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Diffusion Rates in Inorganic Nuclear Materials

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The tracer diffusion coefficient, the self-diffusion coefficient, the intrinsic diffusion coefficient and the interdiffusion coefficient are briefly described. Grain boundary and lattice (volume) diffusion are contrasted. The frequency factors (D_0) and activation energies (Q) are tabulated for diffusion in the borides, carbides, and oxides of Be, Hf, Mo, Nb, Ta, Th, Ti, and Zr and for diffusion of C, N, and O in these metals. The purity of the solvent media, the preparation and properties of the samples, the method, the type of diffusion coefficient measured and the temperature range are also specified.

Key Words: Chemical interdiffusion, grain-boundary diffusion, intrinsic diffusion, lattice diffusion, self-diffusion, tracer diffusion.

1. Introduction

Since diffusion is often the rate controlling step in kinetic processes in solids—such as sintering, creep, precipitation, and corrosion—diffusion data have a necessary part in deciding the role of many metals and their compounds in high-temperature nuclear technology. Borides, carbides, nitrides, and oxides of plutonium and uranium, as well as the alloys of Pu and U with refractory metals, are potential high-temperature nuclear fuels. Refractory metals, such as Hf, Mo, Nb, Ta, Ti, and Zr also may be used as structural and cladding materials. Thorium compounds can be transmuted to ^{233}U-fuels in breeder reactors, and BeO can serve as a neutron moderator and reflector.

In this compilation diffusion data are presented for the borides, carbides, and oxides of Be, Hf, Mo, Nb, Ta, Th, Ti, and Zr. No diffusion data are available to date for the nitrides nor for plutonium compounds. A similar compilation of the very extensive data for uranium compounds is now in progress. Since corrosion of the metals by C, N, and O often proceeds by reactive diffusion, diffusion data for C, N, and O diffusion in the eight metals listed above have been included (data for B diffusion in these metals were not available).

2. Diffusion Coefficients

In general, a diffusion coefficient D is defined by Fick's first law as the constant which relates the flux of matter J to the concentration gradient causing the flow. The gradient usually is taken to be only in the x direction, thus

$$J = -D(\partial C/\partial x). \tag{1}$$

In the case of solids, three different diffusion coefficients—tracer diffusion (D_T), intrinsic diffusion (D_i) and chemical interdiffusion ($\tilde{D}$)—can be considered depending on the experimental conditions. The tracer and intrinsic diffusion coefficients apply to the diffusion of a single species; whereas the interdiffusion coefficient applies to the intermingling of species.

In the case of tracer diffusion, only a trace amount of species "i" diffuses into a homogeneous solid from a very thin layer at the surface of the sample. In the absence of any external force field and of the influence of other species, the i-atoms will diffuse in a random manner toward an equilibrium distribution due only to their own concentration gradient ($\partial C_i/\partial x$). If the tracer is the same as one of the elements of the solid matrix, D_T becomes the self-diffusion coefficient, D^*. The tracer and self-diffusion coefficients can be determined by a wide variety of techniques which are noted in the tables.

The intrinsic diffusion coefficient takes into account the atom flux resulting from (1) the redistribution described by D_T, (2) the effect of a nonideal and nonhomogeneous solid solution of "i," and (3) the influence of the driving forces of the other species on the diffusion of "i." When substituted into eq (1), D_i describes the flux of "i" with respect to a local lattice plane in a nonhomogeneous, nonideal, solid solution which is not subject to any external driving force. The driving forces in a nonideal, nonhomogeneous solid solution are the chemical potential gradients ($\partial \mu_i/\partial x$) of the various constituents of the material. The intrinsic diffusion coefficient generally is not measured experimentally, but it can be calculated if tracer diffusion coefficients of the species and the variation of the activity coefficient γ_i with respect to the mole fraction N_i of "i" are known.

If the rates of diffusion of different ionic species are not equalized by an internal potential gradient or by external forces, their interdiffusion will be accompanied by a net flow of imperfections. This flow of imperfections can be observed by inert marker techniques as a net movement of the lattice with respect to some fixed plane (e.g., the end of the sample). Thus, if the net flow of species is measured with respect to a fixed plane outside the diffusion zone, diffusion and the movement of the local lattice planes together will be measured. The chemical interdiffusion coefficient (or merely the "chemical diffusion coefficient") $\tilde{D}$ is obtained from eq (1) if the flux J in this equation is measured with respect to a fixed plane outside the diffusion zone. If it is assumed that $\tilde{D}$ is a function of the ratio $x/\sqrt{t}$, where t is time, $\tilde{D}$ can be determined by the classical method of Boltzmann [1][1] and Matano [2]. If there is no net flow of imperfections during diffusion, $\tilde{D}$ for interdiffusion in a binary system equals the intrinsic diffusion coefficients of the two species (D_{12} will be used in this case).

It should be emphasized that D_T can be determined only in a homogeneous solid. If the solid is nonhomogeneous, then $\tilde{D}$, and in some cases D_i, can be determined if the flux with respect to a fixed plane is known. These three diffusion coefficients apply to diffusion through the lattice.

In addition, diffusion can take place along grain boundaries. Grain-boundary diffusion of a tracer into a solid gives a nearly linear [3–6] decrease of $\ln C_i$ with penetration depth x, whereas $\ln C_i$ varies linearly with x^2 for lattice (volume) diffusion. The grain-boundary diffusion coefficient is represented in the tables by D_{gr}.

Diffusion coefficients for the borides, carbides, and oxides of Be, Ti, Zr, Hf, Nb, Ta, Mo, and Th have been measured generally for the cations and occasionally for the anions. The self-diffusion and tracer diffusion coefficients correspond empirically to the Arrhenius relation

$$D=D_0 \exp(-Q/RT) \tag{2}$$

where D_0 is the frequency factor, Q is the activation energy, R is the ideal gas constant and T is the absolute temperature. Although the chemical and intrinsic diffusion coefficients may be expressed in terms of eq (2), $\tilde{D}$ and D_i have a more complex temperature dependence.

3. Experimental Methods

In general, there are two modes of determining D. The direct method measures the distribution of concentration through the solid at a time t. The indirect method determines the diffusion coefficient by measuring a diffusion controlled phenomenon: attenuation of radioactivity, exchange of isotopes between a solid and a gas, release of anelastic strain, change of a physical property of the surface or the release of rare gases.

4. Reliability

Most of the diffusion values in the tables are "preliminary." That is, they are the only values presently available, and they will suffice for rough estimates of the behavior of materials in technological applications.

The immediate needs of technology have provided the rationale for including many of the diffusion values in this compilation. Since the ratios of two independent measurements of the diffusion coefficient can be as great as 10^6 (see Be diffusion in BeO, low temperatures) due primarily to differences in materials and experimental methods, caution is required in the use of diffusion values. To this end, diffusion values from more than one source have been tabulated when they have been available and auxiliary information and comments have been included in the tables.

To go beyond the rough estimate to the fundamental understanding of the properties of solids requires that a very exacting set of criteria be placed upon materials and methods. The solvent medium should be a very pure, well-characterized single crystal. In the case of chemical diffusion, the concentration dependence of the diffusion coefficient should be determined or the diffusion coefficient should be determined at given concentrations. Indirect determinations of D should be compared with direct determinations of D from chemical or isotopic concentration profiles. Measurements of a physical property related to the concentration do not establish the concentration profile unless the property's functional dependence on concentration is determined (e.g., the assumption of linearity is not sufficient). Diffusion anneals should be carried out above one-half the melting point temperature so that extrinsic diffusion is avoided, unless impurity effects are to be measured. These anneals must be carried out under thermodynamically specifiable conditions—temperatures and partial pressures must be known.

The scope of this compilation prevented a detailed use of these criteria in establishing the degree of reliability of each diffusion coefficient. Critical evaluations also were limited by the lack of first-hand experience with most of the experimental techniques, and by the absence of experimental details, of tabulated data and of careful error analyses in many of the original works. Nevertheless, some general comments can be made.

Much of the unreliability results from the specimens used, and high impurity concentrations are foremost among the causes. Impurity controlled diffusion rates (extrinsic diffusion) are to be expected when impurities with valences other than that of the diffusing species are present in concentrations greater than 100 ppm and when the annealing temperature is low with respect to the melting point. Diffusion coefficients measured under such conditions are strictly only characteristic of the specimen studied and are not "intrinsic" to the material.

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[1] Figures in brackets indicate the literature references at the end of this paper.

