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REGIONS OF EXISTENCE OF SPECIAL AND NON-SPECIAL GRAIN BOUNDARIES

L. S. SHVINDLERMAN and B. B. STRAUMAL
Group of the Interfaces in Metals, Institute of Solid State Physics, Academy of Sciences of the U.S.S.R., Chernogolovka, Moscow distr. 142432, U.S.S.R.

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Abstract—The whole complex of experimental results on the structure and properties of grain boundaries in different materials has been analysed on the basis of the original works available by the present time. This has made it possible to show that (a) special boundaries exist in a certain, finite interval of misorientation angles, the magnitude of this interval decreasing with increasing Σ, that is, reciprocal density of coincident sites; (b) special boundaries exist in a finite temperature interval, and the "special boundary–non-special boundary" transition can occur below the melting temperature, the temperature of this transition decreasing with an increase of Σ; (c) there is a threshold value of $\Sigma = \Sigma_{max}$ that is temperature dependent and decreases with rising temperature. Above Σ_{max} for a given temperature the boundaries with special misorientation angles are not different in properties from those of the general type. The analogy has been formulated between special and non-special grain boundaries with commensurate and incommensurate phases in adsorbed layers on the external surface.

Résumé—Dans cette article on analise un ensemble des resultats expérimentaux sur la structure et les propriétes des joints de grains dans des matériaux differents à la base des travaux originals connus au présent. De ce fait on a construit les diagrammes d'existence des joints de grains spécials et non-spécials. Des données expérimentaux reçus ont montré que (a) des joints spécials existent à certaine intervalle finie des angles de désorientation dont la valeur déminue exponentiellement aux basses temperatures avec la croissance Σ-inverse de la densité des noeuds de coincidence; (b) des joints spécials existent à l'intervalle finie des temperatures, avec cela la transition "une joint spécial–joint non-spécial" peut se passer au-dessous de la temperature de fusion et la temperature de cette transition déminue avee la croissance de Σ; (c) on existe une valeur limite de $\Sigma = \Sigma_{max}$ qui depend de la temperature et réduit avec la croissance de la temperature. Au dessus Σ_{max} pour la temperature donnée des joints avec des angles spécials des désorientation ne distinguent pas d'avec les joints du type general par les propriétés. Dans cette article on a suivi une analogie entre des joints de grains spécials et non-specials et des phases comparables et non-comparables dans des couches adsorbées sur la surface exterieure.

Zusammenfassung—Im Artikel wird die Gesamtheit von Experimentalergebnissen über die Struktur und Eigenschaften von Korngenzen in verschiedenen Materialen auf der Basis der z. Z. bekannten Originalarbeiten analysiert. Anhand dieser Gesamtheit wurden Diagramme der Existenz von speziellen und nichtspeziellen Korngrenzen zusammengestellt. Der Zusammenschluss der Experimentalwerte in ein einheitliches Bild erlaubte zu zeigen, dass (a) die speziellen Grenzen in einem bestimmten Endintervall der Misorientierungswinkel existieren, wobei die Grösse dieses Intervalls bei tiefen Temperaturen mit der Erhöhung Σ der Rückdichte der zusammenfallenden Gitterplätze exponential abnimmt; (b) die speziellen Grenzen im Endtemperaturintervall existieren, wobei der Übergang "spezielle Grenze–nichtspezielle Grenze" bei der Temperatur tiefer als die Schmelztemperatur stattfinden kann und die Temperatur dieses Überganges mit dem Wachstum von tiefer wird; (c) es besteht Grenzwert $\Sigma = \Sigma_{max}$, das von der Temperatur abhängt und mit der Erhöhung der Temperatur abnimmt. Über Σ_{max} für die gegebene Temperatur unterscheiden sich nicht die Grenzen mit den speziellen Auseinanderorientierungswinkel den Eigenschaften nach von den Grenzen des Gesamttyps. In der Arbeit wird die Ähnlichkeit zwischen den speziellen und nichtspeziellen Korngrenzen und den vergleichbaren und nicht vergleichbaren Phasen in den adsorbierten Schichten auf der Aussenoberfläche formuliert.

INTRODUCTION

To date vast experimental material has been stored on the structure and properties of grain boundaries. Traditionally, grain boundaries are divided into two broad classes, namely, special boundaries and general boundaries (non-special). The properties of special boundaries differ dramatically from those of general boundaries. Orientational dependences of surface tension, grain boundary diffusion parameters, grain boundary migration etc have a sharply non-monotonic character with extrema on special "angles" [1,101–105]. The geometrical models predicting the existence of special boundaries were developed rather a long time ago. The first of these was the coincidence site lattice model (CSL) in terms of which it was shown that at particular misorientation angles a portion of interpenetrating-lattice sites coincide.

The CSL is characterised by the Σ value, that is, the reciprocal density of coincident sites. It turned out that angular coordinates of the boundaries exhibiting special properties do coincide with the angular values for the CSL with low Σ. Conventionally, this is attributed to the fact that the grain boundary occurring in the CSL with low Σ demonstrates a periodic structure and a lower energy as compared with general boundaries. Although the CSL is violated at any small departure from a special angle, the properties of special boundaries differ from those of general boundaries in a certain finite interval of misorientation angles. This is attributed to the special-boundary structure accomodation by means of grain boundary dislocations. [2, 3]. The Burgers vectors of these dislocations are determined by the DSC-lattice [3]. The greater the Σ value the smaller the length of such a Burgers vector b. The geometrical models available make it possible, in principle, to describe the structure of any special boundary, to predict special misorientation parameters. The authors of these models realized that large Σ values and small lengths of Burgers vector of grain boundary dislocations have no physical sense. The applicability limits of geometrical models of grain boundary structure have been discussed for a long time, but the question remains obscure so far. [4, 3]. Thus, in particular, the problem is not solved on a maximal value of Σ, at which special boundaries are still different in properties from general boundaries. It is not clear whether special boundaries remain special in those temperature intervals, and if there is Σ_{max} then how does it depend on the temperature? It must be found out what determines the width of the angular interval wherein a special boundary manifests its special properties and its structure consists of alternating singular regions and misfit grain boundary dislocations.

The purpose of this work is to analyse these questions. Firstly, using the published experimental data we shall plot the regions of existence of special boundaries in the "temperature–misorientation angle" coordinates.

ANALYSIS OF THE EXPERIMENTAL DATA ON SPECIAL AND NON-SPECIAL BOUNDARIES

Table 1 presents the experimental data available on special and non-special grain boundaries. The data are grouped in order of increasing Σ, and for each one Σ in order of decreasing homological temperature, $t (t = T/T_m)$. Using t enables one to unite and generalize the results of investigation of the same boundaries in different materials. This is, to a certain extent, equivalent to the grain boundary study in the same material but at different temperatures. The data on structure and properties of boundaries are not so numerous, therefore we do not discriminate between grain boundaries of different types, i.e. tilt and twist boundaries, although tilt and twist special boundaries exhibit different sets of misfit dislocations: walls and networks, accordingly, one-dimensional or two-dimensional misfit accomodation.

For each case the table presents the experimental temperature T, the method to investigate the structure or properties of the boundaries, the deflection angle $\Delta\theta$ from exact misorientation θ_Σ for a particular Σ, the boundary type (tilt or twist), if it is known. It is shown whether the particular boundary is a special one at the given values temperature and angle. The references are mentioned too.

