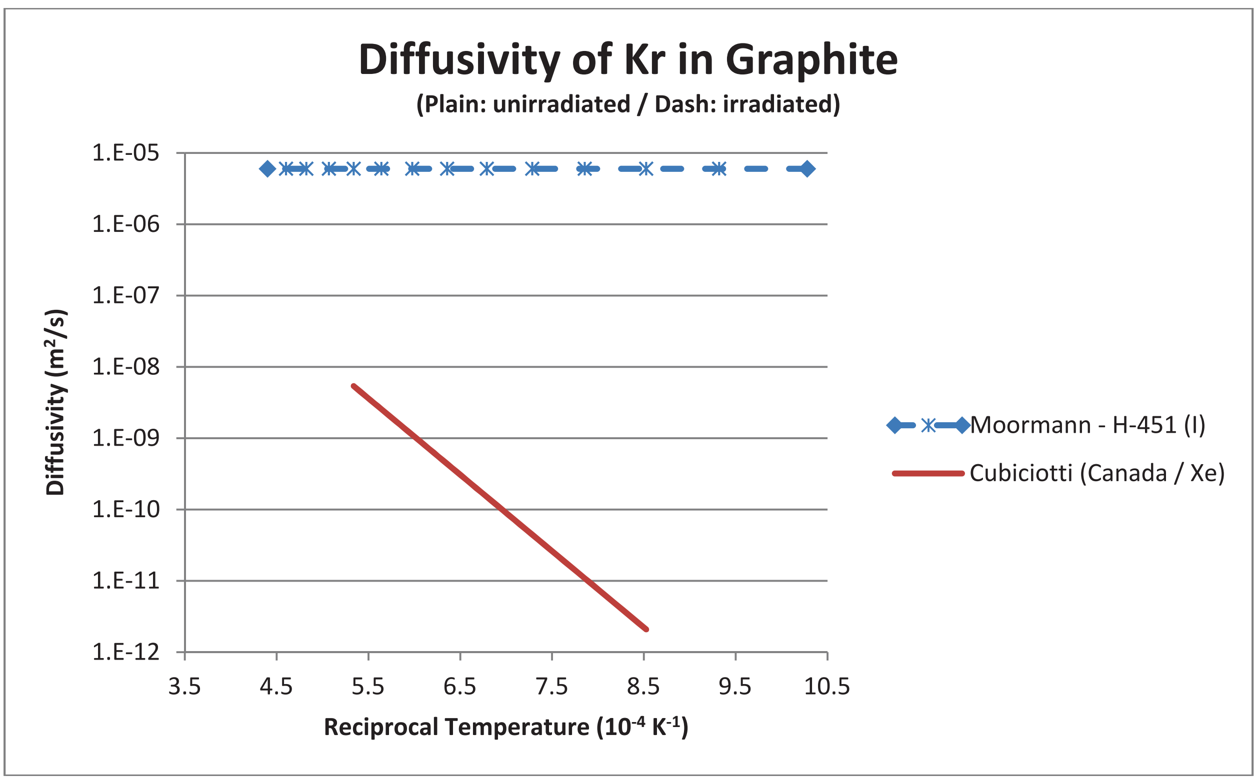
Diffusivities in structural graphite

Appendix F
Diffusivities in structural graphite






Diffusivity of Sr in Graphite
(Plain: unirradiated / Dash: irradiated)
Diffusivity (m²/s)
1.E-07
1.E-08
1.E-09
1.E-10
1.E-11
1.E-12
1.E-13
1.E-14
1.E-15
1.E-16
1.E-17
3.5
4.5
5.5
6.5
7.5
8.5
9.5
10.5
Reciprocal Temperature (10⁻⁴ K⁻¹)
Moormann - H-451
Myers(1) - Various
Nabielek(2) (UK)


Diffusivity of Kr in Graphite
(Plain: unirradiated / Dash: irradiated)
Diffusivity (m²/s)
1.E-05
1.E-06
1.E-07
1.E-08
1.E-09
1.E-10
1.E-11
1.E-12
3.5
4.5
5.5
6.5
7.5
8.5
9.5
10.5
Reciprocal Temperature (10⁻⁴ K⁻¹)
Moormann - H-451 (I)
Cubiciotti (Canada / Xe)