Several errors can arise from the use of polycrystalline materials. Grain boundaries and pores provide high diffusivity paths. Experimental observations of these effects and experiments in which these may have been a major factor have been noted in the tables. These high diffusivity paths probably contributed measureably to the observed rates in experiments carried out below 700 to 1000 °C, but it has not been possible to assess the magnitude of these contributions here. Grain orientation is important when the material has less than cubic symmetry because the diffusion coefficient is a second rank tensor and, therefore, depends on crystallographic direction.

Dislocations, subgrain boundaries and microcleavages due to surface damage are other sources of high diffusivity paths which can occur in both single and polycrystalline specimens. These sources of error have been overlooked by most investigators.

Diffusion coefficients from any experiments in which chemical concentration gradients were present, such as oxidation of metals, have been classed as chemical diffusion coefficients. Apparent agreement between such diffusion coefficients and self-diffusion coefficients should be considered fortuitous. Furthermore, when these diffusion coefficients have been obtained by assuming that they are independent of concentration, they are first order approximations for the overall diffusion zone in the specimen studied.

Experimental methods are the second area in which problems arise. Indirect measurements usually depend upon the change of a physical property which is assumed to depend on concentration. In some cases, notably anelastic strain measurements, such methods can be very reliable. However, indirect methods usually do not reveal the concentration dependence of the chemical diffusion coefficient nor the presence of high diffusivity paths.

In regard to both indirect and direct methods, the functional dependence of the measured property on concentration often has not been demonstrated and the influence of other factors has not been determined. Microhardness, for example, depends on microstructure, impurities, and preferred orientation of the grains as well as on chemical composition, and it is not necessarily a linear function of concentration. The absorption of beta radiation by a solid is generally more complex than a mere exponential function of distance. If the functional relationship only has been assumed, the reported diffusion coefficient should be considered a preliminary value.

Some other sources of unreliability which the user of the tables should determine from the original work if accuracy is very important are:

(1) temperature control and measurement;

(2) failure to satisfy the boundary conditions of the diffusion problem;

(3) change in the characteristics of the specimen during the diffusion anneal due to sintering, vaporization, annihilation or production of defects and reaction with components of the furnace; and

(4) hysteresis in the response of the measuring instrument.

5. Key to the Tables

Each table contains data for a metal and its borides, carbides, and oxides. The data in each table is ordered first according to the solvent medium, i.e., the matrix metal or compound. First the matrix metal is presented, followed in turn by the borides, the carbides and the oxides. For example, in the table for thorium, thorium metal occurs first followed by ThO_2 (there is no data for the borides and carbides).

The data for the diffusion in the metallic solvent medium is ordered alphabetically with respect to the diffusing element (C, N, or O). A further ordering with respect to the metallic phase is used if this distinction is important (e.g., C-diffusion in α-Ti precedes C-diffusion in β-Ti).

The compound solvent medium (e.g., oxides) is subdivided first with respect to the number of cations per molecule. For example, the niobium carbides have the following order: $NbC \rightarrow Nb_2C \rightarrow Nb_4C_3 \rightarrow$ mixed carbides. Each compound subdivision next is arranged alphabetically with respect to the diffusing element. The order for BeO is: $Be \rightarrow O \rightarrow T(^3H) \rightarrow Xe$.

In addition to specifying the solvent medium and diffusing element, each entry gives the purity of the solvent medium, the preparation and properties of the diffusion sample, the method used to measure the diffusion coefficient, the type of diffusion coefficient measured, the temperature range, the frequency factor (D_0) and the activation energy (Q), in cal/mol (1 cal = 4.184 J).

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Solvent medium	Diffusing element	Purity[a]	Preparation and properties	Method	Diffusion coefficient	Temperature range, °C	D_0 cm²/s	Q cal/mol	Comments	Ref.
BeO.......	Be[b]......	Al, 15; Fe, 200; Pb, 20; Si, 500.	Polycrystalline, cold-pressed and sintered, 96–98% of theoretical density.	Determination of the radioisotope distribution by sectioning.	D^* (self-diffusion).	1180–1800	2.49×10^{-3}	62,500	Grain-boundary diffusion was considered insignificant because grain size exceeded diffusion depth; impurity content was probably important.	[1]
BeO.......	Be.........	Al, 3000; Ca, 330; Fe < 25; Si < 77; Ti, 61; P < 500.	Polycrystalline, slip cast and sintered 92–93% of theoretical density.	Determination of the radioisotope distribution by sectioning.	D^* D^*	1550–1730 1730–1960	5.56×10^{-3} 6.14×10^{-2}	111,600 66,100	Variation in diffusion coefficient was primarily due to impurity content; scatter in data makes the actual magnitude of curvature uncertain. "Tailing" of concentration distribution curve in single crystal specimens (which is suggestive of grain boundary diffusion in polycrystalline samples) was ascribed to microcleavages due to grinding.	[2]
BeO.......	Be.........	Al < 160; Fe, 43; Si, 60; Ti, 33; P < 500.	Polycrystalline, hot-pressed, 99.3% of theoretical density.	Determination of the radioisotope distribution by sectioning.	D^* D^*	1550–1725 1725–2000	1.35 1.07×10^{-6}	92,000 36,000		[2]
BeO.......	Be.........	Mo micro-inclusions; all other impurities under 100.	Single crystal; grown in lithium molybdate flux.	Determination of the radioisotope distribution by sectioning.	D^* D^*	1500–1760 1720–1975	1.27×10^{-3} 1.23×10^{-6}	64,000 36,000		[2, 3]
BeO.......	O..........	Al, 3000; Ca, 330; Fe < 25; Si, < 77; Ti, 61; P < 500.	Polycrystalline, slip cast and sintered, 92–93% of theoretical density.	Heterogeneous isotopic exchange between a solid sample and a gas.	D^*	1600–1900	5.2×10^{-7}	42,900	Evidence of significant grain-boundary diffusion; the rates may also be affected by the impurity concentration.	[2, 4, 5]
BeO.......	O..........	Fe, 25; Li, 20; Mo, 1200; all others ≦ 10.	Single crystal; grown in a molybdate flux.	Heterogeneous isotopic exchange between a solid sample and a gas.	D^*	1300–1700	2.95×10^{-5}	68,500	Grain boundary effects were removed by use of single crystal.	[6]
BeO.......	T(^{3}H)......	Not stated.	Commerical BeO powder (Brush UOX).	Rate of fission gas release from irradiated powder, spherical particles were assumed.	D_T (tracer diffusion)	673–923	6.6×10^{-13}	24,500	T was assayed as T_2O, recovery as T_2O was quantitative. The very low values for both D_0 and Q are suggestive of significant grain boundary diffusion.	[7]
BeO.......	T..........	Not stated.	Commerical BeO powder (Brush Minox).	Rate of fission gas release from irradiated powder, spherical particles were assumed.	D_T	673–873	7.6×10^{-13}	24,000		[7]
BeO.......	T..........	Not stated.	Sintered compacts and powders were investigated; powder data was considered more reliable.	Rate of fission gas release from irradiated powder, spherical particles were assumed.	D_T	700–1000	0.131	70,000	Data indicated a lower activation energy below 700 °C; T was assayed as HT, a correction was required for the loss as HTO.	[8]
BeO.......	Xe.........	Samples were obtained from S. B. Austerman, Ref. 2, 3.	Pyramidal, single-crystals, were assumed to be spherical for calculation of D.	Hahn emanation technique, Xe recoiled into oxide when oxide was irradiated in contact with UO_2.	D_T	800–1500	3.0×10^{-6}	63,500		[9]

[a] Impurity concentrations are given in ppm unless otherwise stated.

[b] Note added in proof: Condit and Hashimoto [10] reported $D = (1 \times 20\, F_p) N_v [10 \times \exp(-62.0\ \mathrm{Kcal}/RT)]$ cm² s⁻¹ for Be diffusion in polycrystalline BeO in the temperature range between 1330 to 2135 °C. F_p is the fraction of porosity and N_v is the molar fraction of vacancies introduced by impurities.