We shall, now, briefly characterize the methods to investigate the grain boundary structure and properties and interpret numerical disignations in the table. We shall explain, too, why in every individual case we attribute grain boundaries to special or non-special (general type). We shall first discuss indirect methods when the needed boundary properties are determined. (1) Method of sintering metallic balls. The idea of this method was suggested by Shewman [128], and first realized by Gleiter and the co-workers. [4, 117, 118]. Using the method (1) they studied the misorientation distribution in microscopic monocrystalline balls sintered on a massive monocrystalline substrate. If there are singular points on the orientational dependence of the boundary surface tension, then the balls can rotate upon anneal to the position with a minimal surface tension, corresponding to these singular points. The rotation occurs under the effect of the grain boundary surface tension gradient between the ball and the substrate $d\delta/d\theta$ that increases on approaching a singular point. Thus,

Table 1. Properties of special boundaries

Σ	T/T_m	T,(°C)	Material	$\Delta\theta$ (deg)	The existence if special structure of properties	Methods' group	The type of boundary	Reference
1	2	3	4	5	6	7	8	9
3	0.99	1063	Cu	± 0.5	+	1		56
	0.99	940.5	Ag	± 0.5	+	1		56
	0.98	930	Ag–1% Au	± 0.5	+	1		95
	0.98	930	Ag–0.2% Bi	± 0.5	+	1		95
	0.96	930	Ag–20% Au	± 0.5	+	1		95
	0.95		Al	± 1	+	7		39
	0.95		NiO	± 0.5	+	2	tilt	30
	0.93	590	Al	± 1	+	7		41
	0.9		Al	± 1	+	7		7
	0.9		Cu	± 1	+	7		7
	0.89	930	Cu	± 0.5	+	1		95
	0.84	500	Al	± 0.5	+	4	tilt	103, 105
	0.82	1100	Si	± 0.5	+	7		28
	0.79	2000	Mo	± 0.5	+	7		93

Table 1. (cont.)

Σ	T/T_m	T,(°C)	Material	Δθ (deg)	The existence if special structure of properties	Methods' group	The type of boundary	Reference
1	2	3	4	5	6	7	8	9
3	0.78	450	Al	±0.5	+	4	tilt	103, 105
	0.73	400	Al	±0.5	+	4	tilt	103, 105
	0.70		Al	±0.5	+	7	tilt	72
	0.66	340	Al	±0.5	+	3	tilt	101, 102
	0.63	310	Al	±0.5	+	3	tilt	101, 102
	0.60	280	Al	±0.5	+	3	tilt	101, 102
	0.60		Al	±1	+	7		39
	0.56	250	Al	±0.5	+	3	tilt	101, 102
	0.56	20	KH_2PO_4	±0.5	+	7	tilt	13
	0.51	407	Au	±0.5	+	7	tilt	58
	0.49	20	Pb	±5	+	8	tilt	73
	0.47	300	Ag	±6	+	8	tilt	64
	0.31	20	Al	±0.5	+	8		78
	0.31	20	Al	±2	+	8		31
	0.22	20	Au	±0.5	+	8		10, 11, 48, 88, 99, 100
	0.22	20	Cu–3%Si	±0.5	+	8		43
	0.17	20	Si	±0.5	+	8		20, 21, 86
	0.17	20	Stainless steel	±0.5	+	8		81, 113
	0.15	20	Ti–15,5% V	±0.5	+	8.10		80
	0.14	20	V	±0.5	+	8	tilt	65
	0.04	−196	Fe 3%Si	±0.5	+	8		71
	0.08	20	W	±0.5	+	8		75
	0.03	−196	W	±0.5	+	11		33, 34, 107
5	0.99	1065	Cu	±1	−	2		46
	0.99	1063	Cu	±0.5	−	1		56
	0.98	940.5	Ag	±0.5		1		56
	0.98	930	Ag–1% Au	±0.5	−	1		95
	0.98	930	Ag 0.2% Bi	±0.5	−	1		95
	0.98	300	Pb	±1;−2	−	4	tilt	92
	0.96	930	Ag 20% Au	±0.5	−	1		95
	0.95		Al	±1	−	7		39
	0.92	275	Pb	−2; +1	−	4	tilt	92
	0.89	930	Cu	±0.5	−	1		56
	0.87	250	Pb	−1.5; +1	+	4	tilt	92
	0.84	500	Al	±0.5	+	4	tilt	104, 105
	0.82	225	Pb	−2; −1.5; +1	+	4	tilt	92
	0.78	200	Pb	−2; −1.5; +1	+	4	tilt	92
	0.78	450	Al	±0.5	+	4	tilt	104,105
	0.78	775	Cu	±0,2	+	3	tilt	89
				+0.3	−	3	tilt	89
				+1.1	−	3	tilt	89
				+1.2	−	3	tilt	89
				+1.4	−	3	tilt	89
				+2.0	−	3	tilt	89
	0.76	750	Cu	+0.2; +0.3; +1.1; +1.2;	+	3	tilt	89
				+1.4; +2.0;	−	3	tilt	89
	0.75	725	Cu	+0.2; +0.3;	+	3	tilt	89
				+1.1; +1.2	+	3	tilt	89
				+1.4; +2.0	−	3	tilt	89
	0.75	725	Cu	+0.2; +0.3;	+	3	tilt	89
				+1.1; 1.2;	+	3	tilt	89
				+1.4	+	3	tilt	89
				+2	−	3	tilt	89
	0.73	700	Cu	+0.2; +0.3	+	3	tilt	89
				+1.1; +1.2;				
				+1.4	+	3	tilt	89
				+2	−	3	tilt	89
	0.73	400	Al	±0.5	+	4	tilt	104,105
	0.71	675	Cu	+0.2; +0.3;				
				+1.1	+	3	tilt	89
				+1.2; 1.4	+	3	tilt	89
				+2	−	3	tilt	89
	0.66	340	Al	±0.5	+	3	tilt	101,102
	0.63	310	Al	±0.5	+	3	tilt	101,102

Table 1. (cont.)

