SAE INTERNATIONAL

AEROSPACE STANDARD

AS5491 | REV. C

Issued 2000-12
Revised 2007-11
Reaffirmed 2013-10

Superseding AS5491B

Calculation of Electron Vacancy Number in Superalloys

RATIONALE

AS5491C has been reaffirmed to comply with the SAE five-year review policy.

1. SCOPE

1.1 Purpose

This SAE Aerospace Standard (AS) establishes a uniform procedure for calculation of electron vacancy numbers in superalloys. It is intended for use by suppliers of raw materials and parts, typically castings, for which control of electron vacancy number is required by the raw material specification.

1.2 Application

This procedure has been used to estimate the potential for alloy phase instability by calculation of the density of electrons per atom in nickel-based superalloys.

1.3 Background

1.3.1 Complex, highly alloyed superalloys have been observed, for some alloy chemistries and under certain conditions, to form precipitated phases which can adversely affect strength and ductility. These phases, typically of a crystalline structure known as topologically close-packed, or TCP, appear after extended exposure at temperatures in the range from 1300 to 1650 °F (704 to 899 °C). Such phases include sigma (σ), mu (μ), or Laves. Their tendency to precipitate from the alloy matrix has been related by researchers such as Boesch and Slaney (see 2.1) and Woodyatt, et al. (see 2.2) to the density of electrons per atom as expressed by the electron vacancy number N_v, as shown in Equation 1, as follows:

$$N_v = \sum_{i=1}^{n} m_i (N_v)_i \qquad \text{(Eq. 1)}$$

TO PLACE A DOCUMENT ORDER: Tel: 877-606-7323 (inside USA and Canada)
Tel: +1 724-776-4970 (outside USA)
Fax: 724-776-0790
Email: CustomerService@sae.org
SAE WEB ADDRESS: http://www.sae.org

where:

N_v is the electron vacancy number for the alloy

m_i is the atomic mass fraction of the ith element in the alloy composition, and

$(N_v)_i$ is the electron vacancy number of the ith element.

Determination of the electron vacancy concentration requires an understanding of the phases which precipitate in superalloys as well as the sequence in which they form in the gamma matrix. In general, this sequence is (a) the precipitation of borides, (b) the precipitation of carbides, and (c) the formation of gamma prime. When these phase reactions are considered, and adjustments made to the composition to take them into account, the residual matrix composition may be determined. From that residual matrix the electron vacancy number is then calculated.

1.3.2 The sequence of precipitation of strengthening phases is addressed as follows:

1.3.2.1 Nickel, chromium, titanium, and molybdenum form a boride as $(Mo_{0.5}, Ti_{0.15}, Cr_{0.25}, Ni_{0.10})_3B_2$.

1.3.2.2 All carbon is assumed to form carbides of the type MC and $M_{23}C_6$. It is assumed that MC carbides take half the carbon, reacting in sequence with tantalum, columbium, zirconium, titanium, and vanadium. The remaining carbon then reacts with chromium, molybdenum, and tungsten to form $Cr_{21}(Mo,W)_2C_6$.

1.3.2.3 Gamma prime is formed from the remaining aluminum, titanium, hafnium, columbium, tantalum, 50 percent of the original amount of vanadium, and 3 percent of the original amount of chromium by combining with three times that total in nickel, i.e., Ni_3 (Al, Ti, Cb, Hf, Ta, 0.5V, 0.03Cr).

1.3.2.4 The remaining chromium content is adjusted for that lost due to formation of borides, carbides, and gamma prime.

1.3.2.5 The remaining nickel content is adjusted for that tied up in boride and gamma prime formation.

2. REFERENCES

2.1 W. J. Boesch and J. S. Slaney: Metal Progress, July 1964, Vol. 86, No. 1, pp 109-111.

2.2 L. R. Woodyatt, C. T. Sims and H. J. Beattie, Jr.: Transactions of the Metallurgical Society of AIME, April, 1966, Volume 236, pp 519-527.

3. TECHNICAL REQUIREMENTS

3.1 Calculation of N_v

3.1.1 N_v shall be calculated in the following order:

3.1.1.1 Conversion of weight percentage to atomic percentage for each element

3.1.1.2 Calculation of boron and carbide precipitation

3.1.1.3 Calculation of gamma prime precipitation

3.1.1.4 Calculation of the residual gamma matrix composition

3.1.1.5 Determination of electron vacancy number, N_v

3.1.2 It may be helpful to set up a matrix similar to Table 1 to facilitate recording compositions through the process of electron vacancy number calculation.