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Hafnium

Solvent medium	Diffusing element	Purity [a]	Preparation and properties	Method	Diffusion coefficient	Temperature range, °C	D_0 cm²/s	Q cal/mol	Comments	Ref.
Hf.........	O.........	Zr < 100; O, 120; N, 16; C, 37.	Zone-refined; oxide layer formed by anodization.	Time rate of change of interference color (i.e., thickness) of oxide film on metal due to solution of film in metal.	$\tilde{D}$ (chemical diffusion).	500–1050	0.660	50,820	$\tilde{D}$ assumed to be independent of concentration.	[1]
Hf..........	O.........	Zr, 1.0 w/o; Al, 1100; Fe, 450; Cu, 60; Cr, 800; Mg, 50; Ti, 300; Ni, 60; all others < 50.	Hot-rolled and annealed at 800° C; machined and polished; oxidized in air.	Determination of concentration gradient by microhardness measurements.	D	700–1200	1.6	49,300	Assumption of linear relationship between oxygen concentration and hardness probably was not justified, according to [4] the relationship is parabolic; nitrogen gradient was superimposed on oxygen gradient.	[2]
$Hf_{0.86}$—..... $Ca_{0.14}$—..... $O_{1.86}$	O.........	Fe_2O_3, 0.012–0.1%; Al_2O_3, 0.012–0.1%; TiO_2, 0.01-0.2%; ZrO_2, 2.5-3%; Nb_2O_5, 0.05–0.1% (weight percent).	Tube closed at one end; density 9.51 g/cm³; porosity ~ 5%.	Determination of the rate of permeation of O_2 through walls of stabilized hafnia tube.	$\tilde{D}$	1100–1600	22	55,700	A large drop in partial pressure between the inside and outside of the tube caused a large chemical potential gradient.	[3]

[a] Impurity concentrations are given in ppm unless otherwise stated.

[1] J. P. Pemsler, J. Electrochem. Soc. **111**, 1185 (1964); J. Electrochem. Soc. **106**, 1067 (1959).
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Molybdenum

Solvent medium	Diffusing element	Purity [a]	Preparation and properties	Method	Diffusion coefficient	Temperature range, °C	D_0 cm²/s	Q cal/mol	Comments	Ref.
Mo_2B.......	B..........	Not stated.	Boride layer was formed on a Mo cylinder by boronizing in boron carbide and borax.	Determination of the concentration gradient by microhardness measurements.	$\tilde{D}$ (chemical diffusion)	1100–1400	0.0696	45,000	$\tilde{D}$ was assumed to be independent of concentration; absence of a homogeneity range [2] was probably a major source of error.	[1]
Mo_2C.......	C..........	Not stated.	Carbide layer was formed on a Mo cylinder by carburizing in graphite.	Determination of the concentration gradient by microhardness measurements.	$\tilde{D}$	1400–1700	1,640	83,000	$\tilde{D}$ was assumed to be independent of concentration; narrow homogeneity range [3].	[1]

[a] Impurity concentrations are given in ppm unless otherwise stated.

[1] G. V. Samsonov and A. P. Epik, Dopovidi Akad. Nauk Ukr. RSR [1], 67 (1964).
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[3] ibid., p. 370.

Niobium

Solvent medium	Diffusing element	Purity [a]	Preparation and properties	Method	Diffusion coefficient	Temperature range, °C	D_0 cm²/s	Q cal/mol	Comments	Ref.
Nb.........	C..........	Not stated.	Not stated.	Measurement of anelastic strain by elastic aftereffect and by internal friction.	D_T (tracer diffusion)	55–160	0.015	27,000	Effects of possible interstitial impurity (C, N, O) interactions were not ascertained.	[1]
Nb.........	C..........	Nb, 99.4 w/o; C, 1000 (max.); Ta, 5000; Ti, 400; Si, 200; Fe, 100. Degassed to reduce O and N damping peaks.	Carbon introduced by pyrolysis of hydrocarbons, and in a few samples by heating wires coated with graphite-water slurry.	Measurement of anelastic strain by elastic aftereffect and by internal friction.	D_T	140–275	0.004	33,020	Effects of interestitial impurity interactions were determined; carbide precipitation was observed at "high" C concentrations.	[2, 3]

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[a] Impurity concentrations are given in ppm unless otherwise stated.

Solvent medium	Diffusing element	Purity[a]	Preparation and properties	Method	Diffusion coefficient	Temperature range, °C	D_0 cm²/s	Q cal/mol	Comments	Ref.
Nb	C	Nb, 99.01 w/o; Ta, 0.94 w/o; O, 400; Ti, Fe, Si and C not detected.	Porosity of metal ~ 13%; ^{14}C labeled emulsion pyrolyzed on specimen, specimens were cleaved and were fastened together in pairs along active faces.	Measurement of attenuation of β-radiation by the method of Gruzin [5] (ratio of activities).	D_T	900–1100	1.09×10^{-5}	32,000	High diffusivity paths probably existed along pores.	[4]
Nb	N	Nb, 99.4 w/o; C, 1000 (max.); Ta, 5000; Ti, 400; Si, 200; Fe, 100. Degassed to remove O and N initially.	N added by absorption of molecular nitrogen or NH_3.	Measurement of anelastic strain by elastic aftereffect and by internal friction.	D_T	150–290	8.6×10^{-3}	34,920	Effects of interstitial impurity interactions were determined.	[2, 3]
Nb	N	Not stated.	N introduced by heating a wire in NH_3, followed by a brief vacuum anneal.	Measurement of anelastic strain by elastic aftereffect.	D_T	285–310	0.098	38,600	Effects of possible interstitial impurity interactions were not ascertained.	[6]
Nb	N	Nb, 99.9 w/o	Nb foil; N introduced by annealing in air.	Measurement of anelastic strain by internal friction.	D_T	563–644		28,100	Effects of possible interstitial impurity interactions were not ascertained.	[7]
Nb	O	Nb, 99.4 w/o; C, 1000 (max.); Ta, 5000; Ti, 400; Si, 200; Fe, 100. Degassed to remove O and N initially.	O introduced by absorption of molecular oxygen.	Measurement of anelastic strain by elastic aftereffect and by internal friction.	D_T	44–150	0.0212	29,910	Effect of interstitial impurity interactions were determined.	[2]
Nb	O	Not stated.	Not stated.	Measurement of anelastic strain by elastic aftereffect.	D_T	148–168	0.0147	27,600	Effects of possible interstitial impurity interactions were not ascertained.	[6]
Nb	O	Nb, 99.9 w/o	Nb foil; O introduced by annealing in air.	Measurement of anelastic strain by internal friction.	D_T	377–423		22,000	Effects of possible interstitial impurity interactions were not ascertained.	[7]
Nb	O	O, 1000; N, 500; C, 300.	Nb cylinders machined from arcmelted buttons; reacted with O_2 in modified Sieverts apparatus; O_2 from decomposition of permanganate.	Determination of the concentration gradient by microhardness measurements.	$\tilde{D}$	600–1000	4.07×10^{-3}	24,900	The following were assumed: (a) $\tilde{D}$ independent of concentration, (b) Nb-Nb oxide boundary stationary.	[8]
NbB_2	B	Not stated.	Boride layer was formed on a Nb cylinder by boronizing in boron carbide and borax.	Determination of the concentration gradient by microhardness measurements.	$\tilde{D}$	1100–1400	2.94	59,000	$\tilde{D}$ was assumed to be independent of the B concentration.	[9]
NbC	C	Not stated.	Niobium sheets heated in presence of CH_4-Ar atmosphere.	Rate of carbide layer growth measured with filar micrometer.	$\tilde{D}$	1900–2300	1.2	79,000	The results represent average values for $\tilde{D}$ over the composition range. $\tilde{D}$ was assumed to be independent of concentration. The boundary compositions of the carbide layer were taken from phase equilibrium diagrams [11].	[10]
NbC	C	Nb slab; W, 290; Fe < 100; C, 100; Si, 50; W, 110; Ta, 600; Zr < 100.	Niobium slabs packed in high-purity lampblack and heated.	Rate of carbide layer growth; movement of inert markers (holes) in diffusion regions of bonded graphite and Nb slabs.	$\tilde{D}$	1700–2300	7.6	88,200	Nb was found to be immobile as compared to C. $\tilde{D}$ was assumed to be independent of concentration. X-ray data indicated higher diffusion rates in the more carbon deficient region of the NbC layer.	[12, 13]

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[a] Impurity concentrations are given in ppm unless otherwise stated.