Σ	T/T_m	T,(°C)	Material	$\Delta\theta$ (deg)	The existence if special structure of properties	Methods' group	The type of boundary	Reference
1	2	3	4	5	6	7	8	9
	0.60	280	Al	±0.5	+	3	tilt	101,102
	0.60		Al	±1	+	7		39
	0.56	250	Al	±0.5	+	3	tilt	101,102
	0.55	1300	Mo	±1	+	7		93
	0.55	1300	Mo	±1.9	+	7		106
	0.31	20	Al	+2.20	+	8		113
	0.24	20	Ge	+0.05	+	8		8
	0.22	20	Au	±0.5	+	8	twist	11,90
				±0.5	+	8	tilt	51;99
				+0.5	+	8	twist	88
	0.22	20	Au	from −2 to +2	+	8	twist	12,98
	0.22	20	Au	±0.5	+	7	tilt	27
	0.17	20	Fe	±0.5	+	1		59
	0.17	20	Stainless steel	±0.5	+	8		14
	0.13	20	NiO	−0.52	+	8	tilt	32
	0.23	20	NiO	±0.5	+	8	twist	70
	0.10	20	MgO	±0.5	+	8	twist	110
	0.10	20	MgO	−4; from −1.5 to +2; +4	+	8	twist	109
	0.10	20	MgO	±0.5	+	1		79
7	0.99	1063	Cu	±0.5	−	1		56
	0.98	940.5	Ag	±0.5	−	1		56
	0.98	930	Ag–1% Au	±0.5	−	1		95
	0.98	930	Ag–0.2% Bi	±0.5	−	1		95
	0.96	930	Ag–20% Au	±0.5	−	1		95
	0.95		Al	±1	−	7		39
	0.88 – −0.94	550 – −600	Al	±0.5	+	7		87
	0.9		Al	±1	−	7		7
	0.9		Al	±1	−	7		7
	0.89	930	Cu	±0.5	−	1		95
	0.84	500	Al	±0.5	+	4	tilt	103,105
	0.79	2000	Mo	±0.5	+	7		93
	0.78	450	Al	±0.5	+	4	tilt	103,105
	0.73	400	Al	±0.5	+	4	tilt	103,105
	0.66	340	Al	±0.5	+	3	tilt	101,102
	0.63	310	Al	±0.5	+	3	tilt	101,102
	0.60	280	Al	±0.5	+	3	tilt	101,102
	0.60		Al	±1	+	7		39
	0.56	250	Al	±0.5	+	3	tilt	101,102
	0.55	1300	Mo	±3	+	7		106
	0.22	20	Au	±1.1, +1.5	+	8		38
	0.22	20	Au	±0.5	+	8		88,99
9	0.99	1063	Cu	±0.5	−	1		56
	0.98	940.5	Ag	±0.5	−	1		56
	0.98	930	Ag–0.2% Bi	±0.5	−	1		95
	0.98	930	Ag–1% Au	±0.5	−; +	1		95
	0.96	930	Ag–20% Au	±0.5	+	1		95
	0.95		Al	±1	+	7		39
	0.95		NiO	±0.5	+	2		30
	0.93	590	Al	±1	+	7		41
	0.9		Al	±1	+	7		7
	0.9		Cu	±1	+	7		7
	0.89	930	Cu	±0.5	+	1		95
	0.84	500	Al	±0.5	+	4	tilt	105
	0.82	1100	Si	±0.5	+	7		28
	0.82	1100	Si	±0.5	+	7		29
	0.79	2000	Mo	±0.5	+	7		93
	0.78	450	Al	±0.5	+	4	tilt	105
	0.73	400	Al	±0.5	+	4	tilt	105
	0.68	650	Cu	±0.5	+	7		108
	0.68		Al	±0.5	+	7	tilt	72
	0.66	850	Fe	±0.5	+	7		106
	0.54	680	Stainless steel	+1.61	+	9		24
	0.52	650	Stainless steel	+1.61	+	9		24
	0.52	650	Stainless steel	±0.5	+	7		103
	0.48	575	Stainless steel	+1.61	+	9		24
	0.24	20	Ge	+0.02	+	8		67,68
	0.24	20	Ge	+0.005	−	8		82
	0.23	20	Cu–3% Si	±0.5	+	8		43
	0.23	20	Cu–6% Si	+0.04	+	8		44

Table 1. (cont.)

Σ	T/T_m	T,(°C)	Material	$\Delta\theta$ (deg)	The existence if special structure of properties	Methods' group	The type of boundary	Reference
1	2	3	4	5	6	7	8	9
9	0.22	20	Au	± 0.5	+	8		47;48;88;100
	0.22	20	Cu	− 0.25	+	8		21;22
	0.22	20	Cu	± 0.5	+	8		23
	0.17	20	Si	± 0.5	+	8		28;29;76;114
	0.17	20	Stainless steel	+ (1.61 ± 0.22)	+	8		25
	0.03	− 196	W	+ 0.2	+	11		107
11	0.99	1063	Cu	± 0.5	+	1		56
				± 0.5	−	1		56
	0.99	940.5	Ag	± 0.5	+	1		56
				± 0.5	−	1		56
	0.98	930	Ag–1% Au	± 0.5	+	1		95
				± 0.5	−	1		95
	0.98	930	Ag–0.2% Bi	± 0.5	−	1		95
	0.96	930	Ag–20% Au	± 0.5	+	1		95
				± 0.5	−	1		95
	0.95		Al	± 1	+	7		39
	0.95		NiO	± 0.5	+	2	tilt	30
	0.93	590	Al	± 1	+	7		41
	0.9		Al	± 1	+	7		7
	0.9		Cu	± 1	+	7		7
	0.89	930	Cu	± 0.5	−	1		95
	0.70		Al	± 0.5	+	7	tilt	72
	0.60		Al	± 1	+	7		39
	0.51	407	Au	± 0.5	+	7	twist	58
	0.31	20	Al	± 0.2	+	8		31
	0.31	20	Al	± 0.2	+	8	twist	58
	0.24	20	Ge	+ 0.02	−	8	tilt	82
	0.22	20	Au	± 0.5	+	8		47,48;60,100
	0.15	20	CdS	± 0.5	+	8		36
	0.03	− 196	W	± 0.5	+	11		35, 107
13	0.99	1065	Cu	± 1	−	2		46
	0.99	1063	Cu	± 0.5	−	1		56
	0.98	940.5	Ag	± 0.5	−	1		56
	0.98	930	Ag–1% Au	± 0.5	−	1		95
	0.98	930	Ag–0.2% Bi	± 0.5	−	1		95
	0.97	300	Pb	+ 0.5; + 1.5	−	4	tilt	92
	0.96–	330	Ag–20% Au	± 0.5	−	1		95
	0.95		Al	± 1	−	7		39
	0.91	550–600	Al	± 0.1	+	7	tilt	87
	0.93	590	Al	± 1	+	7		41
	0.92	275	Pb	+ 0.5; + 1.5	+	4	tilt	92
	0.89	930	Cu	± 0.5	−	1		95
	0.87	250	Pb	+ 0.5	−	4	tilt	92
				+ 1.5	+	4	tilt	92
	0.84	500	Al	+ 0.5	+	4	tilt	104,105
	0.82	225	Pb	+ 0.5; + 1.5	+	4	tilt	92
				± 0.2	−	4	tilt	92
	0.79	2000	Mo	± 0.5	+	7		93
	0.78	200	Pb	+ 1.5; + 0.5	+	4	tilt	92
				± 2	−	4	tilt	92
	0.78	450	Al	± 0.5	+	4	tilt	104,105
	0.73	400	Al	± 0.5	+	4	tilt	104,105
	0.66	850	Fe	+ 0.2; + 0.6	+	7		106
				+ 0.8; − 1.6	+	7		106
	0.66	340	Al	± 0.5	+	3	tilt	101,102
	0.63	310	Al	± 0.5	+	3	tilt	101,102
	0.60	280	Al	± 0.5	+	3	tilt	101,102
	0.60		Al	± 0.5	+	7		39
	0.56	250	Al	± 0.5	+	3	tilt	101,102
	0.55	1300	Mo	± 0.1	+	7		93
	0.55	1300	Mo	+ 1.3; − 1.6	+	7		106
	0.33	20	Al 4.4% Mg	± 0.2	+	8		77
	0.24	20	Ag	± 0.2	+	10	twist	18
	0.22	20	Au	from − 1 to + 1	+	8	twist	12
	0.22	20	Au	± 1.61 + 1.91	+	8	twist	38
	0.22	20	Au	± 0.5	+	8	twist	18,51,90,99
	0.22	20	Au	± 0.5	+	10	tilt	50
	0.17	20	Fe	± 0.5	+	1		59
	0.17	20	Stainless steel	± 0.5	+	8		14
	0.13	20	NiO	± 0.5	+	8		70
	0.10	20	Nb	± 0.5	+	5		20
	0.10	20	Nb	± 0.5	+	6		91

Table 1. (cont.)