TABLE 1 - MATRIX FOR CALCULATION OF N_v (ELECTRON VACANCY NUMBER)

	Element	Wt %	Atomic Weight	Wt %/ At. Wt	Atomic Fraction	Precip. Adj.	Matrix Atomic Fraction	N_v	Nv Product
Column		A	B	C	D	E	F	G	H
Row 1	Cr		52.00					4.66	
Row 2	Ti		47.90					6.66	
Row 3	Mo		95.94					4.66	
Row 4	Al		26.98					7.66	
Row 5	Co		58.93					1.71	
Row 6	B		10.81					7.66	
Row 7	Zr		91.22					6.66	
Row 8	C		12.01					–	
Row 9	Si		28.09					6.66	
Row 10	Mn		54.94					3.66	
Row 11	Fe		55.85					2.66	
Row 12	Cu		63.54					0.00	
Row 13	V		50.94					5.66	
Row 14	W		183.85					4.66	
Row 15	Ta		180.95					5.66	
Row 16	Cb		92.91					5.66	
Row 17	Hf		178.49					6.66	
Row 18	Re		186.21					4.66	
Row 19	Ni		58.71					0.61	
Sum									

TABLE 1 (CONTINUED)

Sample Calculation based on AMS 5410:

Element	Wt. %	Element	Wt. %
Cr	15.8	Mn	0.03
Ti	3.45	Fe	0.35
Mo	1.65	Cu	0.00
Al	3.45	V	0.00
Co	8.5	W	2.5
B	0.01	Ta	1.75
Zr	0.04	Cb	0.00
C	0.17	Hf	0.00
Si	0.03	Re	0.00

Matrix for Calculation of N_v (Electron Vacancy Number)

	Element	Wt%	Atomic Weight	Wt%/Atomic Weight	Atomic Fraction	Precip. Adj.	Matrix Atomic Fraction	Nv	Nv Product
Column		A	B	C	D	E	F	G	H
Row 1	Cr	15.8	52.00	0.3038	0.1744	0.1521	0.3077	4.66	1.434
Row 2	Ti	3.45	47.90	0.0720	0.0406	0.0000	0.0000	6.66	0.000
Row 3	Mo	1.65	95.94	0.0172	0.0097	0.0086	0.0173	4.66	0.081
Row 4	Al	3.45	26.98	0.1279	0.0721	0.0000	0.0000	7.66	0.000
Row 5	Co	8.5	58.93	0.1442	0.0814	0.0814	0.1646	1.71	0.281
Row 6	B	0.01	10.81	0.0009	0.0005	0.0000	0.0000	7.66	0.000
Row 7	Zr	0.04	91.22	0.0004	0.0002	0.0002	0.0005	6.66	0.003
Row 8	C	0.17	12.01	0.0142	0.0080	0.0000	0.0000	-	0.000
Row 9	Si	0.03	28.09	0.0011	0.0006	0.0006	0.0012	6.66	0.008
Row 10	Mn	0.03	54.94	0.0005	0.0003	0.0003	0.0006	3.66	0.002
Row 11	Fe	0.35	55.85	0.0063	0.0035	0.0035	0.0072	2.66	0.019
Row 12	Cu	0	63.54	0.0000	0.0000	0.0000	0.0000	0.00	0.000
Row 13	V	0	50.94	0.0000	0.0000	0.0000	0.0000	5.66	0.000
Row 14	W	2.5	183.85	0.0136	0.0077	0.0071	0.0143	4.66	0.067
Row 15	Ta	1.75	180.95	0.0097	0.0055	0.0000	0.0000	5.66	0.000
Row 16	Cb	0	92.91	0.0000	0.0000	0.0000	0.0000	5.66	0.000
Row 17	Hf	0	178.49	0.0000	0.0000	0.0000	0.0000	6.66	0.000
Row 18	Re	0	186.21	0.0000	0.0000	0.0000	0.0000	4.66	0.000
Row 19	Ni	62.27	58.71	1.0606	0.5984	0.2405	0.4865	0.61	0.297
Sum		100		1.7725		0.4943			**2.19**

3.2 Conversion to Atomic Fraction

3.2.1 Enter in column A the weight percent of the individual elements by row. When the weight percent is unknown, or the element is not found in the alloy, enter zero (0). The weight percent of nickel is determined by adding the percentages of the other elements and subtracting the sum from 100.

3.2.2 Divide the weight percent of each element (the entries in column A) by their respective atomic weights (from column B) and enter this value in column C in the table. Sum the entries in column C; then individually divide the entries for each element in column C by the sum of column C. Enter this value in column D. This is the atomic fraction of that element.

3.3 Calculation of Phase Precipitations

For the next series of calculations, reference will be made to cell locations in the table, such that D1 refers to the value of the entry in column D, row 1 (for example, the atomic fraction chromium) and E5 is the residual matrix atomic percent of cobalt, adjusted for precipitation of second phases.

3.4 Boride and Carbide Precipitation

3.4.1 Chromium

Multiply D1 by 0.97 and subtract the quantity [(0.375)(D6) + (1.75)(D8)], where:

D1 is the atomic fraction of Cr
D6 is the atomic fraction of B
D8 is the atomic fraction of C

Enter the result in E1.

3.4.2 Molybdenum

From D3, subtract the quantity {[(0.75)(D6)] + (0.167)[(D8)(D3)/(D3+D14)]}, where:

D3 is the atomic fraction of Mo
D6 is the atomic fraction of B
D8 is the atomic fraction of C
D14 is the atomic fraction of W

Enter the result in E3.