Solvent medium	Diffusing element	Purity[a]	Preparation and properties	Method	Diffusion coefficient	Temperature range, °C	D_0 cm²/s	Q cal/mol	Comments	Ref.
$NbC_{0.98}$.....	C...........	Not stated.	Nb carbides were synthesized from Nb_2O_5.	Measurement of attenuation of β-radiation by the method of Gruzin [5] (ratio of activities).	D^* (self-diffusion)	1600–2000	1.0×10^{-6}	32,300	High diffusivity paths probably existed along pores.	[4]
$NbC_{0.98}$.....	Nb.........	Not stated.	Nb carbides were synthesized from Nb_2O_5.	Measurement of attenuation of β-radiation by the method of Gruzin [5] (ratio of activities).	D^*	1800–2200	5.5×10^{-6}	55,000	High diffusivity paths probably existed along pores.	[4]
Nb_2C........	C...........	Not stated.	Nb carbides were synthesized from Nb_2O_5.	Measurement of attenuation of β-radiation by the method of Gruzin [5] (ratio of activities).	D^*	1600–2000	5.7×10^{-6}	29,800	High diffusivity paths probably existed along pores.	[4]
Nb_4C_3......	C...........	Not stated.	Nb carbides were synthesized from Nb_2O_5.	Measurement of attenuation of β-radiation by the method of Gruzin [5] (ratio of activities).	D^*	1600–2000	8.8×10^{-6}	35,300	High diffusivity paths probably existed along pores.	[4]
NbC:TiC...	Nb.........	Starting materials: TiO_2 99.7 w/o; Nb 98 w/o; lamp black with 4 w/o ash residue.	TiO_2-Nb mixture carbidized with lamp black in graphite furnace, carbide powder pressed and sintered; density 6.55 g/cm³; grain size 20–30 μm.	Measurement of attenuation of β-radiation by the method of Zhukhovitskii and Geodakyan [15] (nonexponential absorption).	D^*	2170–2280	470	120,000		[14]
$Nb_2O_{4.978}$ ..	O...........	Ta_2O_5, 0.01 w/o; SiO_2, 0.02 w/o; TiO_2, 0.005 w/o; Fe_2O_3, 0.003 w/o.	Hot-pressed anion-deficient oxide slabs, density of 4.55 g/cm³.	Microphotometric determination of the color change associated with the advance of an "oxygen-rich" front into an oxygen deficient oxide slab.	$\tilde{D}$	500–900	0.038	28,200	$\tilde{D}$ was measured for the particular oxide composition given.	[16]
Nb_2O_5 + 1 m/o ZrO_2.	O	Impurity content of Nb_2O_5 same as given above.	Hot-pressed anion-deficient oxide slabs, densities varied between 4.52 and 4.55 g/cm³.	Microphotometric determination of the color change associated with the advance of an "oxygen-rich" front into an oxygen-deficient oxide slab.	$\tilde{D}$	500–900	0.00201	24,000		[16]
Nb_2O_5 + 1 m/o TiO_2.	O...........	Impurity content of Nb_2O_5 same as given above.	Hot-pressed anion-deficient oxide slabs, densities varied between 4.52 and 4.55 g/cm³.	Microphotometric determination of the color change associated with the advance of an "oxygen-rich" front into an oxygen-deficient oxide slab.	$\tilde{D}$	500–900	0.0262	30,700		[16]
Nb_2O_5 + 1 m/o. V_2O_5.	O...........	Impurity content of Nb_2O_5 same as given above.	Hot-pressed anion-deficient oxide slabs, densities varied between 4.52 and 4.55 g/cm³.	Microphotometric determination of the color change associated with the advance of an "oxygen-rich" front into an oxygen-deficient oxide slab.	$\tilde{D}$	500–900	0.0432	32,400		[16]

[a] Impurity concentrations are given in ppm unless otherwise stated.

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Tantalum

Solvent medium	Diffusing element	Purity [a]	Preparation and properties	Method	Diffusion coefficient	Temperature range, °C	D_0 cm²/s	Q cal/mol	Comments	Ref.
Ta	C	Not stated.	Not stated.	Measurement of anelastic strain by after-effect and by internal friction.	D_T (tracer diffusion)	55–160	0.015	27,000	Effects of possible interstitial impurity (C, N, O) interactions were not ascertained.	[1]
Ta	C	Metallic contaminants not stated; 99.9 w/o Ta; C, 100–900.	C was added to a degassed wire by pyrolysis of carbonaceous vapor or by heating a wire coated with a carbon black-water slurry.	Measurement of anelastic strain by elastic after-effect and by internal friction.	D_T	193–350	6.1×10^{-3}	38,510	Effects of interstitial impurity interactions were determined; carbide precipitation was observed at "high" C concentrations.	[2]
Ta	C	C, 1000.	^{14}C was introduced into about 10 mm center portion of a 70 mm Ta wire.	Determination of the concentration gradient by radioisotope distribution.	D_T	600–2600	2.78×10^{-3}	24,600	An increase in the activation energy was observed below 800 °C.	[3]
Ta	N	Metallic contaminants not stated; 99.9 w/o Ta; O, 320; N, 50–1000.	Degassed wire was enriched in N by heating in N_2 or NH_3 at low partial pressure.	Measurement of anelastic strain by elastic after-effect and by internal friction.	D_T	187–350	5.6×10^{-3}	37,840	Effects of interstitial impurity were determined.	[2]
Ta	N	Not stated.	N introduced by heating a wire in NH_3, followed by a brief vacuum anneal.	Measurement of anelastic strain by elastic after-effect and by internal friction.	D_T	360–662	0.0123	39,800	Effects of possible interstitial impurity interactions were not ascertained.	[4]
Ta	N	C, 60; N < 20; W, 1000; Cu < 40; Fe < 50; Si < 100; Ti < 50; Mo < 80; Sn < 40; Nb, 500; O, 60; all others < 20.	Cold-rolled specimens were polished, annealed, etched; reacted with N_2 (99.995 v/o).	Determination of the concentration gradient by microhardness measurements.	$\bar{D}$ (chemical diffusion)	800–1000	0.024	40,900	Linear dependence of hardness on N concentration was demonstrated by Gebhardt et al. [13]; $\bar{D}$ was assumed to be independent of the N concentration.	[5]
Ta	N	O, 16; N, 10; C, 30; Nb, 100–300; Cu, 30; all others < 10.	Ta plates were used below 1000 °C, cylindrical specimens were used above 1000 °C: vacuum annealed; reacted with prepurified N_2 (99.996 v/o).	Determination of concentration gradient by microhardness measurements.	$\bar{D}$	800–1300	0.0182	41,100	$\bar{D}$ was assumed to be independent of the N concentration.	[6]
Ta	O	Metallic contaminants not stated; 99.9 w/o Ta; O, 90–1630; N, 50.	Degassed Ta wire loaded with O by heating in O_2 at low partial pressure.	Measurement of anelastic strain by elastic after-effect and by internal friction.	D_T	38–250	4.4×10^{-3}	25,450	Effects of interstitial impurity interactions were determined.	[2]
Ta	O	Not stated.	Not stated.	Measurement of anelastic strain by elastic after-effect and by internal friction.	D_T	155–355	0.0190	27,300	Effects of possible interstitial impurity interactions were not ascertained.	[4]
Ta	O	Not stated.	Band-shaped specimens with one section enriched in O used.	Determination of the concentration gradient by microhardness measurements.	$\bar{D}$	700–1400	0.015	26,700	Linear dependence of hardness on O concentration was demonstrated up to 1.1 at. % O. D was assumed to be independent of the O concentration.	[7]
Ta	O	O, 16; N, 10; C, 30; Nb, 100–300; Cu, 30; all others < 10.	Ta plates were used below 1000 °C, cylindrical specimens were used above 1000 °C; vacuum annealed; reacted with O_2 from decomposition of permanganate.	Determination of the concentration gradient by microhardness measurements.	$\bar{D}$	900–1200	2.14×10^{-3}	22,900	Linear dependence of hardness on O concentration was established at low concentrations by [8]. D was assumed to be independent of the O concentration.	[6]
TaB_2	B	Not stated.	Boride layer was formed on a Ta cylinder by boronizing in boron carbide and borax.	Determination of the concentration gradient by microhardness measurements.	$\bar{D}$	1100–1400	9.44×10^{-4}	47,000	D was assumed to be independent of the B concentration.	[9]

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[a] Impurity concentrations are given in ppm unless otherwise stated.