Σ	T/T_m	T,(°C)	Material	Δθ (deg)	The existence if special structure of properties	Methods' group	The type of boundary	Reference
1	2	3	4	5	6	7	8	9
13	0.10	20	MgO	±0.5	+	8		110
	0.10	20	MgO	from−0.5 to +0.5	+	8		109
	0.10	20	MgO	±0.5	+	1		79
15	0.99	1063	Cu	±0.5	−	1		56
	0.99	940.5	Ag	±0.5	−	1		56
	0.98	930	Ag − 1% Au	±0.5	−	1		95
	0.96	930	Ag − 20% Au	±0.5	−	1		95
	0.89	930	Cu	±0.5	−	1		95
	0.66	850	Fe	+1.5	+	7		106
	0.55	1300	Mo	±0.5	+	7		93
	0.31	20	Al	±0.2	+	8		31
17	0.99	1065	Cu	±1	−	2		46
	0.99	1063	Cu	±0.5	−	1		56
	0.99	940.5	Ag	±0.5	−	1		56
	0.98	930	Ag-1% Au	±0.5	−	1		95
	0.98	930	Ag-0.2% Bi	±0.5	−	1		95
	0.97	300	Pb	±0.5	−	4	tilt	92
	0.96	930	Ag-20% Au	±0.5	−	1		95
	0.95		Al	±1	+	7		39
	0.93	590	Al	±1	+	7		41
	0.92	275	Pb	±0.5	−	4	tilt	92
	0.9		Al	±1	+	7		7
	0.9		Cu	±1	+	7		7
	0.89	930	Cu	±0.5	−	1		95
	0.87	250	Pb	+0.2	−	4	tilt	92
				+1	+	4	tilt	92
	0.84	500	Al	±0.5	+	4	tilt	104,105
	0.82	225	Pb	+0.2	−	4	tilt	92
	0.79	2000	Mo	±0.5	+	7		93
	0.78	200	Pb	+0.2	+	4	tilt	92
				+1	+	4	tilt	92
	0.78	450	Al	±0.5	+	4		95
	0.73	400	Al	±0.5	+	4		95
	0.66	850	Fe	+1.9	+	7		106
	0.66	340	Al	±0.5	+	3	tilt	101,102
	0.63	310	Al	±0.5	+	3	tilt	101,102
	0.60	280	Al	±0.5	+	3	tilt	101,102
	0.60		Al	±0.5	+	7		39,40
	0.56	250	Al	±0.5	+	3	tilt	101,102
	0.55	1300	Mo	±1	+	7		93
	0.22	20	Cu	±0.5	+	8	tilt	63
	0.22	20	Au	from −0.9 to +0.9	+	8		12,98
	0.22	20	Au	±0.5	+	8	twist	99,100 111
	0.17	20	Fe	±0.5	+	1		59
	0.10	20	Nb	±0.5	+	5		20
	0.10	20	Nb	±0.5	+	6		91
	0.10	20	MgO	±0.5	+	1		79
	0.10	20	MgO	from −0.5 to +0.5	+	8	twist	108
19	0.99	1063	Cu	±0.5	−	1		56
	0.98	940.5	Ag	±0.5	−	1		56
	0.98	930	Ag-1% Au	±0.5	−	1		95
	0.98	930	Ag-0.2% Bi	±0.5	−	1		95
	0.96	930	Ag-20% Au	±0.5	−	1		95
	0.91 ± 0.3	550–600	Al	±0.1	−	7		87
	0.89	930	Cu	±0.1	−	1		95
	0.84	500	Al	±0.5	+	4	tilt	105
	0.78	450	Al	±0.5	+	4	tilt	105
	0.73	400	Al	±0.5	+	4	tilt	105
	0.66	850	Fe	+1	+	7		106
	0.66	340	Al	±0.5	+	3		101,102
	0.63	310	Al	±0.5	+	3		101,102
	0.60	280	Al	±0.5	+	3		101,102
	0.56	250	Al	±0.5	+	3		101,102
	0.22	20	Au	±1.9, +2.21	+	8		38
	0.10	20	Nb	±0.5	+	5		20
21	0.95		Al	±1	−	7		39
	0.91 ± 0.3	550–600	Al	±0.1	+	7	tilt	87
	0.60		Al	±0.5	+	7		39
	0.55	1300	Mo	±0.5	+	7		93
	0.22	20	Au	±0.5	+	8	tilt	99
23	0.55	1300	Mo	±1.6	+	7		106

Table 1. (cont.)

Σ	T/T_m	T,(°C)	Material	Δθ (deg)	The existence if special structure of properties	Methods' group	The type of boundary	Reference
1	2	3	4	5	6	7	8	9
25	0.66	850	Fe	+0.7	+	7		106
	0.55	1300	Mo	±1	+	7		93
	0.55	1300	Mo	+0.7; +1.9	+	7		106
	0.24	20	Ge	+0.9	+	8	tilt	9
				+0.25	+	8	tilt	9
				+0.02	+	8	tilt	9
	0.24	20	Ge	+0.05	+	8		15
	0.22	20	Au	±0.5	+	8	twist	10,98,111
	0.22	20	Au	±0.5	+	7		27
	0.10	20	MgO	±0.05	+	1		79
	0.10	20	MgO	±0.5	+	8	twist	111
27	0.99	1063	Cu	±0.5	−	1		56
	0.99	940.5	Ag	±0.5	−	1		56
	0.98	930	Ag − 1% Au	±0.5	−	1		95
	0.96	930	Ag–20% Au	±0.5	−	1		95
	0.89	930	Cu	±0.5	−	1		95
	0.68	650	Cu	±0.5	+	7		93
	0.55	1300	Mo	±1	+	7		108
	0.52	650	Stainless steel	±0.5	+	7		103
	0.31	20	Al	+0.34	+	8		113
	0.24	20	Ge	+0.007	+	8		9
	0.22	20	Cu–3% Si	±0.5	+	8		43
	0.22	20	Cu	±0.5	+	8		113
	0.22	20	Cu–Ni	−0.85	+	8		61
	0.17	20	Si	±0.5	+	8		28,29
29	0.314	20	Al	+2.1	+	8		113
	0.17	20	Fe	±0.5	+	1		59
	0.17	20	Stainless steel	±0.5	+	8		14
	0.10	20	MgO	from −0.2 to +0.2	+	8		109
31	0.66	850	Fe	±1	−	7		106
	0.56	725	Stainless steel	−0.45	−	9		24
	0.55	1300	Mo	±1	+	7		93
	0.55	1300	Mo	±1	+	7		106
	0.51	625	Stainless steel	−0.45	+	9		24
	0.49	600	Stainless steel	−0.45	+	9		24
	0.46	550	Stainless steel	−0.45	+	9		24
	0.44	500	Stainless steel	−0.45	+	9		24
	0.22	20	Au	±0.5	+	8	twist	38
	0.22	20	Cu	±0.5	+	8		113
33	0.99	1063	Cu	±0.5	−	1		56
	0.99	940.5	Ag	±0.5	−	1		56
	0.98	930	Ag–1% Au	±0.5	−	1		95
	0.98	930	Ag–0.2% Bi	±0.5	−	1		95
	0.96	930	Ag–20% Au	±0.5	−	1		95
	0.89	930	Cu	±0.5	−	1		95
	0.66	850	Fe	±0.5	−	1		106
	0.55	1300	Mo	±1	−	7		93
	0.22	20	Au	±1	+	7		47,48
	0.14	20	V	±0.5	+	8		65
	0.03	−196	W	±0.5	+	11		107
37	0.22	20	Au	±0.5	+	7		
	0.17	20	Fe	±0.5	+	1		
41	0.66	850	Fe	±1	−	7		106
	0.55	1300	Mo	±1	−	7		106
	0.55	1300	Mo	±1	−	7		93
	0.31	20	Al	±0.2	+	8		31
	0.31	20	Al	±0.2	+	8		86
	0.24	20	Ge	±0.1	+	8	tilt	9
	0.22	20	Au	±0.5	+	10		50
	0.22	20	Au	±0.5	+	7		27
	0.17	20	Fe	±0.5	+	1		59
	0.10	20	Mo	±0.5	+	8		85
	0.10	20	MgO	±0.2	+	1		79
43	0.22	20	Au	±0.5	+	8	twist	38
51	0.17	20	Fe–3% Si	±0.5	+	8	tilt	52
53	0.22	20	Au	±1	−	8		99
	0.10	20	MgO	±0.5	+	1		79
	0.10	20	MgO	+0.5	+	8	twist	109
57	0.24	20	Cu–8% Si	+0.9	+	8		45