Tantalum — Continued

Solvent medium	Diffusing element	Purity [a]	Preparation and properties	Method	Diffusion coefficient	Temperature range, °C	D_0 cm²/s	Q cal/mol	Comments	Ref.
TaC.........	C...........	Nb, 40–50; Ti, < 25; Mo, < 40; W < 40; all others < 50; O_2 and $N_2 \sim 100$ in carbide slab.	Slabs with marker holes near the surface were carburized in high purity graphite powder, for Kirckendall shift measurements. TaC slabs with low carbon content (45 to 46 at pct C) were heated in CH_4-Ar mixture for chemical diffusion measurements.	Determination of carbon concentration profile by x-ray diffraction analysis; A Matano analysis was performed, but values of D_0 and Q were calculated from values of $\tilde{D}$ averaged over the slab.	$\tilde{D}$	1700–2700	0.18	85,000	The marker movement study indicated that D_c: $D_{Ta} \cong 80:1$ in TaC at 2500 °C. The Matano analysis indicated that $\tilde{D}$ had a complicated dependence on C concentration. Grain boundary diffusion was not important.	[10]
TaC.........	C...........	Not stated.		Determination of carbon concentration profiles by electron microprobe analysis.	$\tilde{D}$	2100–2650	1.8	87,000	The carbon concentration profiles were found to be nonlinear in the TaC layer.	[11]
TaC.........	C...........	Nb, 50; Ti < 25; Fe, 10; Mo < 50; W < 50; all other metals < 50; O, 15–75; N, 10–30; C, 10–30.	Carbide layer was formed by heating Ta sheets in an Ar-methane atmosphere.	Measurement of the rate of movement of the TaC-Ta_2C and Ta_2C-Ta interfaces.	$\tilde{D}$	1800–2700	1.04	86,000	Rate of movement of the interfaces was assumed to be controlled by diffusion through the carbide layers. D was assumed to be independent of the C concentration.	[12]
TaC.........	W.........	Free C, 500; Fe, 800.	Carbide was formed by carburization in graphite charge; carbide powder sintered; density 14.2 g/cm³; porosity 3 %; grain size 50–100 μm.	Measurement of the attenuation of the β-radiation by the method of Kryukov and Zhukhovitskii [14].	D^* (self-diffusion)	2130–2300	19.2	142,000	There may be some error in this data due to vaporization of the radioactive layer.	[13]
Ta_2C........	C...........	Nb, 50; Ti < 25; Fe, 10; Mo < 50; W < 50; all other metals < 50; O, 15–75; N, 10–30; C, 10–30.	Carbide layer was formed by heating Ta sheets in Ar-methane atmosphere.	Measurement of the rate of movement of TaC-Ta_2C and Ta_2C-Ta infaces.	$\tilde{D}$	1800–2700	7.0	89,000	Rate of movement of the interfaces was assumed to be controlled by diffusion through the carbide layers. D was assumed to be independent of C concentration.	[15]

[a] Impurity concentrations are given in ppm unless otherwise stated.

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Thorium

Solvent medium	Diffusing element	Purity [a]	Preparation and properties	Method	Diffusion coefficient	Temperature range, °C	D_0 cm²/s	Q cal/mol	Comments	Ref.
Th...........	C, 0.4 w/o.	Not stated.	Thorium cylinders were carburized in a graphite charge.	Determination of the concentration gradient by chemical analysis.	$\tilde{D}$ (chemical diffusion)	1000–1200	~ 0.03	38,200	The concentration dependence of D was determined by the method of Smith and Danielson [2]; D_0 has a large uncertainty.	[1]
ThO_2........	Ce..........	Not stated.	Grain size 0.2 μm; irradiated with 3.8×10^{17} fast neutrons/cm².	Determination of the rate of leaching of fission products into molten NaCl.	D_T (tracer diffusion)	910–1010	5.5×10^{-7}	70,000		[3]

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[a] Impurity concentrations are given in ppm unless otherwise stated.

Solvent medium	Diffusing element	Purity[a]	Preparation and properties	Method	Diffusion coefficient	Temperature range, °C	D_0 cm²/s	Q cal/mol	Comments	Ref.
ThO_2	I	Not stated.	ThO_2 powder, was irradiated for 32 days at 3×10^{13} n/cm²/s (fast); post-irradiation anneals, I collected on Ag wool at 400 °C.	Measurement of the rate of release of fission gas from irradiated powder.	D_T	800–1220	7×10^{-11}	28,600		[4]
ThO_2	Kr	Not stated.	Sintered ThO_2; Kr was introduced by ion bombardment.	Measurement of the rate of Kr release from ion bombarded sample.	D_T	1100–1350		104,000	D_0 was assumed to be $\sim 3\times10^{-1\pm1}$ cm²/s for purposes of calculating D from the release data.	[5]
ThO_2	Kr	Si ~ 3; Mg and Cu ~ 1; all other elements were not detectable.	ThO_2 powder; irradiated with fast neutron, dosage 10^{20} nvt.[b]	Measurement of the rate of Kr release neutron irradiated powder.	D_T	600–1200	2.5×10^{-10}	32,300		[6]
ThO_2	Nb	Not stated.	Grain size 0.2 μm; irradiated with 3.8×10^{17} fast neutrons/cm².	Determination of the rate of leaching of fission products into molten NaCl.	D_T	820–960	8.3×10^{-6}	65,400		[3]
ThO_2	O	Not stated.	Grain size about 10 μm.	Heterogeneous isotopic exchange between a solid sample and a gas.	D^* (self-diffusion)	800–1420	1×10^{-8}	14,700	Low values of D_0 and Q are suggestive of grain-boundary diffusion.	[7]
ThO_2	O	Co, Mg, Fe each < 100.	ThO_2 powder fused into spheres in a plasma torch.	Heterogeneous isotopic exchange between a solid sample and a gas.	D^*	800–1500	4.4	65,800	Finite rate of exchange accounted for in treatment of results.	[8]
ThO_2	Rn	Not stated.	ThO_2 was labeled with Rn by recoil from α-decay of Ra adsorbed on the powder; the Ra was quantitatively removed after labeling.	Measurement of the rate of release of Rn from recoil labeled powder.	D_T	565–1515		59,000		[4]
ThO_2	Rn	Not stated.	Sintered ThO_2; Rn was introduced by recoil from α-decay of Ra on one face of sample; the Ra was quantitatively removed after labeling.	Measurement of the rate of release of Rn from recoil labeled disk.	D_T	1100–1300		93,000	D_0 was assumed to be $\sim 3\times10^{-1\pm1}$ cm²/s for purposes of calculating D from the release data.	[5]
ThO_2	Th	Not stated.	ThO_2 pellets; 97.5% of theoretical density.	Determination of isotopic concentration gradient by mass spectrometric analysis of thin sections.	D^*	925–1480	4×10^{-8}	27,000	Data was adjusted to eliminate grain-boundary contribution.	[9]
ThO_2	Xe	Not stated.	ThO_2 powder was irradiated for 32 days at 1.5×10^{14} n/cm² (thermal), post-irradiation anneals.	Measurement of the rate of release of fission gas from irradiated powder.	D_T	700–1220		30,000		[4]
ThO_2	Xe	Not stated.	Single crystal ThO_2; neutron dose $\sim 3\times10^{16}$ n/cm² (fast).	Measurement of the rate of release of fission gas from irradiated crystals.	D_T	1200–2000	1×10^{-4} -2×10^{-2}	81,000	Based on preliminary D/a^2 values (a = average particle radius).	[10]
ThO_2	Xe	Not stated.	Polycrystalline ThO_2; neutron dose 7×10^{15} n/cm² (fast).	Measurement of the rate of release of fission gas from irradiated powder.	D_T	500–1100		37,000	Evaluated as D/a^2 values after subtraction of the initial burst.	[10]
ThO_2	Xe	Th, 99.23 m/o; U 0.77 m/o.	ThO_2 powder; neutron dose $\sim 2.4\times10^{12}$ nvt (thermal).	Measurement of the rate of release of fission gas from irradiated powder.	D_T	800–1600		50,000		[11]

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[a] Impurity concentrations are given in ppm unless otherwise stated.

[b] The notation "nvt" represents a quantity of neutron exposure and has the units neutron–cm^{-2}.

Solvent medium	Diffusing element	Purity [a]	Preparation and properties	Method	Diffusion coefficient	Temperature range, °C	D_0 cm²/s	Q cal/mol	Comments	Ref.
ThO_2........	Zr..........	Not stated.	Grain size 0.2 μ; irradiated with 3.8×10^{17} fast neutrons/cm².	Determination of the rate of leaching of fission products into molten NaCl.	D_T	840–960	6.9×10^{-7}	62,300		[3]
ThO_2 + 12%UO_2.	Kr.........	Not stated.	Sintered ThO_2-UO_2 compact; Kr was introduced by ion bombardment.	Measurement of the rate of Kr release from ion bombarded sample.	D_T	1250–1350		110,000	D_0 was assumed to be ~ $3 \times 10^{-1 \pm 1}$ cm²/s for purposes of calculating D from the release data.	[5]
ThO_2 + 10%Y_2O_3	Se.........	Th 89.39 m/o; U, 0.70 m/o; Y, 9.91 m/o.	Neutron dose ~ 2.4 $\times 10^{17}$ nvt (thermal)	Measurement of the rate of release of fission gas from irradiated powder.	D_T	1000–1600		75,000		[11]
ThO_2 + 30%Y_2O_3	Se.........	Th 69.48 m/o; U, 0.74 m/o; Y 29.78 m/o.	Neutron dose ~ 2.4 $\times 10^{17}$ nvt (thermal)	Measurement of the rate of release of fission gas from irradiated powder.	D_T	900–1600		90,000		[11]

[a] Impurity concentrations are given in ppm unless otherwise stated.

[b] The notation "nvt" represents a quantity of neutron exposure and has the units neutron-cm^{-2}.

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Titanium

Solvent medium	Diffusing element	Purity [a]	Preparation and properties	Method	Diffusion coefficient	Temperature range, °C	D_0 cm²/s	Q cal/mol	Comments	Ref.
α-Ti.........	C..........	Other than C: O, 180–2360 (highest in C-Ti alloy); H, 90–200; N, 110–340; Al, 30; Fe, 10–70; Si, 20–50; Mn, 10–30; all others ≦ 10.	C-Ti alloy (0.4 w/o or higher in C) buttwelded to high purity Ti (0.038 w/o C).	Determination of the concentration gradient by chemical analysis.	$\tilde{D}$ (chemical diffusion coefficient).	736–882	5.06	43,500	$\tilde{D}$ was assumed to be independent of C concentration.	[1]
β-Ti.........	C..........		C-Ti alloy (0.4 w/o or higher in C) buttwelded to high purity Ti (0.038 w/o C).	Determination of the concentration gradient by chemical analysis.	D	920–1150	108	48,400	$\tilde{D}$ was assumed to be independent of concentration.	[1]
β-Ti.........	N..........	Principal impurities: C, 360; Mn, 300; O, 110; Al, 100. Commercial N_2 passed through liquid N_2 trap or tube furnace with Ti turnings.	Argon-arc-melted iodide Ti, hot-forged and rolled, swaged cold to rod-shaped, machined into cylindrical specimens.	Determination of the concentration gradient by chemical analysis (Kjeldahl).	$\tilde{D}$	800–1400	3.5×10^{-2}	33,800	Measurements were complicated by formation of outer nitride layer and α-phase, but less than 3% of cylindrical radius; $\tilde{D}$ was assumed to be independent of concentration.	[2]
α-Ti.........	O..........	Not stated.	VT-1 Ti, samples were polished and then etched for 60 s in 7% Hf in HNO_3.	Determination of the concentration gradient by microhardness measurements.	$\tilde{\bar{D}}$	800–900	1.80×10^{-3}	35,900	$\tilde{D}$ was assumed to be independent of concentration; hardness was assumed to be linearly dependent on the concentration of O.	[3]
α-Ti.........	O..........	Fe, Mn, Al, Sn, Mg and Cr, each 100; Cu, 10.	Electron-beam-melted titanium.	Determination of the concentration gradient by microhardness measurements.	$\tilde{D}$	800–1000	0.5	51,000	$\tilde{D}$ was assumed to be independent of concentration; hardness was assumed to be linearly dependent on concentration of O.	[4]

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[a] Impurity concentrations are given in ppm unless otherwise stated.

Solvent medium	Diffusing element	Purity [a]	Preparation and properties	Method	Diffusion coefficient	Temperature range, °C	D_0 cm²/s	Q cal/mol	Comments	Ref.
α-Ti........	O..........	Si, 600; Fe, 1500; Al, 2000; Mg, 200; Mn, 100–500; W, 300; N, 100; all others ≦ 100.	Ti bars were oxidized by TiO_2 powder.	Determination of the concentration gradient by microhardness measurements.	$\tilde{D}$	700–850	5.08×10^{-3}	33,500	$\tilde{D}$ was assumed to be independent of concentration; hardness was assumed to be linearly dependent on the concentration of O.	[5]
β-Ti........	O..........	Principal impurities: C, 360; Mn, 300; O, 110; Al, 100. Dried commercial O_2 and O_2 from decomposition of permanganate were used.	Argon-arc-melted iodide Ti, hot-forged and rolled, swaged cold to rod-shape, machined into cylindrical specimens.	Determination of the concentration gradient by chemical analysis (vacuum fusion with tin).	$\tilde{D}$	950–1414	1.6	48,200	$\tilde{D}$ was assumed to be independent of concentration.	[2]
β-Ti........	O..........	Si, 600; Fe, 1500; Al, 2000; Mg, 200; Mn, 10–50; W, 300; Ni, 10; all others ≦ 100.	Ti cylinders were oxidized by TiO_2 powder.	Determination of the concentration gradient by microhardness measurements.	$\tilde{D}$	930–1150	3.14×10^{4}	68,700	Measurements were complicated by grain growth and formation of the α-phase. $\tilde{D}$ was assumed to be independent of concentration; hardness was assumed to be linearly dependent on concentration.	[5]
β-Ti........	O..........	Ti, 99.7 w/o, Cu major impurity.	Ti-wire (Ti-75A); initially ~ 1 mm section of wire oxidized in O_2.	Determination of the concentration gradient by change in resistance along the sample.	$\tilde{D}$	1130–1350	0.083	31,200	Results may be complicated by formation of α-phase which would be stabilized by oxygen atoms in the metal; linear dependence of resistance on O concentration up 1% O was verified by [24].	[6]
TiB_2........	B..........	Not stated.	Boronization of surface of Ti-cylinder by heating in a boron carbide-borax charge.	Determination of the concentration gradient by microhardness measurements.	$\tilde{D}$	1100–1400	8.9×10^{-5}	30,600	$\tilde{D}$ was assumed to be independent of B concentration.	[7]
TiC..........	C..........	Not stated.	Carburization of the surface of Ti cylinder by heating in a boron carbide-borax charge.	Determination of the concentration gradient by microhardness measurements.	$\tilde{D}$	900–1300	2.04×10^{-3}	33,000	$\tilde{D}$ was assumed to be independent of concentration.	[7]
TiC..........	Nb........	Free C, 4000; Fe, 150; N, 350.	Carburization of TiO_2+C in vacuum furnace with graphite heater, carbide was crushed, Fe was removed with HCl; density approximated theoretical values.	Method of Zhukhovitskii and Geodakyan [8]; nonexponential attenuation of β-radiation when a radioisotope diffuses into a solid.	D_T (tracer diffusion).	1935–2170	2.4	84,000		[9]
TiC · NbC.. (1:1)	Nb........	Free C, 2600; Fe 200; N, 700.	Carburization of $TiO_2+NbC+C$ in vacuum furnace, etc.	Method of Zhukhovitskii and Geodakyan.	D^* (self-diffusion).	2170–2280	470	120,000		[9]
TiC..........	W..........	Free C, 1100	Carburization of TiO_2 in vacuum furnace; porosity up to 0.2%; grain size 50–100 μm; density 4.97 g/cm³.	Method of Kryukov and Zhukhovitskii [10]; diffusion of thin radioactive layer into thin sample (30 to 100 μm).	D_T	2130–2300	7.7	115,000	There may be some error in this data due to vaporization of the radioactive layer.	[11]
TiC · WC... (77:23)	W..........	Free C, 1700.	Carburization in vacuum furnace; porosity 0.2%; grain size 50–70 μm; density 7.35 g/cm³.	Method of Kryukov and Zhukhovitskii.	D^*	2130–2300	31.6	138,000	Measurements also were made on other mixed carbides, but these appear to have large errors due to vaporization of the radioactive layer.	[11]

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[a] Impurity concentrations are given in ppm unless otherwise stated.