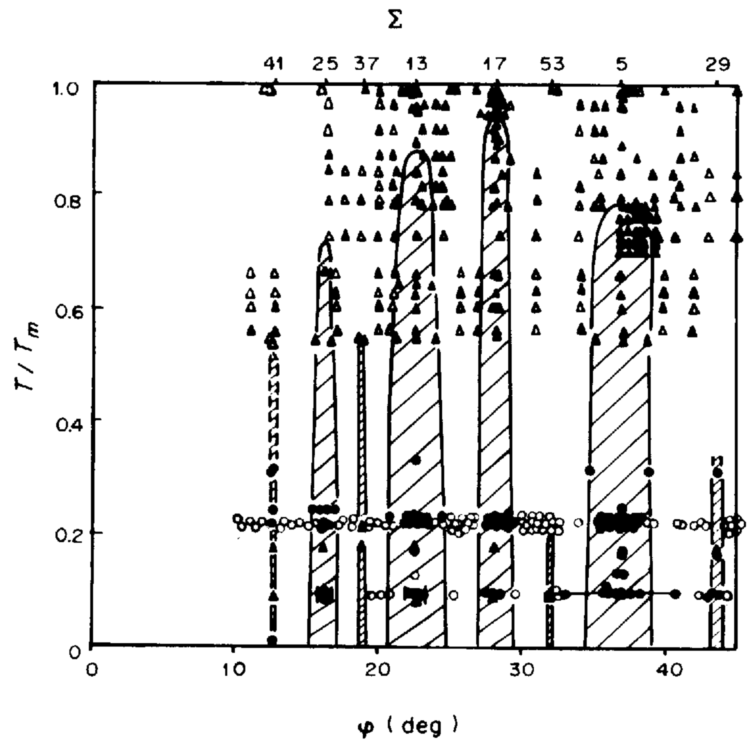

Fig. 1. The existence diagram of special and non-special [001] grain boundaries (see Table 1); ▲—boundaries with special properties; △—boundaries with non-special properties; ●—boundaries with special structure; ○—boundaries with non-special structure.

the angles at which drastic differences in the number of balls from an average value were observed correspond to boundaries with low surface tension (special boundaries). If at the angles corresponding to the particular Σ no peaks in the distribution of balls are observed, the boundaries with this Σ are not different in the surface tension from general boundaries, thus they are not special.

Note, that Table 1 and Fig. 1 demonstrate that the number of special boundaries increases with decreasing temperature. This effect was observed in the works of Gleiter and the co-workers [117] using method (1): as the temperature decreases the number of peaks on the misorientational distributions of the balls increases. An increase in the number of peaks is also observed with increasing pressure [118]. The authors interpret these results as manifestations of phase transitions on the boundaries [4, 119]. Unfortunately, the authors of [117, 118] do not present the Σ values corresponding to the boundaries in question, therefore these important results are not incorporated in Table 1 and Fig. 1.

The next group involves methods using the data on special grain boundaries which were obtained from the orientational dependences of thermodynamic and kinetic properties of grain boundaries. Bicrystalline samples with individual grain boundaries with known crystallographic parameters (normally with an accuracy $\pm 0.5^\circ$) were employed to measure the properties of the surface tension (2), diffusivity (3), mobility (4), microhardness (5) and parameters of intercrystalline corrosion (6). These orientational dependences are nonmonotonic with minima or maxima corresponding to special boundaries. Of special interest is the work [89] where the coefficients of grain boundary diffusion of nickel in copper were studied in tilt boundaries with misorientation angles close for a special one for $\Sigma = 5$ in the interval $\Delta\theta < 2^\circ$. In the authors' opinion [89] the jumps on the temperature and angular dependences of diffusivity indicated the "special boundary-general boundary" phase transition.

The techniques grouped as (7) are used to study the misorientational distribution of grains after recrystallization anneals. In principle, this technique is close to the method (1) but it is still more "indirect" than (1) since the angular distribution, in this case, is determined by the properties of individual boundaries between the balls and the substrate, and at recrystallization the angular distribution is established in the course of evolution of a large system of interconnected and, therefore strongly interacting, grain boundaries. Misorientation angles of the boundaries are determined by X-ray or electron microscopy methods. These data are sometimes supplemented by investigation of boundary faceting, since only special boundaries are faceted.

The direct methods to determine special boundaries involve the examination of grain boundary structure by means of electron microscopy and electron diffractometry [at room temperature (8) and with heating *in situ* (9)], X-ray diffraction (10) and field ion microscopy (11). In these cases the boundaries exhibiting a network of grain boundary dis-

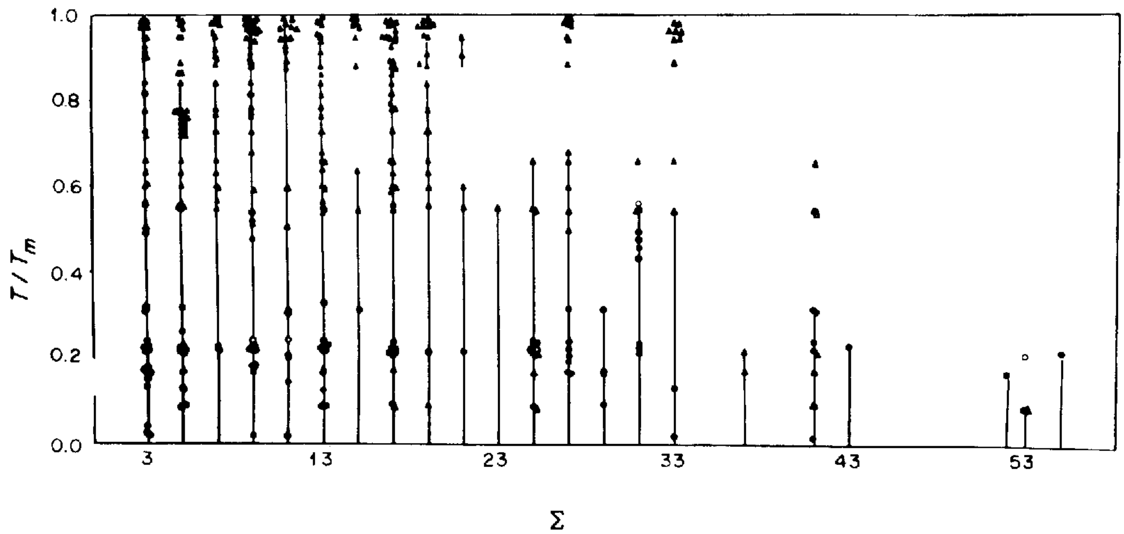

Fig. 2. The existence temperature of special and non-special grain boundaries as a function of the reciprocal coincidence sites density Σ. The symbols as in Fig. 1.

locations that accomodate, in terms of Brandon's model [2, 121], a departure of the grain boundary misorientation angle from the special one are assumed to be special. Application of the methods [8–11] gives a more correct determination (to $\pm 0.01°$) of the angular interval of existence of special boundaries. We treat as special not only the boundaries exhibiting the equilibrium network of grain boundary dislocations with the Burgers vector corresponding to the DSC-lattice [3, 4] but, also, those which exhibit localized grain boundary dislocations formed due, for example, to dissociation of the boundary-absorbed lattice dislocations. Of particular interest are the detailed investigations of < 100 > twist boundaries in gold and magnesium oxide, carried out by Balluffi and the co-workers [11, 12, 109] and the work [24] dealing with grain boundary dislocations in stainless steel at different temperatures. In [24] the electron microscopic images of grain boundary dislocations were smeared at the boundary $\Sigma = 31$ in transiting from 625° to 725°C. We interpreted it as transition from special to general boundary.

The diagram present in Fig. 1 is based on the data of Table 1. It demonstrates the data for < 100 > grain boundaries (tilt and twist). Homological temperature lays off as ordinate, misorientation angle, varying from 0 to 45°, as abscissa. There are four types of points on the diagram. Solid symbols indicate the values of misorientation angles and temperatures at which grain boundaries exhibited special properties, open symbols indicate the boundaries of the general type. Circles indicate the results of direct experiments, triangles of indirect ones. The lines in Fig. 1, based on the experimental data, both direct and indirect, discriminate between the regions of existence of special boundaries with different Σ and the single region of existence of general boundaries. It appears that only special boundaries with low Σ manifest themselves as special up to T. The boundaries with higher Σ remain special only to a certain finite temperature. Note, too, that the angular interval of existence of special boundaries decreases with growing Σ.

Figure 2 presents the data on the intervals of existence of special boundaries plotted on the base of Table 1. As contrasted from Fig. 1, here the Σ lays off as abcissa. The angular interval of existence of special boundaries is not shown. Figure 2 enables one to estimate the temperature at which special-properties are lost for the boundaries with a particular Σ.

ANALOGY BETWEEN SPECIAL AND NON-SPECIAL GRAIN BOUNDARIES AND COMMENSURATE AND INCOMMENSURATE PHASES IN THE SURFACE ADSORBED LAYERS

The authors of [136] purposed that there is a deep analogy between commensurate and incommensurate phases in the surface adsorbed layers and special and non-special grain boundaries. There is also the analogy between the secondary grain boundary dislocations and the domain walls in weak-incommensurate structures [136]. The regularities that determine the conditions of existence of commensurate and incommensurate phases on the surface were obtained theoretically by Pokrovskii and Talapov [5, 6, 122]. Their works treat a monolayer of adsorbed atoms that is influenced by a periodic potential of a monocrystalline substrate $V(\mathbf{h})$ (vector of reciprocal lattice of the substrate $\mathbf{b}$). The monolayer is in equilibrium state with a gas phase of the adsorbate. At the appropriate gas pressure the adsorbed atoms form a regular lattice with vectors $\mathbf{R}$ (vectors of the reciprocal lattice $\mathbf{g}$) on absolute smooth substrate $V(\mathbf{h})$. The lattice of adatoms is distorted under the influence of the substrate periodic potential the interaction with the substrate, described by the periodic function $f(\phi)$, tends to fit the adsorbed atoms on the substrate periodic potential minima. Alternatively, the interaction between the adsorbed atoms tends to fit them on their own regular lattice. By minimising the interaction energy between the atoms and the substrate, the authors of [6] obtain the solutions of two types: in one case the adsorbate lattice is commensurate with the substrate along the x-axis ($\mathbf{q}$-$\mathbf{b} = 0$) in the other case not all the adsorbate-atom positions correspond to the energy minima of the substrate, that is, the monolayer and the substrate lattices are incommensurate. Commensurate phase exists in a particular pressure range, ρ. These phases occur in the vicinities, δ, of all the points where the b/q ratio is rational

$$B/q = M/N + \delta.$$

The N value is the order of commensurability. The δ value decreases exponentially with an increase of N. In the work [6] the behaviour of the monolayer at a finite, not equal to zero temperature was studied too. Using a renormalization group method the authors of [6] show that under a particular temperature T, a long-range order in commensurate phase disappears and it becomes incommensurate. Commensurate phases of higher orders disappear at $T = T_1/N^2$.

Consider the analogy between surface phases and grain boundaries. In the case of grain boundaries the superstructure on the boundary is formed, too, at rational ratios of the lattice periods of two grains at their mutual rotation. In this case, analog of the gas pressure will be a misorientation angle θ, and analog of the commensurability parameter the Σ value. "Commensurate phases"—special boundaries—also exist in a particular interval of angles $\Delta\theta$ near to a special misorientation θ_Σ. In the interval $\theta_\Sigma \pm \Delta\theta$ the special-boundary structure involves alternating singular regions and misfit dislocations that accomodate a misfit $\Delta\theta$. With $\Delta\theta \to 0$ the spacing between the grain boundary dislocations tends to infinity, and with sufficiently small no misfit dislocations are observed. (For example, in the work [82] with $\Delta\theta = 0.005°$ for $\Sigma = 9$ and $\Delta\theta = 0.02°$ for $\Sigma = 11$ no misfit dislocations were observed, and with $\Delta\theta = 0.1°$, $\Sigma = 9$ [67, 68] and $\Sigma = 11$ [31, 78] they were observed on the electron micrographs, see also Fig. 3.) As $\Delta\theta$ grows the energy of the misfit-dislocation system grows and at particular values of $\Delta\theta$ "incommensurate phase" becomes more favourable, that is, non-special grain boundary of the general type with the structure that can be described by the O-lattice [111].

Based on this analogy, one may apply the conclusion of Pokrovskii's and Talapov's theory to grain boundaries. Strictly speaking, applicability of the results [6] is limited by tilt boundaries where accomodation $\Delta\theta$ occurs by means of a wall of dislocations since the works [6] treats quasi-one-dimensional case. For twist boundaries on which a dislocation network is formed this model needs to be refined.

The results of Fig. 2 and Table 1 enable one to check up whether the theory [6] is applicable to grain boundaries. Figure 4 gives the temperature at which

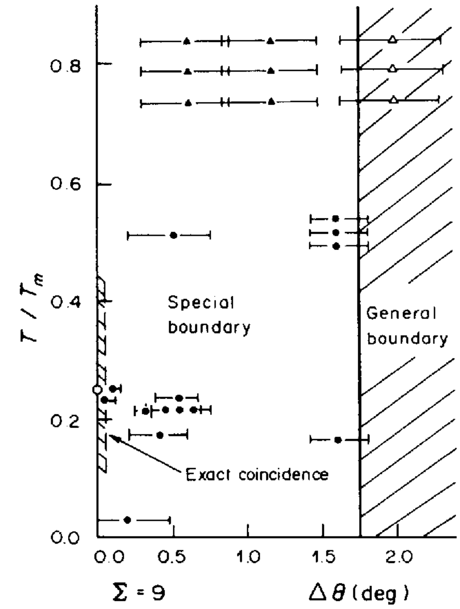

Fig. 3. The existence diagram of special grain boundary $\Sigma = 9$ (see Table 1), the symbols as in Fig. 1.

the transition occurs from special to non-special boundary as a function of Σ. The upper boundaries of the temperature intervals presented correspond to minimal trempeature values at which no special properties were observed on the boundaries in question, the lower boundaries correspond to maximal temperatures at which these boundaries still behaved as special. Due to shortage of the experimental data upper boundaries of the temperature intervals are lacking for a number of values. Figure 4 shows evidence that the transition temperature from a special boundary to a non-special one does drop with increasing Σ, i.e. the commensurability parameter for the boundaries, and at a particular temperature the special properties are minifested only at the boundaries with Σ less than a certain Σ_{max}. Figure 5 presents the logarithm of the angular interval $\Delta\theta$ of the existence of special boundaries the Σ. With changing $\Delta\theta$ by two orders of magnitude, the points fall well on the straight line. Hence, the angular interval of the existence of the special boundaries does decrease exponentially with an increase of Σ.