Solvent medium	Diffusing element	Purity [a]	Preparation and properties	Method	Diffusion coefficient	Temperature range, °C	D_0 cm²/s	Q cal/mol	Comments	Ref.
TiO_2	Ba	Rutile: traces of Si and Fe Ba: Ca, 2; Mg, 1; Cu, 1; Na, 1.	^{133}Ba labeled carbonate was decomposed to oxide on TiO_2 single crystal in O_2 atmosphere, second-phase region formed in TiO_2.	Determination of the concentration gradient by radioisotope distribution, Matano analysis [12, 13].	$\tilde{D}$, perpendicular to C axis of crystal.	1100–1200		~ 59,000		[14]
TiO_2	Ba	Rutile: traces of Si and Fe Ba: Ca, 2; Mg, 1; Cu, 1; Na, 1.	^{133}Ba labeled carbonate was decomposed to oxide on TiO_2 single crystal in O_2 atmosphere, second-phase region formed in TiO_2.	Determination of the concentration gradient by radioisotope distribution, Matano analysis.	$\tilde{D}$, parallel to C axis of crystal.	1100–1200		~ 43,000		[14]
TiO_2	Fe	Impurities not precipitated with NH_3, 1000; Fe, 100; heavy metals of sulfide type, 500.	TiO_2 powder was compressed into pellets and sintered at 1100 °C; ^{59}Fe was vacuum deposited on pellet face.	Determination of the concentration gradient by radioisotope distribution.	D_T (air)	800–1000	1.98×10^{-2}	55,000		[15]
TiO_2	Fe	Impurities not precipitated with NH_3, 1000; Fe, 100; heavy metals of sulfide type, 500.	TiO_2 powder was compressed into pellets and sintered at 1100 °C; ^{59}Fe was vacuum deposited on pellet face.	Determination of the concentration gradient bv radioisotope distribution.	D_T (vacuum).	770–1000	0.192	55,400		[15]
TiO_2	Fe	Impurities not precipitated with NH_3, 1000; Fe, 100; heavy metals of sulfide type, 500.	TiO_2 powder was compressed into pellets and sintered at 1100 °C; ^{59}Fe was vacuum deposited on pellet face.	Determination of the concentration gradient by radioisotope distribution.	D_{gr}, grain-boundary diffusion in the presence of air.	800–1000	1.56×10^{-5}	34,000		[15]
TiO_2	Fe	Impurities not precipitated with NH_3, 1000; Fe, 100; heavy metals of sulfide type, 500.	TiO_2 powder was compressed into pellets and sintered at 1100 °C; ^{59}Fe was vacuum deposited on pellet face.	Determination of the concentration gradient by radioisotope distribution.	D_{gr} (vacuum).	770–1000	1.13×10^{-3}	34,700		[15]
TiO_2	Li	Not stated.	Single crystal TiO_2 doped uniformly with Li.	Measurement of the change in optical absorption due to the diffusion of Li out of the crystal.	$\tilde{D}$, parallel to C axis of crystal.	80–550	0.295	7,610	Impurity concentration and surface damage were observed to affect diffusion rates; impurities were minimized by taking cuts near center of boule; abrasion of surfaces was used to control diffusion direction.	[16]
TiO_2	O	Al_2O_3, 100 to 200; infrared measurements showed that OH-groups were present.	Single crystal TiO_2 pulverized to 10–250 μm.	Heterogeneous isotopic exchange between solid sample and a gas.	D^* (self-diffusion).	700–1300	2.0×10^{-3}	60,000	"High" Al_2O_3 concentration may have caused extrinsic diffusion.	[17, 18]
TiO_2	Rn	Not stated.	TiO_2 powder labeled with Rn by recoil from Ra decay.	Hahn emanation technique, modified by mixing oxide powder with Ra salt allowing Rn to recoil into oxide and then dissolving away the Ra.	D_T	315–1150		22,000		[19]
TiO_2	Sn	Not stated.	TiO_2 single crystal; SnO_2 applied to face of crystal.	Determination of the concentration gradient by x-ray analysis (change in the intensity of x rays reflected as TiK_{α} and $SnL_{\alpha 1}$).	D_T, parallel to C axis of crystal.	900–1050	0.16	80,000		[20]

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[a] Impurity concentrations are given in ppm unless otherwise stated.

Titanium—Continued

Solvent medium	Diffusing element	Purity[a]	Preparation and properties	Method	Diffusion coefficient	Temperature range, °C	D_0 cm²/s	Q cal/mol	Comments	Ref.
$BaTiO_3$.....	Ba..........	Not stated.	$BaCO_3$ reacted with TiO_2 to form $BaTiO_3$; compressed and sintered, 80% of theoretical density.	Determination of the concentration gradient by radioisotope distribution.	D^*	884–1180	0.8	89,000		[21]
$SrTiO_3$......	O...........	Mg ≦ 1; Si ~ ~~100~~; Al ≦ 10; Au ≦ 1; Pb, 10.	Single crystal; dislocation density of ~ 1.4 × 10⁶/cm².	Heterogeneous isotopic exchange between a solid sample and a gas.	D^*	825–1200	1.6×10^{-7}	15,500	Low frequency factor, D_0, was taken as evidence for extrinsic diffusion; diffusion rate was found to depend on dislocation density.	[22]
$SrTiO_3$......	O...........	Mg ≦ ; Si ~ 10; Al ≦ 10; Au ≦ 1; Pb, 10.	Single crystal; dislocation density ~ 6.6 × 10⁵/cm².	Heterogeneous isotopic exchange between a solid sample and a gas.	D^*	850–1525	1.2×10^{-5}	29,300	Possible extrinsic diffusion; diffusion rate was found to depend on dislocation density.	[22]
$SrTiO_3$......	Sr.........	Not stated.	$SrCO_3$ was reacted with anatase to form $SrTiO_3$; compressed and sintered; 95% theoretical density.	Method of Kryukov and Zhukhovitskii.	D^*	1000–3000	4.0	70,000		[23]

[a] Impurity concentrations are given in ppm unless otherwise stated.

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Zirconium

Solvent medium	Diffusing element	Purity[a]	Preparation and properties	Method	Diffusion coefficient	Temperature range, °C	D_0 cm²/s	Q cal/mol	Comments	Ref.
β-Zr.........	C...........	Hf, 700; N, 140; Fe, 400; Si, 500.	Zr-bars were melted in an electron arc furnace; ¹⁴C was added to some specimens which were continually remelted to obtain uniform distribution.	Determination of the concentration gradient by radioisotope distribution.	$\tilde{D}$ (chemical diffusion).	900–1260	0.0048	26,700	$\tilde{D}$ was assumed to be independent of concentration.	[1]
β-Zr.........	N...........	Hf, 150; Fe, 250; Si, 100; Sn, 100; all others < 100.	Zr: iodide-crystal bars were produced by deBoer process, double arc melted, cold rolled into rods. Prepurified tank N_2 was passed over heated Zr turnings and then through a cold-trap.	Determination of the concentration gradient by chemical analysis (Kjeldahl).	$\tilde{D}$	920–1640	0.015	30,700	$\tilde{D}$ was assumed to be independent of concentration.	[2]

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[a] Impurity concentrations are given in ppm unless otherwise stated.