So, the main theoretical predictions [6] agree well with the experimental data. We shall formulate the

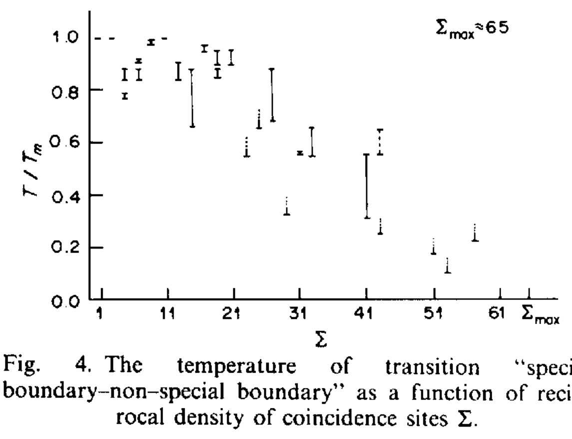

Fig. 4. The temperature of transition "special boundary–non-special boundary" as a function of reciprocal density of coincidence sites Σ.

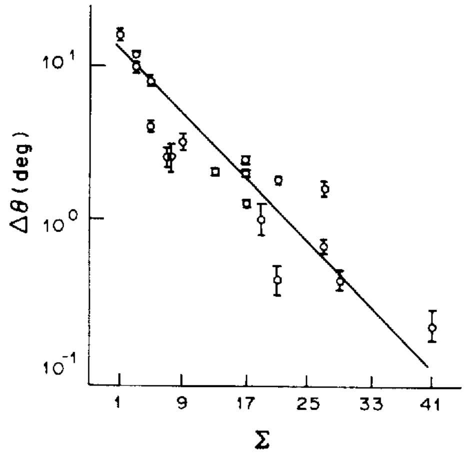

Fig. 5. The interval of misorientation angles where the special boundaries exist at the low temperatures as a function of reciprocal density of coincidence sites Σ.

principal conclusions drawn from our analysis of the experimental data on the investigation of the structure and properties of grain boundaries and from the analogy between grain boundaries and surface adsorbed layers. These conclusions are, simultaneously, the answers to the questions put at the beginning of the paper.

(1) Special boundaries manifest their special properties in a particular temperature and angular interval.

(2) The transition temperature of special boundaries to general-type boundaries decreases with growing Σ that plays the role of the commensurability parameter for grain boundaries.

(3) At a particular temperature the special properties are manifested only by the boundaries with Σ less than some Σ_{max}. With a decrease of the temperature (to be more accurate T/T_m) still larger number of the boundaries manifest the special properties at the same temperature in the materials with a higher the special properties will be exhibited by the boundaries with higher Σ too.

(4) The angular interval of the existence of special boundaries at low temperatures descreases exponentially with increasing Σ.

NON-SPECIAL BOUNDARIES (GENERAL BOUNDARIES) AND A MAXIMAL Σ VALUE

One of the most important results of this work is the conclusion that there is a threshold value of Σ, i.e. Σ_{max}, at which the properties of special boundaries are still different from those of general ones, the Σ_{max} decreasing with growing temperature. The problem of the existence of the maximal Σ value is discussed, in particular, in the paper by Zisman and Ribin [127] This work shows grain boundaries can be described by the DSC-lattice only as long as the DSC-lattice period (or of grain boundary displacement lattice [3]) is larger than the thermal fluctuations amplitude. The existence of Σ_{max} implies that at a particular temperature only the boundaries with $\Sigma < \Sigma_{max}$ exhibit special properties. Hence, the extrema on the orientational dependences of the properties will be observed only at special angles for which $\Sigma < \Sigma_{max}$. At the same time the parameters of the boundaries with $\Sigma \geqslant \Sigma_{max}$ will not be distinguished at the background on non-special boundaries (general boundaries). These considerations suggest that if we plot the properties of special boundaries Σ and extrapolate this dependence towards larger Σ, the range of the values for general boundaries will, approximately, indicate (at the extrapolated portion of the straight line) Σ_{max} for the experimental temperature interval.

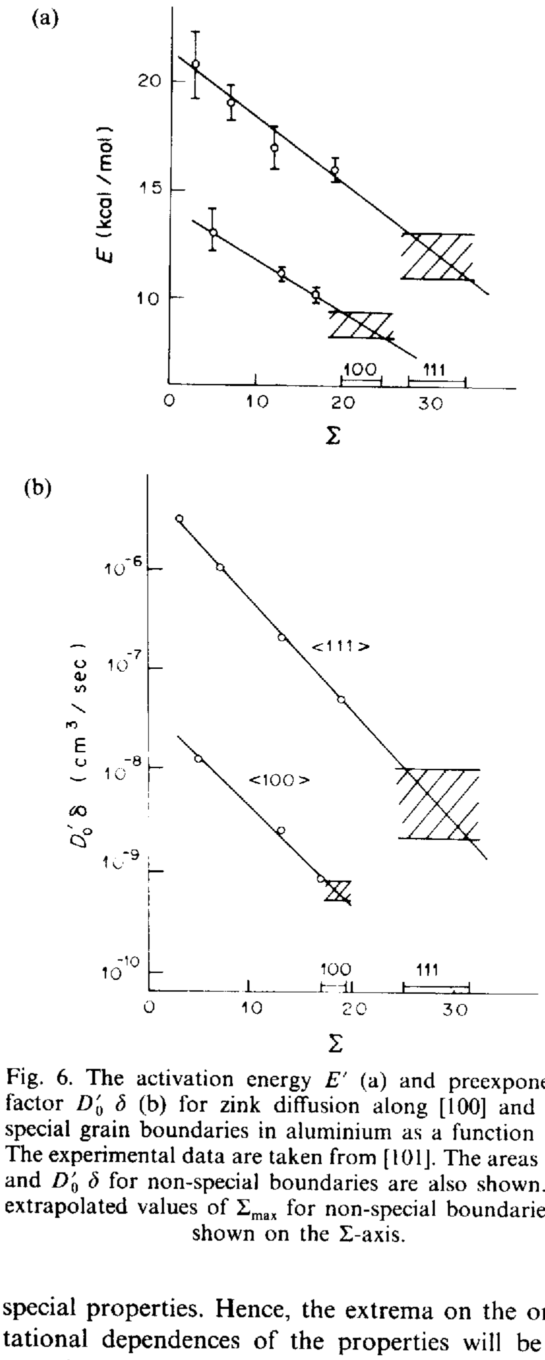

Fig. 6. The activation energy E' (a) and preexponential factor $D_0' \delta$ (b) for zink diffusion along [100] and [111] special grain boundaries in aluminium as a function of Σ. The experimental data are taken from [101]. The areas of E' and $D_0' \delta$ for non-special boundaries are also shown. The extrapolated values of Σ_{max} for non-special boundaries are shown on the Σ-axis.