Solvent medium	Diffusing element	Purity [a]	Preparation and properties	Method	Diffusion coefficient	Temperature range, °C	D_0 cm²/s	Q cal/mol	Comments	Ref.
β-Zr.........	N...........	Hf, 1.8–2.2 w/o; O, N, H, Fe, Si, totaling < 100.	Cylindrical specimens were machined from outgassed iodide Zr bars. Commercial N_2 was dried by Mg perchlorate.	Determination of the concentration gradient by chemical analysis (Kjeldahl).	$\tilde{D}$	900–1600	0.003	33,600	$\tilde{D}$ was assumed to be independent of concentration.	[3]
α-Zr.........	O...........	O, 300; C, 150; Fe, 120; Al, 50; P < 75; Cr, 40.	Oxide films grown on Zr plates in the presence of O_2 at one atm pressure.	Determination of the concentration gradient by microhardness measurement and analysis of the reaction rates.	D_{gr} (grain-boundary). $\tilde{D}$	400–650 650–850	4.57×10^{-4} 224	35,000 59,700	Electron microscope studies of fracture surfaces of the metal suggested that grain boundary diffusion was the predominant mode at low temperatures.	[4]
α-Zr.........	O...........	High temperature samples: O, 1300; N, 240; Hf, 2.04 w/o; Fe, 190; Al, 95; Ba < 650; Si < 650. Low temperature samples: O, 600; Fe, 170; Al, 290; Cr < 650.	Vacuum annealed Zr plates were oxidized in O_2 at high temperatures plus one sample in O_2-bearing Na. Low temperature oxidations in O_2-bearing Na or CO_2.	Determination of the concentration gradient by microhardness measurements.	$\tilde{D}$ $\tilde{D}$	400–700 700–850	9.13×10^{-5} 69.2	29,800 56,190	Use of O_2-bearing sodium gave diffusion results similar to O_2 oxidations. D-values were calculated only over range where linearity existed between hardness and O concentration.	[5]
α-Zr.........	O...........	Low Hf content, concentrations of impurities not stated.	Rolled stock annealed, polished and etched; samples anodized in KOH solution to form the oxide film.	Time rate of change of the interference color (i.e., thickness) of the oxide film due to solution of the film in the metal.	$\tilde{D}$	400–585	9.4	51,780	$\tilde{D}$ was assumed to be independent of concentration.	[6]
α-Zr.........	O...........	Al, 45; C, 50; Fe, 218; Hf, 68; Mo, 25; O, 140; Si < 40; Zr < 50; all others < 25.	Iodide-refined Zr, polished. O_2 (99.6 v/o pure) was passed through heated cupric oxide, Ascarite, Linde 5A molecular sieves and cold trap.	Determination of the concentration gradient by microhardness measurements.	$\tilde{D}$	400–850	28.8	53,400	$\tilde{D}$ was assumed to be independent of concentration.	[7]
α-Zr.........	O...........	Zr sample: Fe < 100; Hf, 55; C, 80; O, 160; all others < 50. Zr-O alloy: Fe, 510; Al, 200; Hf, < 300; C, 200; H, 57; N, 89; O, 3100; all others < 50.	Oxygen enriched Zr disk was pressure bonded to low oxygen Zr disk at 675 °C to form the diffusion couple.	Determination of the concentration gradient by microhardness measurements.	$\tilde{D}$	622–840	3.3	49,500	Linearity of concentration to hardness was demonstrated for O-Zr alloys with less than 2.4 a/o oxygen; linearity of the probability plot indicated that $\tilde{D}$ was independent of concentration.	[8]
α-Zr.........	O...........	Al, 100; Fe, 1000; Si, 425; Ca, 200; Hf, 200; N, 437; O, 800; all others < 50.	Zr bars; annealed, polished and etched; surface oxidized in O_2.	Determination of the concentration gradient by microhardness measurements; gravimetric determinations also were used.	$\tilde{D}$	550–650 650–850	7.9×10^{-5} 0.22	30,500 47,000	$\tilde{D}$ was assumed to be independent of concentration. Grain boundary diffusion probably was important at low temperatures.	[9]
α-Zr.........	O...........				$\tilde{D}$	400–850	6.81 ±2.9	51,200 ±800	Combined data; data from only the high temperature ranges of [5] and [9] were used. This agreement is remarkable.	[5–9]
ZrB_2.........	B...........	Not stated.	Boride layer was formed on a Zr cylinder by boronizing in boron carbide and borax.	Determination of the concentration gradient by microhardness measurements.	$\tilde{D}$	1100–1400	1.26×10^{-4}	34,500	$\tilde{D}$ was assumed to be independent of concentration; narrow homogeneity range [11] may be a major source of error in the results.	[10]

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[a] Impurity concentrations are given in ppm unless otherwise stated.

Solvent medium	Diffusing element	Purity [a]	Preparation and properties	Method	Diffusion coefficient	Temperature range, °C	D_0 cm²/s	Q cal/mol	Comments	Ref.
ZrC..........	C..........	Not stated.	Carbide layer was formed on a Zr cylinder by carburizing in graphite.	Determination of the concentration gradient by microhardness	$\tilde{D}$	900–1300	0.0344	41,000	$\tilde{D}$ was assumed to be independent of concentration.	[10]
ZrC..........	C..........	Zirconium: Cr, 84; Fe, 570; Hf, 68; O, 375; all others <50. Graphite: Ca, 140; Fe, 73; all others < 50.	ZrC layer formed between liquid Zr and graphite crucible.	Determination of the rate of growth of ZrC layer from photomicrographs of longitudinal sections of the samples.	$\tilde{D}$	2000–2860	0.95	78,700	D was assumed to be independent of concentration. The boundary concentrations were taken from phase diagrams [13, 14].	[12]
ZrO_2........	O..........	Zr substrate: O, 300; C, 150; Fe, 120; Al, 50; P < 75; Cr, 40.	Oxide layers grown on Zr plates in O_2; monoclinic oxide studied.	Determination of rate of oxide layer growth	$\tilde{D}$	400–850	1.05×10^{-3}	29,300		[4]
ZrO_2........	O.......... vacancies	Impurities in metal substrate not stated.	Oxide layers formed on crystal bar Zr in O_2, then the anion vacancy concentration in the oxide equilibrated by annealing in vacuum; approximate composition, $ZrO_{1.926}$; monoclinic phase.	Interruption kinetics technique of Rosenburg [16]: rate of oxygen uptake by oxygen deficient ZrO_{2-x}.	$\tilde{D}$	300–386	9.0×10^{-4}	28,700	Comparison of $\tilde{D}$ for vacancy diffusion with O-anion diffusion requires the use of an unknown correlatior factor. The anion vacancy concentration in the deficient oxide was $\sim 7 \times 10^{-3}$ g atom/cm³ (386 °C).	[15]
$ZrO_{1.994}$....	O..........	SiO_2, 0.15 w/o; TiO_2, 50; Fe_2O_3, 30; MgO, 300.	Hot pressed nonstoichiometric oxide compacts; density 5.82 g/cm³; monoclinic phase.	Determination of the rate of migration of stoichiometric oxide front into nonstoichiometric grains.	$\tilde{D}$	700–1000	0.055	33,400	Rapid grain boundary diffusion into the compacts was noted so that the re-oxidation of individual grains was measured. A comparison with [4] and [15] above suggests that (a) grain boundary effects may be small in coherent oxide layers, (b) $\tilde{D}$ does not vary strongly with composition nor with crystallographic direction, and (c) the correlation factor may be near unity.	[17]
$Zr_{0.84}$-$Ca_{0.16}$-$O_{1.84}$.	Ca.........	99.95 w/o ZrO_2 and $CaCO_3$ used in fabrication; W < 100.	Calcined mixture of ZrO_2 and $CaCO_3$ pressed into pellets, fused with plasma torch; grain size 0.2–1.0 mm; porosity 0.0–0.5%; cubic phase.	Determination of the concentration gradient by radioisotope distributions.	D^*	1700–2100	0.444	100,200	The error due to grain boundary diffusion was within the experimental uncertainty of the data.	[18]
$Zr_{0.92}$-$Ca_{0.08}$-$O_{1.85}$	O..........	HfO_2, 1.5%; SiO_2, 0.5%; MgO, 0.20%; Fe_2O_3, 0.10%; Al_2O_3, 0.17%; TiO_2, 0.11%. (weight percent).	Tube closed at one end; density 5.4 g/cm³; porosity ~ 5%; pores not connected; cubic phase.	Determination of the rate of permeation of O_2 through the walls.	$\tilde{D}$	1100–1600	185	57,600	A large drop in O_2 partial pressure between the inside and outside caused a large chemical potential gradient.	[19]
$Zr_{0.858}$-$Ca_{0.142}$-$O_{1.858}$	O..........	Not stated.	Polycrystalline samples: porosity 3–6%; grain size 100 μm. Single crystal sample: verneuil method; crack-free specimens used; cubic phase.	Heterogeneous isotopic exchange between solid sample and ^{18}O-enriched O_2.	D^*	780–1100	0.018	31,200	D_0 and Q were determined from the combined data from both types of samples.	[20]
$Zr_{0.85}$-$Ca_{0.15}$-$O_{1.85}$	O..........	Not stated.	Arc-fused, polycrystalline spheres.	Heterogenous isotopic exchange.	D^*	700–1100	6.9×10^{-3}	30,400	D_0 and Q are given as recalculated by Simpson and Carter [20].	[21]

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[a] Impurity concentrations are given in ppm unless otherwise stated.

Zirconium – Continued

Solvent medium	Diffusing element	Purity [a]	Preparation and properties	Method	Diffusion coefficient	Temperature range, °C	D_0 cm²/s	Q cal/mol	Comments	Ref.
$Zr_{0.84}$-$Ca_{0.16}$-$O_{1.84}$; $Zr_{0.88}$-$Ca_{0.12}$-$O_{1.88}$	Zr..........	99.95 w/o ZrO_2 and $CaCO_3$ used in fabrication; W < 100.	Calcined mixture of ZrO_2 and $CaCO_3$ pressed into pellets, fused with plasma torch; grain size 0.2-1.0 mm; porosity 0.0-0.5%; cubic phase.	Determination of the concentration gradient by radioisotope distribution.	D^*	1700–2150	0.035	92,500	D_0 and Q represent the combined results for the two compositions. The error due to grain boundary diffusion was within the experimental error of the data.	[18]

[a] Impurity concentrations are given in ppm unless otherwise stated.

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