Figure 6(a) and 6(b) presents the dependences of the activation energy E' and of preexponential factor $D_0'\delta$ for zinc diffusion on < 100 > and < 111 > special tilt boundaries in aluminium [101]. The region of E' and D_0' δ values for general boundaries is hatched. This region corresponds on the Σ axis to the interval of 18–32. Σ_{max} for the temperature region

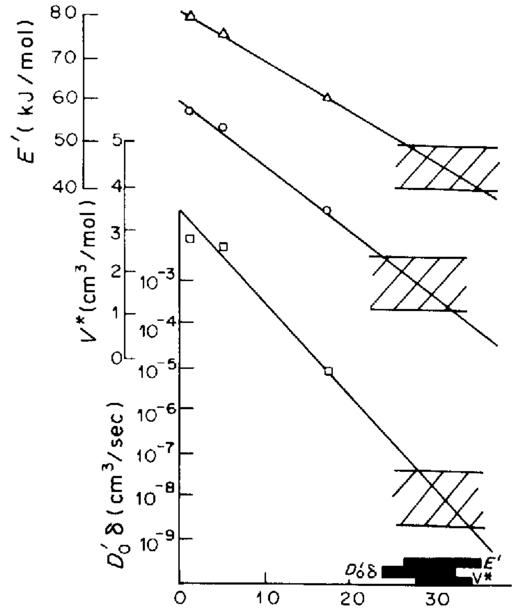

Fig. 7. The activation energy E' preexponential factor D'_0 δ and activation volume V^* for tin diffusion along [100] twist special interphase boundaries Sn–Gle as a function of Σ. The experimental data are taken from [124,125]. The areas of E', D'_0 δ and V^* for non-special boundaries are also shown. The extrapolated values of Σ_{max} for non-special boundaries are shown on the Σ-axis.

wherein the diffusion was measured (T/T_m = 0.55–0.65) equals 20–30 (see Fig. 4). Figure 7 presents the analogous dependences of the E', D_0 δ and V^* (activation volume) on Σ for the indium diffusion on tin–germanium < 001 > twist interphase boundaries [124, 125]. The Σ interval corresponding to E', D'_0 δ and V^* for general boundaries is 24–35. The Σ_{max} for the temperatures of the diffusional measurements T/T_m = 0.6–0.85 range from 19 to 35.

A fair agreement is thus observed between a maximal Σ values for general boundaries, obtained by extrapolation of the experimental data for special boundaries, and Σ_{max}, predicted on the base of Fig. 4. This agreement, on the one side, confirms the existence of Σ_{max} as a function of temperature and, on the other side, it implies that the properties of general boundaries correspond to particular Σ_{max} values rather than to abstract extrapolation $\Sigma \to \infty$.

DIAGRAM OF EXISTENCE OF SPECIAL AND NON-SPECIAL BOUNDARIES AND PHASE TRANSITIONS ON THE BOUNDARIES

The question of phase transitions on grain boundaries has long been discussed in the literature. Thermodynamics of these transitions is considered in the works [1, 123]. Showing that at the points of phase transitions at the grain boundaries bendings are to be observed on the temperature dependences of the surface tension, and bending or jumps on the temperature dependences of the kinetic properties (diffusion coefficients, migration rate etc). The experimental data on the grain boundary phase transitions are, however, very scarce, they are contradictory and do not form, presently a general picture (see, for instance the review [4]).

This situation differs dramatically from that in the study of external surfaces where the number of the works dealing with phase transitions is approaching 500. Numerous experimental data have made it possible to develop a strong theory. In particular the phenomena connected with intertransitions of commensurate and incommensurate phases are described in detail and generalized. Critical phenomena in 2D-systems are much more diverse than in the bulk, i.e. the number of universality classes for critical phenomena is much greater [133]. First experimental works appear, too, on the determination of critical indices for 2D phase transitions on the external surface [134, 135].

These interesting phenomena exist, to our belief, for the grain boundaries too. The description of grain boundaries in terms of the models like in [5,6, 122] enables one to indicate the regions of temperature and misorientation parameters wherein one has to see phase transitions at the boundaries and, likely, the critical phenomena connected with these. The results of this work make it possible, in particular, to explain incontroversally several interesting facts.

First come the results of Gleiter and the coworkers who observed an increase in the number of special boundaries with decreasing temperature and increasing pressure. This implies, in particular, that at high pressures the shape of phase diagrams, like that of Fig. 4, changes significantly. However, the works dealing with investigations of the boundary properties under pressure are scarce. In addition to [118] one can mention only the investigations of grain boundary migration in tin [126] and tin–germanium interphase boundary diffusion [125].

In the experiments of Balluffi and the co-workers grain boundary dislocations were observed on < 100 > special boundaries in magnesium oxide to $\Sigma = 53$ [109], and on < 100 > boundaries in gold only to $\Sigma \leq 25$ [11, 12]. This can be attributed to the fact that T/T_m for magnesium oxide makes up 0.095 whereas for gold it is 0.219, and in the interval from 0.095 to 0.219 special boundaries with $\Sigma = 29,41,53$ (and, likely, 25) transit to non-special ones (see Fig. 1). The authors of [4] observed a marked disappearance of misfit dislocations on a non-coherent α-brass–β-brass interphase boundaries. Dislocations disappear at a small change of the misorientation angle although they should still be easily resolved in an electron microscope. The analogous phenomenon was observed, as evidenced by the author of [4], on grain boundaries in gold as well. Disappearance of dislocations in these cases, to our opinion, is attributed to the transition via a critical angle $\Delta\theta$ that separates the region of existence of a particular special boundary from that of a general boundary. The analogous transformation, that is manifested in disappearance of structural grain boundary dislocation images was observed, as we suppose, on

< 110 > grain boundaries in stainless steel [24]. The difference from [4] is in the fact that here the transition was observed through the critical temperature T_c at which a special boundary with $\Sigma = 31$ is transformed to a non-special one. The first work which accomplised a purposeful search for "special boundary-general boundary" phase transition is the above mentioned investigation on tilt boundaries with $\Sigma = 5$ in copper [89].

Note, that in the other work by the same authors [120] on the investigation of the surface tension σ on the same $\Sigma = 5$ boundaries in copper a singularity of the angular dependence is observed in a very narrow vicinity of $\Sigma = 5$, at $\Delta\theta < 0.2°$. The authors of [120] attribute it to still another hypothetical transition connected with grain boundary dislocation dissociation. The results of the authors of [82] who did not observe grain boundary dislocations on the boundaries deviating from $\Sigma = 9$ by 0.005° and from $\Sigma = 11$ by 0.1° may be an indirect evidence for such a transition.

Recently, several works have been published in which structural transitions on the boundaries were observed at computer simulation of their structure [129, 130, 132]. We suppose that a still greater variety of phase transitions is possible at interphase boundaries formed, as contrasted from grain boundaries from different materials. Geometrical models for their description are rather complicated [131]. There are a number of interesting questions to be answered, namely, how does the "special boundary–general boundary" transition occur? What kind is it? What is its kinetics? How does it influence the boundary properties? Are there differences at the "angular" and "temperatural" transitions and at transitions on tilt and twist boundaries? Are there critical phenomena in the pre-transitional regions on the boundary?

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